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A SPECTRAL METHOD ON TETRAHEDRA USING RATIONAL BASIS FUNCTIONS

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Abstract. A spectral method using fully tensorial rational basis functions on tetrahedron, obtained from the polynomials on the reference cube through a collapsed coordinate transform, is proposed and analyzed. Theoretical and numerical results show that the rational approximation is as accurate as the polynomial approximation, but with a more effective implementation.

Key Words. Spectral methods on tetrahedra, rational basis functions, spectral accuracy.

1. Introduction

Spectral/*hp* element methods, which are capable of extending the merits of spectral methods to complex geometries, have become increasingly popular in computational fluid dynamics, atmospheric modeling and many other fields [6, 15, 5]. While the quadrilateral/hexahedral spectral element methods (QSEM) have achieved tremendous advances since the 80s [21, 18], considerable progress has been made recently in the triangular/tetrahedral element methods (TSEM). The TSEM have proven to be more flexible for complex domains and for adaptivity, and the currently existing approaches can be roughly classified as (i) the use of Koornwinder-Dubiner polynomials [7, 23, 15]; (ii) approximations by non-polynomials on triangular elements [3, 13], and (iii) approximations by polynomials on triangular elements using special nodal points such as Fekete points [14, 24, 19].

Although the use of polynomials on triangles/tetrahedra seems to be natural, this also brings the loss of some flexibility and some difficult implementation issues. For example, the Koornwinder-Dubiner polynomial basis functions, obtained from the collapsed transform, are based on a warped tensor product, which is more complicated in implementation and analysis than the standard tensorial case. However, if one drops the requirement of being polynomials on the triangular/tetrahedral elements, such issues can be circumvented. In a very recent paper [22], we proposed a fully tensorial TSEM using rational basis functions obtained from the polynomials in the reference square through a collapsed coordinate transform. This approach was shown to be at least as accurate as the warped tensorial TSEM using Koornwinder-Dubiner polynomials, and be able to be effectively implemented as

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the QSEM due to the fully tensorial nature and the availability of the nodal basis. In this paper, we discuss the generalization of this method to the case of three dimensional tetrahedron with an aim towards an adaptive element method on unstructured meshes. The extension to three dimensions is nontrivial for several reasons. Firstly, the collapsed transform from a tetrahedron to the reference cube induces severer singularities (i.e., two faces of the cube are collapsed into one edge and one vertex of the tetrahedron) than that of the two dimensional case. Hence, much care has to be taken for dealing with the singularities in both implementations and analysis. On the other hand, the complication of geometry leads to some additional difficulties for the construction of modal/nodal basis functions, and numerical implementations as well.

The outline of the paper is as follows. In Section 2, we introduce the collapsed coordinate transform and the rational basis functions. We also present some results on the approximation properties of the new basis in Sobolev spaces. In Section 3, we implement the rational spectral methods for some model equations on tetrahedron. The final section is for the extension to the tetrahedral spectral elements and some discussions. We end this section with some notations to be used throughout the paper.

- Let $\Omega \subseteq \mathbb{R}^3$ be a bounded domain, and ω be a generic positive weight function which is not necessary in $L^1(\Omega)$. Denote by $(u,v)_{\omega,\Omega} := \int_\Omega uv\omega d\Omega$ the inner product of $L^2_\omega(\Omega)$ whose norm is denoted by $\|\cdot\|_{\omega,\Omega}$. For any $m \ge 0$, we use $H^m_\omega(\Omega)$ and $H^m_{0,\omega}(\Omega)$ to denote the usual weighted Sobolev spaces, whose norm and semi-norms are denoted by $\|u\|_{m,\omega,\Omega}$ and $|u|_{m,\omega,\Omega}$, respectively. In case of no confusion would arise, ω (if $\omega \equiv 1$) may be dropped from the notations.
- Let $\mathbb{N}$ be the set of non-negative integers and $\mathbb{Z}^-$ the set of negative integers. For any $N \in \mathbb{N}$, we set $I = (-1,1)$ and denote by $\mathcal{P}_N(I)$ the set of all polynomials of degree $\le N$, and set $\mathcal{P}^0_N(I) := \{\phi \in \mathcal{P}_N(I) : \phi(\pm 1) = 0\}$.
- We use the expression $A \lesssim B$ to mean that $A \le cB$, where c is a generic positive constant independent of any function and of any discretization parameters.

2. Rational basis functions and approximations on tetrahedra

We introduce in this section a family of orthogonal rational basis functions on tetrahedra, and study its approximation properties in Sobolev spaces.

2.1. The collapsed coordinate transform. It is known that there exists an affine mapping between the reference tetrahedron:

$$\mathcal{T} = \{(x,y,z) :\ 0 < x,y,z,x+y+z < 1\}, \tag{2.1}$$

and any arbitrary tetrahedron $\mathcal{T}_P$ with vertices $P_0 = (u_0,v_0,w_0)^{\mathsf{tr}}$, $P_1 = (u_1,v_1,w_1)^{\mathsf{tr}}$, $P_2 = (u_2,v_2,w_2)^{\mathsf{tr}}$ and $P_3 = (u_3,v_3,w_3)^{\mathsf{tr}}$, which takes the form

$$\begin{cases} u = u_0(1-x-y-z) + u_1x + u_2y + u_3z, \\ v = v_0(1-x-y-z) + v_1x + v_2y + v_3z, \\ w = w_0(1-x-y-z) + w_1x + w_2y + w_3z. \end{cases}$$

In view of this, we shall restrict our attentions to the reference tetrahedron $\mathcal{T}$. We also introduce a second coordinate $(\xi,\eta,\zeta)-$system on the reference cube $\mathcal{Q} :=$

$(-1,1)^3$. The so-called *collapsed coordinate transform* between $\mathcal{Q}$ and $\mathcal{T}$ is given by

$$x=\frac{1+\xi}{2}\frac{1-\eta}{2}\frac{1-\zeta}{2},\quad y=\frac{1+\eta}{2}\frac{1-\zeta}{2},\quad z=\frac{1+\zeta}{2},\quad \forall\ (\xi,\eta,\zeta)\in\mathcal{Q}, \tag{2.2}$$

with the inversion:

$$\xi=\frac{2x}{1-y-z}-1,\quad \eta=\frac{2y}{1-z}-1,\quad \zeta=2z-1,\quad \forall\ (x,y,z)\in\mathcal{T}. \tag{2.3}$$

As illustrated in Figure 2.1, this transform collapses the faces $\big\{(\xi,\eta,\zeta)\in\overline{\mathcal{Q}}:\ \zeta=1\big\}$ and $\big\{(\xi,\eta,\zeta)\in\overline{\mathcal{Q}}:\ \eta=1\big\}$ of $\mathcal{Q}$ into the vertex $(0,0,1)$ and the edge $\big\{(x,y,z)\in\overline{\mathcal{T}}:\ x=0,\ y+z=1\big\}$ of $\mathcal{T}$, respectively. Hence, it is referred to as the collapsed coordinate transform (also known as the Duffy system [8]), which is one of the indispensable building blocks of the spectral/*hp* element methods in [15].

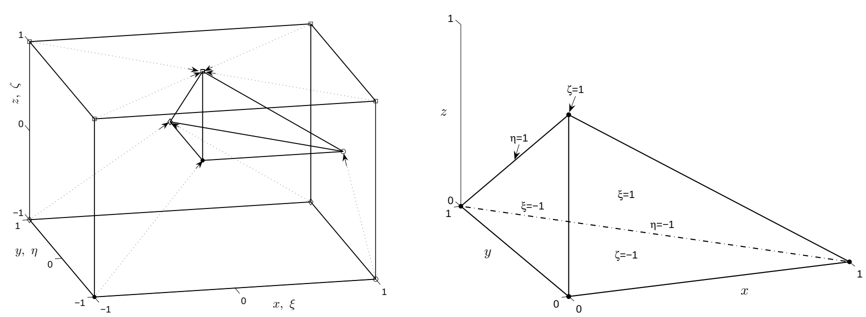

FIGURE 2.1. The collapsed transform between the cube $\mathcal{Q}$ and the tetrahedron $\mathcal{T}$.

It is important to point out that the vertex $(x,y,z)=(0,0,1)$ and the edge $\big\{(x,y,z)\in\overline{\mathcal{T}}:\ x=0;\ y+z=1\big\}$ are multi-valued, since both of them correspond to a face of $\mathcal{Q}$. However, there hold

$$\begin{aligned}&0\le\frac{y}{1-z}=\frac{1+\eta}{2}\le 1,\qquad \text{as } (y,z)\to(0,1) \text{ or } \zeta\to 1,\\ &0\le\frac{x}{1-y-z}=\frac{1+\xi}{2}\le 1,\qquad \text{as } (x,y,z)\to(0,0,1) \text{ or } \zeta\to 1.\end{aligned} \tag{2.4}$$

This situation is reminiscent of the coordinate singularity of the polar and spherical coordinates.

The following calculus associated with the transform (2.2)–(2.3) will be used frequently throughout this paper:

$$\begin{cases}\dfrac{\partial\xi}{\partial x}=\dfrac{2}{1-y-z}=\dfrac{8}{(1-\eta)(1-\zeta)}, & \dfrac{\partial\eta}{\partial x}=0, & \dfrac{\partial\zeta}{\partial x}=0,\\ \dfrac{\partial\xi}{\partial y}=\dfrac{2x}{(1-y-z)^2}=\dfrac{4(1+\xi)}{(1-\eta)(1-\zeta)}, & \dfrac{\partial\eta}{\partial y}=\dfrac{2}{1-z}=\dfrac{4}{1-\zeta}, & \dfrac{\partial\zeta}{\partial y}=0,\\ \dfrac{\partial\xi}{\partial z}=\dfrac{2x}{(1-y-z)^2}=\dfrac{4(1+\xi)}{(1-\eta)(1-\zeta)}, & \dfrac{\partial\eta}{\partial z}=\dfrac{2y}{(1-z)^2}=\dfrac{2(1+\eta)}{1-\zeta}, & \dfrac{\partial\zeta}{\partial z}=2,\end{cases} \tag{2.5}$$

and

(2.6)
$$\begin{cases} \dfrac{\partial x}{\partial \xi} = \dfrac{(1-\eta)(1-\zeta)}{8} = \dfrac{1-y-z}{2}, & \dfrac{\partial x}{\partial \eta} = 0, & \dfrac{\partial x}{\partial \zeta} = 0, \\ \dfrac{\partial y}{\partial \xi} = -\dfrac{(1+\xi)(1-\zeta)}{8} = -\dfrac{x(1-z)}{2(1-y-z)}, & \dfrac{\partial y}{\partial \eta} = \dfrac{1-\zeta}{4} = \dfrac{1-z}{2}, & \dfrac{\partial y}{\partial \zeta} = 0, \\ \dfrac{\partial z}{\partial \xi} = -\dfrac{(1+\xi)(1-\eta)}{8} = -\dfrac{x}{2(1-z)}, & \dfrac{\partial z}{\partial \eta} = -\dfrac{1+\eta}{4} = -\dfrac{y}{2(1-z)}, & \dfrac{\partial z}{\partial \zeta} = \dfrac{1}{2}. \end{cases}$$

Hence, the determinant of the Jacobian of (2.2)–(2.3) is

$$\frac{\partial(x,y,z)}{\partial(\xi,\eta,\zeta)} = \frac{(1-\eta)(1-\zeta)^2}{64} = \frac{(1-y-z)(1-z)}{8}. \tag{2.7}$$

Throughout this paper, we shall associate a function u in $\mathcal{T}$ with a function v in $\mathcal{Q}$ through

$$v(\xi,\eta,\zeta) = u(x,y,z), \quad \forall (x,y,z) \in \mathcal{T},\ \forall (\xi,\eta,\zeta) \in \mathcal{Q}. \tag{2.8}$$

One verifies readily that

$$\begin{aligned} \partial_x u &= \frac{8}{(1-\eta)(1-\zeta)}\partial_\xi v = \frac{2}{1-y-z}\partial_\xi v, \\ \partial_y u &= \frac{4}{1-\zeta}\partial_\eta v + \frac{4(1+\xi)}{(1-\eta)(1-\zeta)}\partial_\xi v = \frac{2}{1-z}\partial_\eta v + \frac{2x}{(1-y-z)^2}\partial_\xi v, \\ \partial_z u &= 2\partial_\zeta v + \frac{2(1+\eta)}{1-\zeta}\partial_\eta v + \frac{4(1+\xi)}{(1-\eta)(1-\zeta)}\partial_\xi v \\ &= 2\partial_\zeta v + \frac{2y}{(1-z)^2}\partial_\eta v + \frac{2x}{(1-y-z)^2}\partial_\xi v, \end{aligned} \tag{2.9}$$

and conversely,

$$\begin{aligned} \partial_\xi v &= \frac{1-y-z}{2}\partial_x u = \frac{(1-\eta)(1-\zeta)}{8}\partial_x u, \\ \partial_\eta v &= \frac{1-z}{2}\partial_y u - \frac{x(1-z)}{2(1-y-z)}\partial_x u = \frac{1-\zeta}{4}\partial_y u - \frac{(1+\xi)(1-\zeta)}{8}\partial_x u, \\ \partial_\zeta v &= \frac{1}{2}\partial_z u - \frac{y}{2(1-z)}\partial_y u - \frac{x}{2(1-z)}\partial_x u \\ &= \frac{1}{2}\partial_z u - \frac{1+\eta}{4}\partial_y u - \frac{(1+\xi)(1-\eta)}{8}\partial_x u. \end{aligned} \tag{2.10}$$

The factors $1/(1-\eta)$ and $1/(1-\zeta)$ in (2.9) play the same role as $1/r$ in the spherical coordinates. We also observe that the collapsed transform implies $v(\xi,\eta,1) = u(0,0,1)$ and $v(\xi,1,\zeta) = u(0,y,1-y)$. As a result,

$$\partial_\xi v(\xi,\eta,1) = \partial_\eta v(\xi,\eta,1) = \partial_\xi v(\xi,1,\zeta) = 0. \tag{2.11}$$

Note that the above corresponds to the pole condition in the polar and spherical coordinates.

2.2. Orthogonal systems on $\mathcal{T}$. Let $\omega^{\alpha,\beta,\gamma,\delta} = \omega^{\alpha,\beta,\gamma,\delta}(x,y,z) := (1-x-y-z)^\alpha x^\beta y^\gamma z^\delta$ with $\alpha,\beta,\gamma,\delta > -1$, be the weight function on the tetrahedron $\mathcal{T}$. Further, let $J_n^{\alpha,\beta}$ be the (generalized) Jacobi polynomials as defined in Appendix A. Karniadakis and Sherwin [23] introduced an orthogonal polynomial system in

$L^2(\mathcal{T})$, which turns to be a special case (with $\alpha=\beta=\gamma=\delta=0$) of the general orthogonal polynomials in $L^2_{\omega^{\alpha,\beta,\gamma,\delta}}(\mathcal{T})$ defined in [25]:

$$\begin{aligned}\mathcal{J}^{\alpha,\beta,\gamma,\delta}_{lmn}(x,y,z) &= (1-y-z)^l J^{\alpha,\beta}_l\Big(\frac{2x}{1-y-z}-1\Big)(1-z)^m \\ &\times J^{2l+1+\alpha+\beta,\gamma}_m\Big(\frac{2y}{1-z}-1\Big)J^{2l+2m+2+\alpha+\beta+\gamma,\delta}_n\big(2z-1\big),\ \forall (x,y,z)\in\mathcal{T}.\end{aligned} \tag{2.12}$$

In fact, the orthogonal polynomials are transformed from a product of one-dimensional polynomials via the mapping (2.3):

$$\begin{aligned}\mathcal{J}^{\alpha,\beta,\gamma,\delta}_{lmn}(x,y,z) =&\mathcal{G}^{\alpha,\beta,\gamma,\delta}_{lmn}(\xi,\eta,\zeta) = J^{\alpha,\beta}_l(\xi)\Big(\frac{1-\eta}{2}\Big)^l J^{2l+1+\alpha+\beta,\gamma}_m(\eta)\\ &\times\Big(\frac{1-\zeta}{2}\Big)^{l+m}J^{2l+2m+2+\alpha+\beta+\gamma,\delta}_n(\zeta), \qquad \forall(\xi,\eta,\zeta)\in\mathcal{Q}.\end{aligned}$$

In contrast to the standard tensor product, the subscripts and superscripts in $\mathcal{J}^{\alpha,\beta,\gamma,\delta}_{lmn}$ are intrinsically dependent, and it is referred to as a *warped* (or *generalized*) tensor product. Such types of polynomials were also considered in [20, 16, 7] in two or three dimensional settings. Tetrahedral spectral/hp element methods using these Koornwinder-Dubiner polynomials on both the tetrahedral elements and the reference cubic elements have been systematically developed in [15]. However, the warped tensor structure of the basis functions makes it difficult to analyze (cf. [12]) and somewhat difficult to implement, particularly, when very high-order polynomials have to be used. Moreover, no nodal basis is available.

In fact, by restricting to polynomials, one may loss some flexibility and face some complicated issues. Motivated by [22], we shall develop a spectral method using fully tensorial rational basis functions, which is easy to implement and is also spectrally accurate. For this purpose, we define

(2.13)
$$\mathcal{R}^{\alpha,\beta,\gamma,\delta}_{lmn}(x,y,z) = J^{\alpha,\beta}_l\Big(\frac{2x}{1-y-z}-1\Big)J^{1+\alpha+\beta,\gamma}_m\Big(\frac{2y}{1-z}-1\Big)J^{2+\alpha+\beta+\gamma,\delta}_n\big(2z-1\big),$$

for all $(x,y,z)\in\mathcal{T}$, which is generated from a tensor product of the Jacobi polynomials

$$\begin{aligned}\mathcal{R}^{\alpha,\beta,\gamma,\delta}_{lmn}(x,y,z) &= \widetilde{\mathcal{R}}^{\alpha,\beta,\gamma,\delta}_{lmn}(\xi,\eta,\zeta)\\ &= J^{\alpha,\beta}_l(\xi)J^{1+\alpha+\beta,\gamma}_m(\eta)J^{2+\alpha+\beta+\gamma,\delta}_n(\zeta), \quad \forall(\xi,\eta,\zeta)\in\mathcal{Q}.\end{aligned} \tag{2.14}$$

By the orthogonality of the Jacobi polynomials and (2.7), we have that

$$\begin{aligned}&\Big(\mathcal{R}^{\alpha,\beta,\gamma,\delta}_{lmn},\mathcal{R}^{\alpha,\beta,\gamma,\delta}_{l'm'n'}\Big)_{\omega^{\alpha,\beta,\gamma,\delta},\mathcal{T}}\\ =&\iiint_{\mathcal{T}}\mathcal{R}^{\alpha,\beta,\gamma,\delta}_{lmn}(x,y,z)\mathcal{R}^{\alpha,\beta,\gamma,\delta}_{l'm'n'}(x,y,z)\omega^{\alpha,\beta,\gamma,\delta}(x,y,z)dxdydz\\ =&\frac{1}{2^{6+3\alpha+3\beta+2\gamma+\delta}}\int_{-1}^1 J^{\alpha,\beta}_l(\xi)J^{\alpha,\beta}_{l'}(\xi)\varpi^{\alpha,\beta}(\xi)d\xi\\ &\times\int_{-1}^1 J^{1+\alpha+\beta,\gamma}_m(\eta)J^{1+\alpha+\beta,\gamma}_{m'}(\eta)\varpi^{1+\alpha+\beta,\gamma}(\eta)d\eta\\ &\times\int_{-1}^1 J^{2+\alpha+\beta+\gamma,\delta}_n(\zeta)J^{2+\alpha+\beta+\gamma,\delta}_{n'}(\zeta)\varpi^{2+\alpha+\beta+\gamma,\delta}(\zeta)d\zeta\\ =&\gamma^{\alpha,\beta}_l\gamma^{1+\alpha+\beta,\gamma}_m\gamma^{2+\alpha+\beta+\gamma,\delta}_n\delta_{ll'}\delta_{mm'}\delta_{nn'} := \gamma^{\alpha,\beta,\gamma,\delta}_{lmn}\delta_{ll'}\delta_{mm'}\delta_{nn'},\end{aligned} \tag{2.15}$$

where $\varpi^{a,b}(t) = (1-t)^a(1+t)^b$ is the Jacobi weight function, and

$$\gamma_l^{\alpha,\beta} = \frac{1}{(2l+\alpha+\beta+1)}\frac{\Gamma(l+\alpha+1)\Gamma(l+\beta+1)}{\Gamma(l+1)\Gamma(l+\alpha+\beta+1)}. \tag{2.16}$$

Consequently, $\{\mathcal{R}_{lmn}^{\alpha,\beta,\gamma,\delta}\}$ are orthogonal in $L^2_{\omega^{\alpha,\beta,\gamma,\delta}}(\mathcal{T})$, and clearly, by dropping the requirement of being polynomials on $\mathcal{T}$, the new basis is formed by a standard tensor product of one-dimensional basis functions. In this paper, we will only use the special case with $\alpha=\beta=\gamma=\delta=0$, so the resultant system is orthogonal with a uniform weight. For notational convenience, we shall omit the superscripts, and simply denote

$$\begin{aligned}\mathcal{R}_{lmn}(x,y,z) &= \mathcal{R}_{lmn}^{0,0,0,0}(x,y,z)\\ &= J_l^{0,0}\Big(\frac{2x}{1-y-z}-1\Big)J_m^{1,0}\Big(\frac{2y}{1-z}-1\Big)J_n^{2,0}\big(2z-1\big)\\ &= \widetilde{\mathcal{R}}_{lmn}(\xi,\eta,\zeta) = J_l^{0,0}(\xi)J_m^{1,0}(\eta)J_n^{2,0}(\zeta),\end{aligned} \tag{2.17}$$

and the constant in (2.15) is

$$\gamma_{lmn} = \gamma_l^{0,0}\gamma_m^{1,0}\gamma_n^{2,0} = \frac{1}{(2l+1)(2m+2)(2n+3)}. \tag{2.18}$$

2.3. Approximations by the rational basis functions. We now analyze the approximations of functions in $L^2(\mathcal{T})$ by the truncated series of the rational basis. At this point, a natural question is whether this rational approximation on the tetrahedron is as accurate as or better than the polynomial approximation? We shall answer this question by performing error analysis in the original coordinates of the tetrahedron, and by presenting illustrative numerical results. The difficulty in obtaining error bounds in the original coordinates is that the collapsed coordinate transform induces a coordinate singularity, similar to the polar and spherical coordinate transforms. However, in polar and spherical geometries, one actually prefers to write the equations in polar and spherical coordinates rather than the original Cartesian coordinates, so it is natural to work in the "transformed" polar or spherical coordinates. But for tetrahedral domains, one obviously prefers to work with the original coordinates.

2.3.1. L^2-projection errors. For any function $u \in L^2(\mathcal{T})$, we write

$$u(x,y,z) = \sum_{l=0}^{\infty}\sum_{m=0}^{\infty}\sum_{n=0}^{\infty}\hat{u}_{lmn}\mathcal{R}_{lmn}(x,y,z). \tag{2.19}$$

Setting

$$\chi^{\alpha_1,\beta_1;\alpha_2,\beta_2;\alpha_3,\beta_3} = \chi^{\alpha_1,\beta_1;\alpha_2,\beta_2;\alpha_3,\beta_3}(\xi,\eta,\zeta) := \varpi^{\alpha_1,\beta_1}(\xi)\varpi^{\alpha_2,\beta_2}(\eta)\varpi^{\alpha_3,\beta_3}(\zeta),$$

and $v(\xi,\eta,\zeta) = u(x,y,z)$, one verifies that $v \in L^2_{\chi^{0,0;1,0;2,0}}(\mathcal{Q})$, and

$$u(x,y,z) = v(\xi,\eta,\zeta) = \sum_{l=0}^{\infty}\sum_{m=0}^{\infty}\sum_{n=0}^{\infty}\hat{v}_{lmn}\widetilde{\mathcal{R}}_{lmn}(\xi,\eta,\zeta), \tag{2.20}$$

where $\{\widetilde{\mathcal{R}}_{lmn}\}$ are defined in (2.14), and

$$\begin{aligned}\hat{u}_{lmn} &= \frac{1}{\gamma_{lmn}}\iiint_{\mathcal{T}} u(x,y)\mathcal{R}_{lmn}(x,y,z)dxdydz\\ &= \frac{1}{2^6\gamma_{lmn}}\iiint_{\mathcal{Q}} v(\xi,\eta,\zeta)\widetilde{\mathcal{R}}_{lmn}(\xi,\eta,\zeta)\chi^{0,0;1,0;2,0}(\xi,\eta,\zeta)d\xi d\eta d\zeta\end{aligned}$$

$$= \frac{1}{2^6\gamma_{lmn}} \int_{-1}^{1} J_n^{2,0}(\zeta)\varpi^{2,0}(\zeta) \int_{-1}^{1} J_m^{1,0}(\eta)\varpi^{1,0}(\eta) \int_{-1}^{1} v(\xi,\eta,\zeta) J_l^{0,0}(\xi) d\xi d\eta d\zeta$$
$$= \hat{v}_{lmn}.$$

Define the finite-dimensional space

$$\Re_{LMN} := \text{span}\big\{\mathcal{R}_{lmn} \ : \ 0 \le l \le L,\ 0 \le m \le M,\ 0 \le n \le N\big\}. \tag{2.21}$$

Define the truncated series

$$\Pi_{LMN} u(x,y,z) = \sum_{l=0}^{L}\sum_{m=0}^{M}\sum_{n=0}^{N} \hat{u}_{lmn}\mathcal{R}_{lmn}(x,y,z) \in \Re_{LMN},$$

and clearly,

$$\iiint_{\mathcal{T}} \big(\Pi_{LMN} u - u\big)\Phi \ dxdydz = 0, \quad \forall \Phi \in \Re_{LMN}. \tag{2.22}$$

For a more precise description of the error, we define the Jacobi weighted space for any $q, r, s \in \mathbb{N}$,

$$\mathcal{H}^{q,r,s}(\mathcal{T}) = \left\{ u \in L^2(\mathcal{T}) \ : \ \|u\|_{\mathcal{H}^{q,r,s}(\mathcal{T})} := \Big(\|u\|_{\mathcal{T}}^2 + |u|^2_{\mathcal{H}^{q,r,s}(\mathcal{T})}\Big)^{\frac{1}{2}} < \infty \right\},$$

where the semi-norm is defined by

$$|u|_{\mathcal{H}^{q,r,s}(\mathcal{T})} = \Big(\|\partial_x^r u\|^2_{\omega^{q,q,0,0},\mathcal{T}} + \sum_{j=0}^{r} \|\partial_y^j(\partial_y - \partial_x)^{r-j} u\|^2_{\omega^{j,r-j,r,0},\mathcal{T}}$$
$$+ \sum_{j=0}^{s}\sum_{k=0}^{s-j} \|\partial_z^j(\partial_z-\partial_y)^k(\partial_z-\partial_x)^{s-j-k}u\|^2_{\omega^{j,s-j-k,k,s},\mathcal{T}} \Big)^{\frac{1}{2}}.$$

Note that the weight functions in the above norms are uniformly bounded, so we have the usual Sobolev space $H^r(\mathcal{T}) \subset \mathcal{H}^{r,r,r}(\mathcal{T})$.

Theorem 2.1. *For any $u \in \mathcal{H}^{q,r,s}(\mathcal{T})$ with integers $q, r, s \ge 0$, we have*

(2.23)

$$\big\|\Pi_{LMN}u - u\big\|_{\mathcal{T}} \lesssim L^{-q}\big\|\partial_x^q u\big\|_{\omega^{q,q,0,0},\mathcal{T}} + M^{-r}\sum_{j=0}^{r}\big\|\partial_y^j(\partial_y-\partial_x)^{r-j}u\big\|_{\omega^{j,r-j,r,0},\mathcal{T}}$$
$$+ N^{-s}\sum_{j=0}^{s}\sum_{k=0}^{s-j}\big\|\partial_z^j(\partial_z-\partial_y)^k(\partial_z-\partial_x)^{s-j-k}u\big\|_{\omega^{j,s-j-k,k,s},\mathcal{T}}.$$

In particular, we denote $\Pi_M = \Pi_{MMM}$. Then for any $u \in H^r(\mathcal{T})$ with integer $r \ge 0$,

$$\big\|\Pi_M u - u\big\|_{\mathcal{T}} \lesssim M^{-r}|u|_{H^r(\mathcal{T})}, \tag{2.24}$$

where the semi-norm $|\cdot|_{H^r(\mathcal{T})}$ is defined by

$$|u|_{H^r(\mathcal{T})} = \left(\sum_{j=0}^{s}\sum_{k=0}^{s-j} \big\|\partial_z^j\partial_y^k\partial_x^{r-j-k}u\big\|^2_{\mathcal{T}} \right)^{\frac{1}{2}}.$$

We postpone the proof of this theorem to Appendix B.

2.3.2. Quadrature and interpolation on the tetrahedron. We now define the quadrature and interpolation on tetrahedron, which are essential for numerical integrations/differentiations in spectral approximations, and also for the introduction of the nodal basis. In view of the singularity of the coordinate transform, it is appropriate to use Gauss-Lobatto points in $\xi-$direction, and Gauss-Radau points in the other two directions.

Let $\{\xi_l\}_{l=0}^{M}$, $\{\eta_m\}_{m=0}^{M}$ and $\{\zeta_n\}_{n=0}^{M}$ be the roots of $(1-\xi^2)J_{M-1}^{1,1}(\xi)$, $(1+\eta)J_M^{1,1}(\eta)$ and $(1+\zeta)J_M^{2,1}(\zeta)$, respectively. Further let

$$\begin{aligned}\omega_l^{\xi} &= \frac{2}{M(M+1)\big[J_M^{0,0}(\xi_l)\big]^2}, \quad 0\le l\le M,\\ \omega_m^{\eta} &= \frac{2(1-\eta_m)}{(M+1)(M+2)\big[J_{M+1}^{0,0}(\eta_m)\big]^2}, \quad 0\le m\le M,\\ \omega_n^{\zeta} &= \frac{4(1-\zeta_n)}{(M+1)(M+3)\big[J_{M+1}^{1,0}(\zeta_n)\big]^2}, \quad 0\le n\le M.\end{aligned}$$

Namely, $\{\xi_l,\omega_l^{\xi}\}_{l=0}^{M}$ are the nodes and weights of the Legendre-Gauss-Lobatto quadrature, $\{\eta_m,\omega_m^{\eta}\}_{m=0}^{M}$ and $\{\zeta_n,\omega_n^{\zeta}\}_{n=0}^{M}$ are the nodes and weights of the Jacobi-Gauss-Radau quadrature with the weight functions $\varpi^{1,0}(\eta)$ and $\varpi^{2,0}(\zeta)$, respectively.

The quadrature grids on $\mathcal{T}$ are defined as

$$x_{lmn} = \frac{1+\xi_l}{2}\frac{1-\eta_m}{2}\frac{1-\zeta_n}{2}, \quad y_{lmn} = \frac{1+\eta_m}{2}\frac{1-\zeta_n}{2}, \quad z_{lmn} = \frac{1+\zeta_n}{2}, \quad 0\le l,m,n\le M. \tag{2.25}$$

Some samples of the points are depicted in Figure 2.2 (left). We further define the discrete inner product on $\mathcal{T}$ by

$$(u,v)_{M,\mathcal{T}} := \frac{1}{64}\sum_{l=0}^{M}\sum_{m=0}^{M}\sum_{n=0}^{M} u(x_{lmn},y_{lmn},z_{lmn})v(x_{lmn},y_{lmn},z_{lmn}) \times \omega_l^{\xi}\omega_m^{\eta}\omega_n^{\zeta}, \qquad \forall u,v\in C(\overline{\mathcal{T}}), \tag{2.26}$$

which is exact, i.e., $(u,v)_{M,\mathcal{T}} = (u,v)_{\mathcal{T}}$, for any $u,v\in\Re_{M-1,M,M}$. Further, we define the rational interpolation operator. For any $u\in C(\overline{\mathcal{T}})$, the interpolant $\mathcal{I}_M u\in\Re_{MMM}$ such that

$$(\mathcal{I}_M u)(x_{lmn},y_{lmn},z_{lmn}) = u(x_{lmn},y_{lmn},z_{lmn}), \quad 0\le l,m,n\le M. \tag{2.27}$$

Finally, we conclude this section with a theorem on the error estimate for the rational interpolation $\mathcal{I}_M$, whose proof will be postponed to Appendix C.

Theorem 2.2. *For any $u\in H^r(\mathcal{T})$, with integers $r\ge 3$, we have*

$$\big\|\mathcal{I}_M u - u\big\|_{\mathcal{T}} \lesssim M^{-r}|u|_{H^r(\mathcal{T})}. \tag{2.28}$$

3. Rational spectral methods on the tetrahedron

Consider the modified Helmholtz equation on the tetrahedron $\mathcal{T}$:

$$-\Delta u + \gamma u = f \quad \text{in } \mathcal{T}; \quad u|_{\partial\mathcal{T}} = 0, \quad \gamma\ge 0. \tag{3.1}$$

The variational formulation of (3.1) is to find $u\in H_0^1(\mathcal{T})$ such that

$$a(u,v) := \big(\nabla u,\nabla v\big)_{\mathcal{T}} + \gamma\big(u,v\big)_{\mathcal{T}} = \big(f,v\big)_{\mathcal{T}}, \quad \forall v\in H_0^1(\mathcal{T}), \tag{3.2}$$

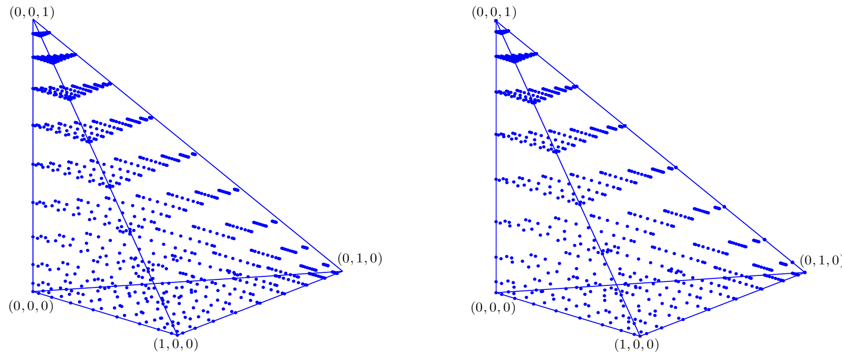

FIGURE 2.2. Distributions of the collocation points ($M = 10$). Left: the transformed points given by (2.25). Right: Legendre-Gauss-Lobatto nodes along all the ξ, η and ζ directions, which will be used to define the nodal basis functions in Section 4.

which, thanks to the Lax-Milgram lemma and the Poincaré inequality, admits a unique solution satisfying

$$\|\nabla u\|_{\mathcal{T}} + \|u\|_{\mathcal{T}} \lesssim \|f\|_{\mathcal{T}}. \tag{3.3}$$

Denote by $\Re_M := \Re_{MMM}$ (cf. (2.21)), and define $X_M^0 = \Re_M \cap H_0^1(\mathcal{T})$. It is clear that the transform (2.2) maps X_M^0 in $\mathcal{T}$ to $\big(\mathcal{P}_M^0(I)\big)^3$ in $\mathcal{Q}$. The rational spectral-Galerkin approximation to (3.2) is to find $u_M \in X_M^0$ such that

$$a(u_M, \varphi) = (\mathcal{I}_M f, \varphi)_{\mathcal{T}}, \quad \forall \varphi \in X_M^0, \tag{3.4}$$

which has a unique solution satisfying (3.3) with u_M and $\mathcal{I}_M f$ in place of u and f, respectively.

3.1. Error estimates. By a standard argument, one derives from (3.2) and (3.4) that

$$\begin{aligned} \|u_M - u\|_{H^1(\mathcal{T})} &\lesssim \inf_{v_M \in X_M^0} \|v_M - u\|_{H^1(\mathcal{T})} + \big\|\mathcal{I}_M f - f\big\|_{L^2(\mathcal{T})} \\ &\lesssim \big\|\Pi_M^{1,0} - u\big\|_{H^1(\mathcal{T})} + \big\|\mathcal{I}_M f - f\big\|_{L^2(\mathcal{T})}, \end{aligned} \tag{3.5}$$

where $\Pi_M^{1,0} : H_0^1(\mathcal{T}) \to X_M^0$ is the H_0^1-orthogonal projection, defined by

$$\big(\nabla(\Pi_M^{1,0} u - u),\ \nabla \Phi\big)_{\mathcal{T}} = 0, \quad \forall \Phi \in X_M^0. \tag{3.6}$$

Hence, to analyze the error, we need the following result.

Lemma 3.1. *For any $u \in H_0^1(\mathcal{T}) \cap H^r(\mathcal{T})$ with $r \ge 1$,*

$$\|\Pi_M^{1,0} u - u\|_{\mu,\mathcal{T}} \lesssim M^{\mu - r} |u|_{H^r(\mathcal{T})}, \quad \mu = 0, 1. \tag{3.7}$$

The argument for this proof is quite similar to that of Theorem 3.2 in [22]. Basically, it is essential to prove the estimate with $\mu = 1$, and the case with $\mu = 0$ can be shown by a duality argument. In contrast with the L^2-estimate, after we transform $\|\Pi_M^{1,0} u - u\|_{1,\mathcal{T}}$ to the corresponding norm in $\mathcal{Q}$, some of the norms may involve Jacobi weights with negative integer parameters -1 or -2. Hence, some one-dimensional generalized Jacobi approximation results (cf. [9, 10]) have to be used to handle the singular weights. Here, we omit the lengthy proof.

We now obtain the following theorem on the error estimates of the rational spectral-Galerkin approximation (3.4).

Theorem 3.1. *Let u and u_M be the solutions of* (3.2) *and* (3.4)*, respectively. If $u \in H_0^1(\mathcal{T}) \cap H^r(\mathcal{T})$ and $f \in H^s(\mathcal{T})$ with $r \geq 1$ and $s \geq 3$, then we have*

$$\|u_M - u\|_{H^\mu(\mathcal{T})} \lesssim M^{\mu-r}|u|_{H^r(\mathcal{T})} + M^{-s}|f|_{H^s(\mathcal{T})}, \quad \mu = 0, 1. \tag{3.8}$$

Proof. Then, applying Lemma 3.1 and Theorem 2.2 to the above, we obtain immediately (3.8) with $\mu = 1$. The result for $\mu = 0$ can then be derived by using a standard duality argument. □

Remark 3.1. Alternative to (3.4), we can also consider the following rational spectral-Galerkin approximation with numerical integration: find $u_M \in X_M^0$ such that

$$a_M(u_M, \varphi) := \gamma(u_M, \varphi)_{M,\mathcal{T}} + (\nabla u_M, \nabla\varphi)_{M,\mathcal{T}} = (f, \varphi)_{M,\mathcal{T}}, \quad \forall \varphi \in X_M^0, \tag{3.9}$$

which is suitable for the approximation on arbitrary tetrahedron. In fact, it can be easily shown that Theorem 3.1 holds for (3.9) as well.

Remark 3.2. The optimal results for polynomial approximation on simplices are established in [4]. However, the results in [4] are expressed in terms of Sturm-Liouville operator on simplices or in terms of polynomial expansion coefficients. It is not a trivial task (cf. [12], [17]) to bound these terms by simple derivative terms as presented here.

3.2. Modal basis functions. In order to treat non-homogeneous boundary conditions and/or to enforce continuity across the interfaces in a tetrahedral spectral-element method, we need to construct basis functions for

$$X_{LMN} = \Re_{LMN} \cap C(\overline{\mathcal{T}}) \cap H^1(\mathcal{T}). \tag{3.10}$$

For this purpose, we first point out that under the mapping (2.2)-(2.3), the space $H^1(\mathcal{T})$ corresponds to the weighted space

$$\widetilde{H}^1(\mathcal{Q}) := \big\{v \in L^2_{\chi^{0,0;1,0;2,0}}(\mathcal{Q}) \ : \partial_\xi v \in L^2_{\chi^{0,0;-1,0;0,0}}(\mathcal{Q}),\ \partial_\eta v \in L^2_{\chi^{0,0;1,0;0,0}}(\mathcal{Q}) \text{ and } \partial_\zeta v \in L^2_{\chi^{0,0;1,0;2,0}}(\mathcal{Q})\big\},$$

with the norm

$$\|v\|_{\widetilde{H}^1(\mathcal{Q})} = \Big(\|\partial_\xi v\|^2_{\chi^{0,0;-1,0;0,0}} + \|\partial_\eta v\|^2_{\chi^{0,0;1,0;0,0}} + \|\partial_\zeta v\|^2_{\chi^{0,0;1,0;2,0}} + \|v\|^2_{\chi^{0,0;1,0;2,0}}\Big)^{\frac{1}{2}}.$$

One verifies the equivalence by using (2.4) and (2.9)–(2.10):

$$\|v\|_{\widetilde{H}^1(\mathcal{Q})} \lesssim \|u\|_{H^1(\mathcal{T})} \lesssim \|v\|_{\widetilde{H}^1(\mathcal{Q})}.$$

Now it can be readily verified that under the transform (2.2), X_{LMN} corresponds to

$$\widetilde{X}_{LMN} := \big\{\Psi \in P_L(I_\xi) \times P_M(I_\eta) \times P_N(I_\zeta) \ : \partial_\xi \Psi(\xi, 1, \zeta) = \partial_\xi \Psi(\xi, \eta, 1) = \partial_\eta \Psi(\xi, \eta, 1) = 0\big\}.$$

Meanwhile, we recall for the following C^0-model basis for $P_L(I_\xi) \times P_M(I_\eta) \times P_N(I_\zeta)$:

$$\Psi_{lmn}(\xi, \eta, \zeta) := \psi_l(\xi)\psi_m(\eta)\psi_n(\zeta), \quad 0 \leq l \leq L,\ 0 \leq m \leq M,\ 0 \leq n \leq N, \tag{3.11}$$

where

$$\psi_k(z) = \begin{cases} \dfrac{1+z}{2} = \dfrac{1}{2}\big(J_0^{0,0}(z) + J_1^{0,0}(z)\big) = J_1^{0,-1}(z), & k = 0, \\ \dfrac{1-z}{2} = \dfrac{1}{2}\big(J_0^{0,0}(z) - J_1^{0,0}(z)\big) = -J_1^{-1,0}(z), & k = 1, \\ J_k^{0,0}(z) - J_{k-2}^{0,0}(z) = \dfrac{2(2k-1)}{k-1} J_k^{-1,-1}(z), & k \geq 2. \end{cases} \tag{3.12}$$

Observe that for any $0 \le l \le L,\ 1 \le m \le M,\ 1 \le n \le N,$

$$\partial_\xi \Psi_{lmn}(\xi,1,\zeta) = \partial_\xi \Psi_{lmn}(\xi,\eta,1) = \partial_\eta \Psi_{lmn}(\xi,\eta,1) = 0.$$

Hence, by adding

$$\begin{aligned} &\Psi_{-1,-1,0}(\xi,\eta,\zeta) := 1 \times 1 \times \psi_0(\zeta) \in \widetilde{X}_{LMN},\\ &\Psi_{-10n}(\xi,\eta,\zeta) := 1 \times \psi_0(\eta)\psi_n(\zeta) \in \widetilde{X}_{LMN}, \quad 1 \le n \le N, \end{aligned} \tag{3.13}$$

we have that

$$\widetilde{X}_{LMN} = \mathrm{span}\big\{\Psi_{lmn}(\xi,\eta,\zeta)\ :\ (l,m,n) \in \Upsilon_{LMN}\big\}, \tag{3.14}$$

where the index set

$$\begin{aligned} \Upsilon_{LMN} := &\big\{(l,m,n)\ :\ 0 \le l \le L,\ 1 \le m \le M,\ 1 \le n \le N\big\}\\ &\cup \big\{(-1,0,n)\ :\ 0 \le n \le N\big\} \cup \big\{(-1,-1,0)\big\}. \end{aligned} \tag{3.15}$$

Let $\Phi_{lmn}(x,y,z) = \Psi_{lmn}(\xi,\eta,\zeta)$ (under the mapping (2.2)–(2.3)), and

$$X_{LMN} = \mathrm{span}\big\{\Phi_{lmn}(x,y,z)\ :\ (l,m,n) \in \Upsilon_{LMN}\big\}. \tag{3.16}$$

Then $\{\Phi_{lmn}\}_{(l,m,n)\in\Upsilon_{LMN}}$ forms a rational C^0-basis of $H^1(\mathcal{T})$. Moreover, as in the $p-$version of finite elements, we can split this modal basis into *interior* and *boundary* modes (including *vertex*, *edge* and *face* modes). All interior modes are zero on the tetrahedron boundary, and the vertex modes have a unit magnitude at one vertex and are zero at all other vertices, while the edge modes only have magnitude along one edge, and the face modes only have magnitude along one face.

- Interior modes:

$$\Phi_{lmn}(x,y,z) = \Psi_{lmn}(\xi,\eta,\zeta), \qquad 2 \le l \le L,\ 2 \le m \le M,\ 2 \le n \le N; \tag{3.17}$$

- Face modes:

(3.18)

$$\begin{cases} x+y+z=1\ (\xi=1): & \Phi_{0mn}(x,y,z) = \Psi_{0mn}(\xi,\eta,\zeta), & 2 \le m \le M,\ 2 \le n \le N,\\ x=0\ (\xi=-1): & \Phi_{1mn}(x,y,z) = \Psi_{1mn}(\xi,\eta,\zeta), & 2 \le m \le M,\ 2 \le n \le N,\\ y=0\ (\eta=-1): & \Phi_{l1n}(x,y,z) = \Psi_{l1n}(\xi,\eta,\zeta), & 2 \le l \le L,\ 2 \le n \le N,\\ z=0\ (\zeta=-1): & \Phi_{lm1}(x,y,z) = \Psi_{lm1}(\xi,\eta,\zeta), & 2 \le l \le L, 2 \le m \le M; \end{cases}$$

- Edge modes:

$$\begin{cases} \begin{matrix} x+y+z=1, y=0\\ (\xi=1,\eta=-1)\end{matrix} : & \Phi_{01n}(x,y,z) = \Psi_{01n}(\xi,\eta,\zeta), & 2 \le n \le N,\\ \begin{matrix} x+y+z=1, x=0\\ (\eta=1)\end{matrix} : & \Phi_{-10n}(x,y,z) = \Psi_{-10n}(\xi,\eta,\zeta), & 2 \le n \le N,\\ \begin{matrix} x+y+z=1, z=0\\ (\xi=1,\zeta=-1)\end{matrix} : & \Phi_{0m1}(x,y,z) = \Psi_{0m1}(\xi,\eta,\zeta), & 2 \le m \le M,\\ x=y=0\ (\xi=\eta=-1): & \Phi_{11n}(x,y,z) = \Psi_{11n}(\xi,\eta,\zeta), & 2 \le n \le N,\\ x=z=0\ (\xi=\zeta=-1): & \Phi_{1m1}(x,y,z) = \Psi_{1m1}(\xi,\eta,\zeta), & 2 \le m \le M,\\ y=z=0\ (\eta=\zeta=-1): & \Phi_{l11}(x,y,z) = \Psi_{l11}(\xi,\eta,\zeta), & 2 \le l \le L; \end{cases} \tag{3.19}$$

- Vertex modes:

$$\begin{cases} \begin{matrix} x=y=z=0 \\ (\xi=\eta=\zeta=-1) \end{matrix} : & \Phi_{111}(x,y,z)=\Psi_{111}(\xi,\eta,\zeta), \\ \begin{matrix} x=1, y=z=0 \\ (\xi=1,\eta=\zeta=-1) \end{matrix} : & \Phi_{011}(x,y,z)=\Psi_{011}(\xi,\eta,\zeta), \\ \begin{matrix} y=1, x=z=0 \\ (\eta=1,\zeta=-1) \end{matrix} : & \Phi_{-101}(x,y,z)=\Psi_{-101}(\xi,\eta,\zeta), \\ \begin{matrix} z=1, x=y=0 \\ (\zeta=1) \end{matrix} : & \Phi_{-1,-1,0}(x,y,z)=\Psi_{-1,-1,0}(\xi,\eta,\zeta). \end{cases} \tag{3.20}$$

In order to enforce C^0-continuity between adjacent tetrahedral elements, we required that $L = M = N$. Accordingly, we denote $X_M = X_{MMM}$ and likewise for $\widetilde{X}_M$ and Υ_M.

3.3. Implementations. We now examine the linear system associated with the spectral-Galerkin approximation (3.4).

For convenience, we shall make use of the following functions and identities:

$$\begin{aligned}
\psi_l^0(\xi) &:= J_l^{0,0}(\xi) - J_{l-2}^{0,0}(\xi) \\
&= \frac{l+1}{2l+1} J_l^{1,0}(\xi) - \frac{l}{2l+1} J_{l-1}^{1,0}(\xi) - \frac{l-1}{2l-3} J_{l-2}^{1,0}(\xi) + \frac{l-2}{2l-3} J_{l-3}^{1,0}(\xi), \\
\psi_l^1(\xi) &:= \partial_\xi \psi_l^0(\xi) = (2l-1) J_{l-1}^{0,0}(\xi) = l J_{l-1}^{1,0}(\xi) - (l-1) J_{l-2}^{1,0}(\xi), \\
\psi_l^2(\xi) &:= (1+\xi)\partial_\xi \psi_l^0(\xi) = l J_l^{0,0}(\xi) + (2l-1) J_{l-1}^{0,0}(\xi) + (l-1) J_{l-2}^{0,0}(\xi) \\
&= \frac{l(l+1)}{2l+1} J_l^{1,0}(\xi) + \frac{l(l+1)}{2l+1} J_{l-1}^{1,0}(\xi) - \frac{(l-2)(l-1)}{2l-3} J_{l-2}^{1,0}(\xi) \\
&\quad - \frac{(l-2)(l-1)}{2l-3} J_{l-3}^{1,0}(\xi), \\
\psi_m^3(\eta) &:= \frac{1}{1-\eta} \psi_m^0(\eta) = -J_{m-1}^{1,0}(\eta) - J_{m-2}^{1,0}(\eta), \\
\psi_n^4(\zeta) &:= (1-\zeta)\partial_\zeta \psi_n^0(\zeta) = -n J_n^{0,0}(\zeta) + (2n-1) J_{n-1}^{0,0}(\zeta) - (n-1) J_{n-2}^{0,0}(\zeta), \\
\psi_n^5(\zeta) &:= (1-\zeta)\psi_l^0(\zeta) = -\frac{n+1}{2n+1} J_{n+1}^{0,0}(\zeta) + J_n^{0,0}(\zeta) + \frac{2n-1}{(2n+1)(2n-3)} J_{n-1}^{0,0}(\zeta) \\
&\quad - J_{n-2}^{0,0}(\zeta) + \frac{n-2}{2n-3} J_{n-3}^{0,0}(\zeta).
\end{aligned}$$

It is easy to verify that

$$\begin{aligned}
&\Phi_{lmn}(x,y,z) = \psi_l^0(\xi) \times \psi_m^0(\eta) \times \varpi^{-1,0}(\zeta)\psi_n^5(\zeta), \\
&\partial_x \Phi_{lmn}(x,y,z) = 8\ \psi_l^1(\xi) \times \psi_m^3(\eta) \times \varpi^{-1,0}(\zeta)\psi_n^0(\zeta), \\
&\partial_y \Phi_{lmn}(x,y,z) = 4\ \psi_l^2(\xi) \times \psi_m^3(\eta) \times \varpi^{-1,0}(\zeta)\psi_n^0(\zeta) \\
&\qquad + 4\ \psi_l^0(\xi) \times \psi_m^1(\eta) \times \varpi^{-1,0}(\zeta)\psi_n^0(\zeta), \\
&\partial_z \Phi_{lmn}(x,y,z) = 4\ \psi_l^2(\xi) \times \psi_m^3(\eta) \times \varpi^{-1,0}(\zeta)\psi_n^0(\zeta) \\
&\qquad + 2\ \psi_l^0(\xi) \times \psi_m^2(\eta) \times \varpi^{-1,0}(\zeta)\psi_n^0(\zeta) + 2\ \psi_l^0(\xi) \times \psi_m^0(\eta) \times \varpi^{-1,0}(\zeta)\psi_n^4(\zeta).
\end{aligned}$$

Let

$$\begin{aligned}
A^{ij} &= (a_{mn}^{ij})_{2\le m,n\le M}, \quad a_{mn}^{ij} = (\psi_m^i, \psi_n^j)_I, \quad 0 \le i,j \le 5, \\
B^{ij} &= (b_{mn}^{ij})_{2\le m,n\le M}, \quad b_{mn}^{ij} = (\psi_m^i, \psi_n^j)_{\varpi^{1,0},I}, \quad 0 \le i,j \le 3.
\end{aligned}$$

Then for any $2 \le l, m, n, l', m', n' \le M$,

$$(\Phi_{lmn}, \Phi_{l'm'n'})_{\mathcal{T}} = \frac{1}{64}\, a^{00}_{ll'}\, b^{00}_{mm'}\, a^{55}_{nn'},$$
$$(\partial_x \Phi_{lmn}, \partial_x \Phi_{l'm'n'})_{\mathcal{T}} = a^{11}_{ll'}\, b^{33}_{mm'}\, a^{00}_{nn'},$$
$$(\partial_y \Phi_{lmn}, \partial_y \Phi_{l'm'n'})_{\mathcal{T}} = \frac{1}{4}\left(a^{22}_{ll'}\, b^{33}_{mm'} + a^{00}_{ll'}\, b^{11}_{mm'} + a^{20}_{ll'}\, b^{31}_{mm'} + a^{02}_{ll'}\, b^{13}_{mm'}\right) a^{00}_{nn'},$$
$$\begin{aligned}(\partial_z \Phi_{lmn}, \partial_z \Phi_{l'm'n'})_{\mathcal{T}} &= \frac{1}{4}\, a^{22}_{ll'}\, b^{33}_{mm'}\, a^{00}_{nn'} + \frac{1}{16}\, a^{00}_{ll'}\, b^{22}_{mm'}\, a^{00}_{nn'} + \frac{1}{16}\, a^{00}_{ll'}\, b^{00}_{mm'}\, a^{44}_{nn'} \\ &+ \frac{1}{8}\, a^{20}_{ll'}\, b^{32}_{mm'}\, a^{00}_{nn'} + \frac{1}{8}\, a^{02}_{ll'}\, b^{23}_{mm'}\, a^{00}_{nn'} + \frac{1}{8}\, a^{20}_{ll'}\, b^{30}_{mm'}\, a^{04}_{nn'} \\ &+ \frac{1}{8}\, a^{02}_{ll'}\, b^{03}_{mm'}\, a^{40}_{nn'} + \frac{1}{16}\, a^{00}_{ll'}\, b^{20}_{mm'}\, a^{04}_{nn'} + \frac{1}{16}\, a^{00}_{ll'}\, b^{02}_{mm'}\, a^{40}_{nn'}.\end{aligned}$$

Set

$$u_M(x,y,z) = \sum_{l=0}^{M-2}\sum_{m=0}^{M-2}\sum_{n=0}^{M-2} \hat{u}_{(M-1)((M-1)l+m)+n}\Phi_{l+2,m+2,n+2}(x,y,z),$$
$$f_{(M-1)((M-1)l+m)+n} = (\mathcal{I}_M f, \Phi_{l+2,m+2,n+2})_{\mathcal{T}}, \quad 0 \le l, m, n \le M-2,$$

and

$$\hat{u} = (\hat{u}_0, \hat{u}_1, \cdots, \hat{u}_{(M-1)^3-1})^{\mathsf{tr}}, \quad \hat{f} = (f_0, f_1, \cdots, f_{(M-1)^3-1})^{\mathsf{tr}}.$$

Further denote by $\otimes$ the tensor product of matrices, i.e., $A \otimes B = (a_{i,j}B)_{0 \le i,j \le M-2}$. Then the linear system resulted from (3.4) becomes

$$(\mathbf{S} + \gamma \mathbf{M})\hat{u} = \hat{f}, \tag{3.21}$$

where

$$\mathbf{M} = \frac{1}{64}\, A^{00} \otimes B^{00} \otimes A^{55},$$

and

$$\begin{aligned}\mathbf{S} = {} & A^{11} \otimes B^{33} \otimes A^{00} \\ & + \frac{1}{4}\big(A^{22} \otimes B^{33} + A^{00} \otimes B^{11} + A^{02} \otimes B^{13} + A^{20} \otimes B^{31}\big) \otimes A^{00} \\ & + \Big\{\big(\frac{1}{4}A^{22} \otimes B^{33} + \frac{1}{16}A^{00} \otimes B^{22} + \frac{1}{8}A^{02} \otimes B^{32} + \frac{1}{8}A^{20} \otimes B^{23}\big) \otimes A^{00} \\ & + \frac{1}{16}A^{00} \otimes \big(B^{00} \otimes A^{44} + B^{02} \otimes A^{40} + B^{20} \otimes A^{04}\big) \\ & + \frac{1}{8}A^{02} \otimes B^{03} \otimes A^{40} + \frac{1}{8}A^{20} \otimes B^{30} \otimes A^{04}\Big\}.\end{aligned}$$

The nonzero entries of these matrices can be exactly evaluated. The structures of the mass matrix $\mathbf{M}$ and the stiffness matrix $\mathbf{S}$ are depicted in Figure 3.2. Therefore, the linear system can be effectively solved by using an efficient sparse solver such as SPARSEPACK.

Alternatively, one may attempt to use a suitable iterative solver. As is typical in a spectral method, the matrix $\mathbf{S}+\gamma\mathbf{M}$ is usually very ill conditioned so it is necessary to construct a suitable preconditioner. We now examine the condition numbers of the stiffness and mass matrices as well as the effect of diagonal preconditioner. For this purpose, let $\mathbf{\Lambda} = \big(\mathrm{diag}(\mathbf{S})\big)^{-1/2}$. We plot below the condition numbers of the matrices $\mathbf{S}$, $\widetilde{\mathbf{S}} = \mathbf{\Lambda}\mathbf{S}\mathbf{\Lambda}$, $\mathbf{T}_\gamma := \mathbf{S} + \gamma\mathbf{M}$ and $\widetilde{\mathbf{T}}_\gamma = \mathbf{\Lambda}\mathbf{T}_\gamma\mathbf{\Lambda}$ for various M and $\gamma = 10^4$.

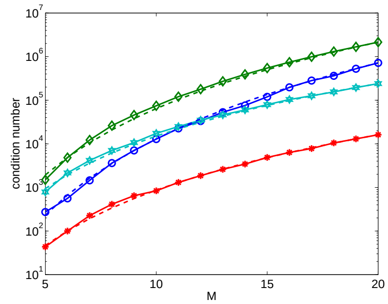

FIGURE 3.1. Condition numbers of $\mathbf{S}$ (marked by 'o'), $\mathbf{S}+\gamma\mathbf{M}$ (marked by '$\diamond$'), $\mathbf{\Lambda S \Lambda}$ (marked by '*') and $\mathbf{\Lambda S\Lambda}+\gamma\mathbf{\Lambda M \Lambda}$ (marked by '$\cdot$') against various M. The accompanied dashed lines are the reference curves for $cM^{5.8}$, $cM^{5.1}$, $cM^{4.2}$ and $cM^{4.0}$.

We observe from the figure that there are visible improvements for the order of the condition numbers versus M after applying the diagonal preconditioner. How to construct a simple and optimal preconditioner in this case is still an open question. We refer to [13] for an attempt using finite difference.

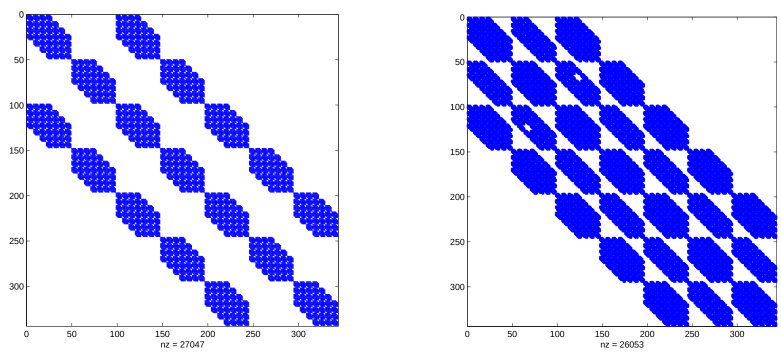

FIGURE 3.2. The structure of the mass matrix (left), and the stiffness matrix (right), where $M = 8$.

3.4. Numerical results. To illustrate the convergence rate of our rational approximation, we implemented the rational approximation to the model equation (3.1) with two exact solutions and we report our numerical results below.

For a given M, we denote the discrete L^2- error by

$$E_M = \sqrt{(u_M - u, u_M - u)_{M,\mathcal{T}}}. \tag{3.22}$$

Example 1. We consider the equation (3.1) with $\gamma = 0$ and the exact solution:

$$u(x,y) = xyz(e^{x+y+z} - e), \quad (x,y,z) \in \mathcal{T}. \tag{3.23}$$

Example 2. We consider the equation (3.1) with $\gamma = 0$ and the exact solution:

$$u(x,y) = \sin\frac{\pi x}{2}\sin\frac{\pi y}{2}\sin\frac{\pi z}{2}\sin\frac{\pi(1-x-y-z)}{2}, \quad (x,y,z) \in \mathcal{T}. \tag{3.24}$$

Since $u \in H^r(\mathcal{T})$ for any $r > 0$, Theorem 3.1 indicates that the error will converge faster than any algebraic order. Indeed, as shown in Figure 3.3 (left), the errors decay exponentially, typical for a spectral approximation to an analytic function. Hence, our numerical results are in good agreement with the error estimates in Theorem 3.1.

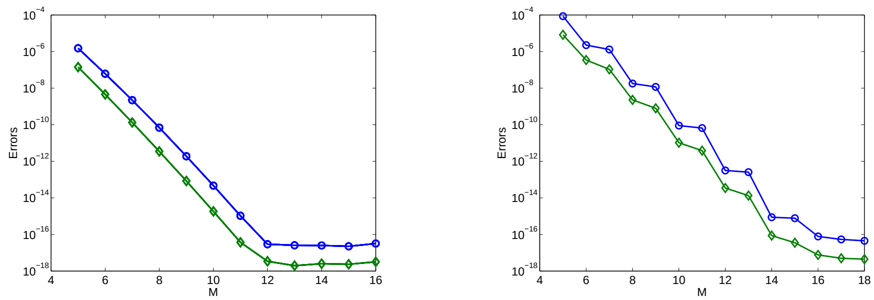

FIGURE 3.3. Maximum pointwise errors (marked by 'o') and L^2-errors (marked by '$\diamond$') against various M. Left: example 1; Right: example 2.

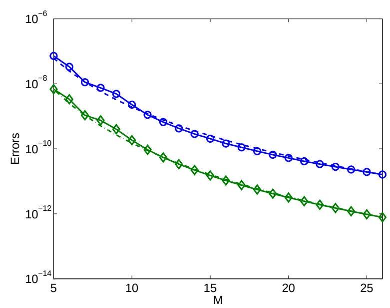

FIGURE 3.4. Maximum pointwise errors (marked by 'o') and L^2-errors (marked by '$\diamond$') against various M for example 3 with $\alpha = 4.3$, $\beta = 3.4$ and $\delta = 2.5$. The dashed and the dash-dot lines are reference curves for $error = cM^{-5}$ and $error = cM^{-5.5}$, respectively.

Example 3. We consider the equation (3.1) with $\gamma = 1$ and the exact solution:

$$u(x,y) = x^{\alpha} y^{\beta} z^{\delta}(1-x-y), \quad \forall\,(x,y,z) \in \mathcal{T}, \;\; \alpha,\beta,\delta > 0. \tag{3.25}$$

If $\alpha, \beta, \delta \in \mathbb{N}$, we expect that our numerical solution converges exponentially to the exact solution. While for α, β and/or δ being non-integer, we can also expect a convergence rate corresponding to the regularity of the exact solution and the right hand side term. In Figure 3.4, we plot the maximum and L^2-errors v.s. various M with $\alpha = 4.3$, $\beta = 3.4$ and $\delta = 2.5$ in the semi-logarithm scale. The algebraic convergence rate is evidenced by the near straight lines in the plot.

4. Extensions and discussions

We introduce in this section a set of nodal basis, which is more computationally practical for the element methods. We also briefly discuss how to extend the previous single domain implementation to multi-domain cases. These serve as important ingredients towards a spectral/hp element method on unstructured tetrahedral meshes.

4.1. Nodal basis. It is more practical to use a nodal basis. Different from the quadrature on $\mathcal{T}$, where the Gauss-Radau points are used, we adopt the Gauss-Lobatto points on $\mathcal{Q}$ in all three directions, which are more suitable for imposing continuity between tetrahedral elements.

Denote by $1 = \xi_0^L > \xi_1^L > \cdots > \xi_L^L = -1$ the $L+1$ roots of the polynomial $(1-\xi^2)J_{L-1}^{1,1}(\xi)$. The Lagrange basis polynomials at the Legendre-Gauss-Lobatto points are

$$\varphi_l^L(\xi) = \prod_{\substack{0\le k\le N\\ k\neq \tilde{l}}} \frac{\xi-\xi_k^L}{\xi_{\tilde{l}}^L-\xi_k} = \frac{1}{2N}\frac{(1-\xi^2)J_{L-1}^{1,1}(\xi)}{(\xi_{\tilde{l}}^L-\xi)J_L^{0,0}(\xi_{\tilde{l}}^L)},$$

where $\tilde{l} = \mathrm{mod}\ (l-1, L+1)$. Besides, we use the notation $\varphi_{-1}^L(\xi) \equiv 1$.

Further denote $\Psi_{lmn}^{LMN}(\xi,\eta,\zeta) = \varphi_l^L(\xi)\varphi_m^M(\eta)\varphi_n^N(\zeta)$. By the same argument as for the modal basis in Section 3, one readily finds that

$$\begin{aligned}\widetilde{X}_{LMN} &= \big\{\Psi \in P_L(I_\xi)\times P_M(I_\eta)\times P_N(I_\zeta)\ :\\ &\qquad \partial_\xi\Psi(\xi,1,\zeta) = \partial_\xi\Psi(\xi,\eta,1) = \partial_\eta\Psi(\xi,\eta,1) = 0\big\}\\ &= \mathrm{span}\big\{\Psi_{lmn}^{LMN}(\xi,\eta,\zeta)\ :\ (l,m,n)\in\Upsilon_{LMN}\big\}.\end{aligned}$$

Recalling that X_{LMN} corresponds to $\widetilde{X}_{LMN}$ under the coordinate transform (2.2), we finally derive the nodal basis of the approximation space X_{LMN},

$$X_{LMN} = \mathrm{span}\big\{\Phi_{lmn}^{LMN}(x,y,z)\ :\ (l,m,n)\in\Upsilon_{LMN}\big\}, \tag{4.1}$$

where $\Phi_{lmn}^{LMN}(x,y,z) = \Psi_{lmn}^{LMN}(\xi,\eta,\zeta)$ under the transform (2.2).

It is worthwhile to note that the nodal basis functions in (4.1) are constructed by the Legendre-Gauss-Lobatto Lagrange basis polynomials for all the ξ-, η- and ζ-directions. Of course, one can also use different types of Lagrange polynomials for different directions, just in the way like the interpolation operator $\mathit{I\!I}_M$ has been defined. Nevertheless, owing to the essential continuity condition of $\widetilde{X}_{LMN}$, one should use only the Jacobi-Gauss-Lobatto Lagrange basis polynomials instead of the Jacobi-Gauss-Radau ones for the construction of the nodal basis functions.

4.2. Multi-domain rational approximations. Let Ω be an open bounded domain. Consider the Poisson type equation:

$$-\Delta u + \gamma u = f \quad \text{in } \Omega; \quad u|_{\partial\Omega} = 0, \quad \gamma \ge 0. \tag{4.2}$$

The variational formulation of (4.2) is to find $u \in H_0^1(\Omega)$ such that

$$a(u,v) = \big(\nabla u, \nabla v\big)_\Omega + \gamma(u,v)_\Omega = (f,v)_\Omega, \quad \forall v \in H_0^1(\Omega). \tag{4.3}$$

We now briefly describe how to setup a multi-domain spectral-element method for (4.3), for more details in this regard, we refer to the books [2, 15]. To simplify the presentation, we shall restrict ourselves to polygonal domains.

Let Ω be an open bounded polygonal domain which can be decomposed as follows:

$$\bar{\Omega} = \cup_{k=1}^K \bar{\Omega}_k, \ \ \Omega_i \cap \Omega_j = \emptyset, \ i \neq j, \tag{4.4}$$

where each Ω_k is either a tetrahedron or a hexahedron. Let F_k be a bijection of class C^∞ which maps $\bar{\hat{\Omega}}$ onto $\bar{\Omega}_k$, where $\hat{\Omega}$ is either the reference tetrahedron $\mathcal{T}$ if Ω_k is a tetrahedron or the reference cube $\mathcal{Q}$ if Ω_k is a hexahedron. We denote

$$\tilde{X}_M^k = \{v_M = \hat{v}_M \circ F_k^{-1} : \hat{v}_M \in \Re_{MMM}(\mathcal{T})\} \quad \text{if } \Omega_k \text{ is a tetrahedron;} \tag{4.5}$$

or

$$\tilde{X}_M^k = \{v_M = \hat{v}_M \circ F_k^{-1} : \hat{v}_M \in [\mathcal{P}_M(I)]^3\} \quad \text{if } \Omega_k \text{ is a hexahedron.} \tag{4.6}$$

Setting

$$\tilde{X}_M = \{v_M \in H^1(\Omega) : v_M|_{\Omega_k} \in \tilde{X}_M^k,\ 1 \le k \le K\}, \quad \tilde{X}_M^0 = \tilde{X}_M \cap H_0^1(\Omega), \tag{4.7}$$

the combined rational function-Legendre spectral-element approximation to (4.3) is: to find $u_M \in \tilde{X}_M^0$ such that

$$\sum_{k=1}^{K} \Big(\gamma(u_M, v_M)_{\Omega_k} + (\nabla u_M, \nabla v_M)_{\Omega_k} \Big) = \sum_{k=1}^{K} (\mathcal{I}_M^k f, v_M)_{\Omega_k}, \quad \forall v_M \in \tilde{X}_M^0, \tag{4.8}$$

where $\mathcal{I}_M^k f \in X_M^k$ such that $\mathcal{I}_M^k f(x_{lmn}^k, y_{lmn}^k, z_{lmn}^k) = f(x_{lmn}^k, y_{lmn}^k, z_{lmn}^k)$, $0 \le l, m, n \le M$, and $(x_{lmn}^k, y_{lmn}^k, z_{lmn}^k) = F_k(\hat{x}_{lmn}^k, \hat{y}_{lmn}^k, \hat{z}_{lmn}^k)$ with $(\hat{x}_{lmn}^k, \hat{y}_{lmn}^k, \hat{z}_{lmn}^k)$, $0 \le l, m, n \le M$, being the collocation points in the reference tetrahedron or reference cube.

Then, using the standard error estimates of the projection and interpolation operators for the Legendre approximation (see, for instance, [1]) and the error estimates of the projection and interpolation operators for the rational approximation established in Section 2, then following procedure similar to that in Section 6.2 of [2], it is expected that the following result can be proved:

Proposition 4.1. *Assuming that the solution of* (4.3) $u \in H_0^1(\Omega)$ *and* $u|_{\Omega_k} \in H^r(\Omega_k)$ *for* $1 \le k \le K$ *with* $r \ge 1$*, and that* $f|_{\Omega_k} \in H^s(\Omega_k)$ *for* $1 \le k \le K$ *with* $s \ge 3$*. Then, the approximate solution* u_M *of* (4.8) *satisfies the following error estimate:*

$$\|u - u_M\|_{1,\Omega} \lesssim \sum_{k=1}^{K} \Big(M^{1-r} \|u\|_{H^r(\Omega_k)} + M^{-s} \|f\|_{H^s(\Omega_k)} \Big). \tag{4.9}$$

Remark 4.1. It can be shown that Proposition 4.1 holds if we replace the inner product in (4.8) in each subdomain by the discrete inner product (cf. Remark 3.1).

4.3. Concluding remarks. We introduced in this paper a rational spectral approximation on tetrahedron. The basis functions were obtained from tensor product of one-dimensional polynomials on the cube through the collapsed coordinate transform (2.2). We presented some error estimates with the norms expressed in the original coordinates on the tetrahedron, which are as accurate as the tensorial polynomial approximations. Furthermore, these rational basis functions appeared to be easier to deal with, both in analysis and in practice, than the Koornwinder-Dubiner polynomial basis functions. Hence, this rational approximation potentially provides a good alternative to the polynomial approximation for tetrahedral domains. We provided the implementation details for the rational spectral-Galerkin approximation to some model equations, and showed that the resulted linear system is sparse and can be efficiently solved, for example, by a sparse solver. We also gave illustrative numerical results which are essentially in agreement with the theoretical estimates.

This work is a first step towards developing a spectral-element method for three-dimensional complex geometries using rational functions on tetrahedron. The fundamental approximation results established here can be used to derive error estimates for the rational interpolations which are essential for a complete analysis for the spectral-element method using rational functions on tetrahedron.

Appendix A. One dimensional approximation results

We derive and refine in this appendix some one-dimensional results on Jacobi polynomial approximations and Jacobi-Gauss-type interpolation approximations, which serve as important tools for error analysis of rational approximation on the tetrahedron $\mathcal{T}$.

A.1. Jacobi polynomials. The classical Jacobi polynomials, denoted by $J_k^{\alpha,\beta}(\zeta)$, $\zeta \in I$ with $\alpha, \beta > -1$, are mutually orthogonal with respect to the Jacobi weight function $\varpi^{\alpha,\beta}(\zeta) = (1-\zeta)^\alpha (1+\zeta)^\beta$:

$$\int_{-1}^{1} J_n^{\alpha,\beta}(\zeta) J_m^{\alpha,\beta}(\zeta)\varpi^{\alpha,\beta}(\zeta)d\zeta = \left\|J_n^{\alpha,\beta}\right\|^2_{\varpi^{\alpha,\beta},I}\delta_{mn}, \tag{A.1}$$

where δ_{mn} is the Kronecker symbol, and

$$\left\|J_n^{\alpha,\beta}\right\|^2_{\varpi^{\alpha,\beta},I} = \frac{2^{\alpha+\beta+1}\Gamma(n+\alpha+1)\Gamma(n+\beta+1)}{(2n+\alpha+\beta+1)\Gamma(n+1)\Gamma(n+\alpha+\beta+1)}. \tag{A.2}$$

Notice that the classical Jacobi polynomials are only defined for $\alpha, \beta > -1$, while in a recent work [9, 22], the definition of Jacobi polynomials are extended to cases where α and/or β are negative integers through the following formula,

$$J_n^{\alpha,\beta}(\zeta) = \begin{cases} \dfrac{\Gamma(n+\alpha+1)\Gamma(n+\beta+1)}{\Gamma(n+1)\Gamma(n+\alpha+\beta+1)}\left(\dfrac{\zeta-1}{2}\right)^{-\alpha} J_{n+\alpha}^{-\alpha,\beta}(\zeta), & \alpha \in \mathbb{Z}^-, \\ \dfrac{\Gamma(n+\alpha+1)\Gamma(n+\beta+1)}{\Gamma(n+1)\Gamma(n+\alpha+\beta+1)}\left(\dfrac{\zeta+1}{2}\right)^{-\beta} J_{n+\beta}^{\alpha,-\beta}(\zeta), & \beta \in \mathbb{Z}^-. \end{cases}$$

The generalized Jacobi polynomials keep the orthogonality (A.1)-(A.2) of the classic Jacobi polynomials. We refer to [22] for more properties of this kind of generalized Jacobi polynomials.

A.2. Jacobi polynomial approximations. We define the orthogonal projection $\pi_N^{\alpha,\beta} : L^2_{\varpi^{\alpha,\beta}}(I) \to \mathcal{P}_N(I) \cap L^2_{\varpi^{\alpha,\beta}}(I)$ by

$$\int_{-1}^{1} \left(\pi_N^{\alpha,\beta} w - w\right)\phi \varpi^{\alpha,\beta} d\zeta = 0, \quad \forall \phi \in \mathcal{P}_N(I) \cap L^2_{\varpi^{\alpha,\beta}}(I). \tag{A.3}$$

Note that for $\alpha, \beta > -1$, we have $\mathcal{P}_N(I) \cap L^2_{\varpi^{\alpha,\beta}}(I) = \mathcal{P}_N(I)$, but when α and/or β are negative integers, suitable boundary conditions are involved. For example, $\mathcal{P}_N(I) \cap L^2_{\varpi^{-1,-1}}(I) = \mathcal{P}_N^0(I) = \mathcal{P}_N(I) \cap H_0^1(I)$.

To describe the approximation errors, we introduce the non-uniformly weighted Sobolev space

$$B^\sigma_{\alpha,\beta}(I) := \left\{ w \in L^2_{\varpi^{\alpha,\beta}}(I) \ : \ w^{(k)}(\zeta) \in L^2_{\varpi^{\alpha+k,\beta+k}}(I),\ 0 \le k \le \sigma \right\},\ \forall\, \sigma \in \mathbb{N}, \tag{A.4}$$

equipped with the norm and semi-norm

$$\|w\|_{B^\sigma_{\alpha,\beta}(I)} := \Big(\sum_{k=0}^{\sigma} \left\|w^{(k)}\right\|^2_{\varpi^{\alpha+k,\beta+k},I}\Big)^{\frac{1}{2}}, \quad |w|_{B^\sigma_{\alpha,\beta}(I)} := \left\|w^{(\sigma)}\right\|_{\varpi^{\alpha+\sigma,\beta+\sigma},I}. \tag{A.5}$$

Let $\mathbb{I}$ be the identity operator. It is obvious that for any $N, M \in \mathbb{N}$ and $N \ge M$, the projection operator $\pi_N^{\alpha,\beta}$ satisfies

$$\left\|\pi_M^{\alpha,\beta} w\right\|_{\varpi^{\alpha,\beta},I} \le \left\|\pi_N^{\alpha,\beta} w\right\|_{\varpi^{\alpha,\beta},I} \le \left\|w\right\|_{\varpi^{\alpha,\beta},I}, \qquad \forall w \in L^2_{\varpi^{\alpha,\beta}}(I), \tag{A.6}$$

$$\left\|\left(\pi_N^{\alpha,\beta} - \mathbb{I}\right)w\right\|_{\varpi^{\alpha,\beta},I} \le \left\|\left(\pi_M^{\alpha,\beta} - \mathbb{I}\right)w\right\|_{\varpi^{\alpha,\beta},I} \le \left\|w\right\|_{\varpi^{\alpha,\beta},I},\ \forall w \in L^2_{\varpi^{\alpha,\beta}}(I). \tag{A.7}$$

Another property is as follows.

Lemma A.1. *If* $w \in L^2_{\varpi^{\alpha,\beta}}(I)$ *and* $w^{(\sigma)} \in L^2_{\varpi^{\alpha+2\sigma,\beta+2\sigma}}(I)$ *with* $\alpha, \beta > -1$ *and integer* $N \geq \sigma > 0$*, then we have*

$$\big\|\big(\pi_N^{\alpha,\beta} - \mathbb{I}\big)w\big\|_{\varpi^{\alpha,\beta},I} \lesssim \big\|w^{(\sigma)}\big\|_{\varpi^{\alpha+2\sigma,\beta+2\sigma},I}. \tag{A.8}$$

Proof. Since (A.8) for $\sigma = 1$ has already been proved in [22], it suffices to prove that for any $0 \leq l \leq \sigma$,

$$\big\|(\pi_l^{\delta,\gamma} - \mathbb{I})w\big\|_{\varpi^{\delta,\gamma},I} \lesssim \big\|(\pi_{l-1}^{\delta+2,\gamma+2} - \mathbb{I})w'\big\|_{\varpi^{\delta+2,\gamma+2},I}, \tag{A.9}$$

if $w \in L^2_{\varpi^{\delta,\gamma}}(I)$ and $w' \in L^2_{\varpi^{\delta+2,\gamma+2}}(I)$ with $\delta, \gamma > -1$.

Integrating by parts yields that for $0 \leq k \leq l$,

$$\begin{aligned}\big((\pi_l^{\delta,\gamma}w - w)', \big(J_k^{\delta,\gamma}\big)'\big)_{\varpi^{\delta+1,\gamma+1},I} &= \big(\pi_l^{\delta,\gamma}w - w, -\varpi^{-\delta,-\gamma}\big(\varpi^{\delta+1,\gamma+1}\big(J_k^{\delta,\gamma}\big)'\big)'\big)_{\varpi^{\delta,\gamma},I}\\ &= \big(\pi_l^{\delta,\gamma}w - w, k(k+\delta+\gamma+1)J_k^{\delta,\gamma}\big)_{\varpi^{\delta,\gamma},I} = 0,\end{aligned}$$

where we use the Sturm-Liouville equation for Jacobi polynomials to derive the second equality sign. Noting that $(\pi_l^{\delta,\gamma}w)'$ is a polynomial of degree $l-1$, we readily find that

$$\big(\pi_l^{\delta,\gamma}w\big)' = \pi_{l-1}^{\delta+1,\gamma+1}w'.$$

Meanwhile, since $\pi_l^{\delta,\gamma}$ recovers any polynomial of degree no greater than l, it holds that

$$\begin{aligned}w - \pi_l^{\delta,\gamma}w &= w - \pi_l^{\delta,\gamma}w + \pi_l^{\delta,\gamma}\pi_l^{\delta+1,\gamma+1}w - \pi_l^{\delta+1,\gamma+1}w\\ &= \big(\mathbb{I} - \pi_l^{\delta,\gamma}\big)\big(\mathbb{I} - \pi_l^{\delta+1,\gamma+1}\big)w.\end{aligned}$$

As an immediate consequence,

$$\begin{aligned}\big\|\big(\mathbb{I} - \pi_l^{\delta,\gamma}\big)w\big\|_{\varpi^{\delta,\gamma},I} &= \big\|\big(\mathbb{I} - \pi_l^{\delta,\gamma}\big)\big(w - \pi_l^{\delta+1,\gamma+1}w\big)\big\|_{\varpi^{\delta,\gamma},I}\\ &\lesssim \big\|\big(w - \pi_l^{\delta+1,\gamma+1}w\big)'\big\|_{\varpi^{\delta+2,\gamma+2},I} = \big\|w' - \pi_{l-1}^{\delta+2,\gamma+2}w'\big\|_{\varpi^{\delta+2,\gamma+2},I}\\ &= \big\|\big(\mathbb{I} - \pi_{l-1}^{\delta+2,\gamma+2}\big)w'\big\|_{\varpi^{\delta+2,\gamma+2},I},\end{aligned}$$

where we use Lemma 2.1 in [22] for obtaining the inequality above. This finally ends the proof. $\square$

The main approximation result is stated in the following lemma.

Lemma A.2 ([22])**.** *Let* $\alpha, \beta > -1$ *or be negative integers. Then for any* $w \in B^\sigma_{\alpha,\beta}(I)$ *with integers* $\sigma \geq \mu \geq 0$,

$$\begin{aligned}\big\|\big(\pi_N^{\alpha,\beta}w - w\big)^{(\mu)}\big\|_{\varpi^{\alpha+\mu,\beta+\mu},I} &\lesssim N^{\mu-\sigma}\big\|\big(\pi_{N-\sigma}^{\alpha+\sigma,\beta+\sigma} - \mathbb{I}\big)w^{(\sigma)}\big\|_{\varpi^{\alpha+\sigma,\beta+\sigma},I}\\ &\lesssim N^{\mu-\sigma}\big\|w^{(\sigma)}\big\|_{\varpi^{\alpha+\sigma,\beta+\sigma},I}.\end{aligned} \tag{A.10}$$

A.3. Jacobi-Gauss-type interpolation approximation. The interpolation on the tetrahedron $\mathcal{T}$ defined in Section 2 is based on a map of the tensorial product of Legendre-Gauss-Lobatto (LGL) and Jacobi-Gauss-Radau (JGR) interpolations on the cube $\mathcal{Q}$.

We first consider the one-dimensional Legendre-Gauss-Lobatto interpolation. Let $\{\xi_j^L\}_{j=0}^N$ be the LGL interpolation points (i.e., zeros of $(1-\xi^2)J_{N-1}^{1,1}(\xi)$) . For any $w \in C(\bar{I})$, the LGL interpolant $\mathcal{I}_N^L w \in \mathcal{P}_N(I)$ and satisfies

$$(\mathcal{I}_N^L w)(\xi_j^L) = w(\xi_j^L), \quad 0 \leq j \leq N. \tag{A.11}$$

We have the following approximation result.

Lemma A.3 ([22]). *If $w \in L^2(I)$ and $w' \in B^{\sigma-1}_{0,0}(I)$ with integers $\sigma \ge \mu \ge 0$ and $\sigma \ge 1$, then we have*

$$\begin{aligned}\big\|(\mathcal{I}^L_N w - w)^{(\mu)}\big\|_{\varpi^{\mu-1,\mu-1},I} &\lesssim N^{\mu-\sigma}\big\|(\pi^{\sigma-1,\sigma-1}_{N-\sigma} - \mathbb{I})w^{(\sigma)}\big\|_{\varpi^{\sigma-1,\sigma-1},I} \\ &\lesssim N^{\mu-\sigma}\big\|w^{(\sigma)}\big\|_{\varpi^{\sigma-1,\sigma-1},I}.\end{aligned} \tag{A.12}$$

We now turn to the Jacobi-Gauss-Radau (JGR) interpolation associated with the weight function $\varpi^{\alpha,0}(\eta) = (1-\eta)^\alpha$. Let $\{\eta^{R,\alpha}_j\}_{j=0}^N$ be the JGR interpolation points (i.e., zeros of $(1+\eta)J^{\alpha,1}_N(\eta)$). For any $w \in C([-1,1))$, the JGR interpolant is defined by $\mathcal{I}^{R,\alpha}_N w \in \mathcal{P}_N(I)$ and

$$(\mathcal{I}^{R,\alpha}_N w)(\eta^{R,\alpha}_j) = w(\eta^{R,\alpha}_j), \quad 0 \le j \le N. \tag{A.13}$$

For $\alpha = 1$, $\mathcal{I}^{R,\alpha}_N$ is reduced to Jacobi-Gauss-Radau interpolation operator $\mathcal{I}^R_N$ analyzed in [22]. In order to establish the error estimate, we use the stability result of the JGR interpolation operator (cf. Theorem 4.5 of [11]). Use Lemma 2.2 of [11] and let the intermediate polynomial $w_N = \hat{P}^1_{N,\alpha,0}w$. Then by a standard argument as in [22], we can derive the following result for $\mathcal{I}^{R,\alpha}_N$.

Lemma A.4. *If $w \in B^\sigma_{\alpha,0}(I)$ with $\alpha > -1$, $\sigma \ge \mu \ge 0$ and $\sigma \ge 1$, then*

$$\begin{aligned}\big\|\big(\mathcal{I}^{R,\alpha}_N w - w\big)^{(\mu)}\big\|_{\varpi^{\mu+\alpha,\mu},I} &\lesssim N^{\mu-\sigma}\big\|\big(\pi^{\sigma+\alpha,\sigma}_{N-\sigma} - \mathbb{I}\big)w^{(\sigma)}\big\|_{\varpi^{\sigma+\alpha,\sigma},I} \\ &\lesssim N^{\mu-\sigma}\big\|w^{(\sigma)}\big\|_{\varpi^{\sigma+\alpha,\sigma},I}.\end{aligned} \tag{A.14}$$

Appendix B. The proof of Theorem 2.1

Let $\pi^{\alpha,\beta}_L : L^2_{\omega^{\alpha,\beta}}(I) \to \mathcal{P}_N(I) \cap L^2_{\omega^{\alpha,\beta}}(I)$ be the one-dimensional orthogonal projection defined in Appendix A. It is obvious that $\Pi_{LMN}u = \pi^{0,0}_{L,\xi}\pi^{1,0}_{M,\eta}\pi^{2,0}_{M,\zeta}v$ (the subscript ξ indicates the operator $\pi^{0,0}_L$ acts on the variable ξ and likewise for η and ζ). A direct calculation, together with (2.7) and (A.6), leads to

$$\begin{aligned}\big\|\Pi_{LMN}u - u\big\|_{\mathcal{T}} &= \frac{1}{8}\big\|\pi^{0,0}_{L,\xi}\pi^{1,0}_{M,\eta}\pi^{2,0}_{N,\zeta}v - v\big\|_{\chi^{0,0;1,0;2,0}} \\ &\le \big\|\pi^{0,0}_{L,\xi}v - v\big\|_{\chi^{0,0;1,0;2,0}} + \big\|\pi^{0,0}_{L,\xi}\big(\pi^{1,0}_{M,\eta}v - v\big)\big\|_{\chi^{0,0;1,0;2,0}} \\ &\quad + \big\|\pi^{0,0}_{L,\xi}\pi^{1,0}_{M,\eta}\big(\pi^{2,0}_{N,\zeta}v - v\big)\big\|_{\chi^{0,0;1,0;2,0}} \\ &\le \big\|\pi^{0,0}_{L,\xi}v - v\big\|_{\chi^{0,0;1,0;2,0}} + \big\|\pi^{1,0}_{M,\eta}v - v\big\|_{\chi^{0,0;1,0;2,0}} + \big\|\pi^{2,0}_{N,\zeta}v - v\big\|_{\chi^{0,0;1,0;2,0}}.\end{aligned}$$

Using (A.10) yields

$$\begin{aligned}\|\Pi_{LMN}u - u\|_{\mathcal{T}} \lesssim{}& L^{-q}\big\|\partial^q_\xi v\big\|_{\chi^{q,q;1,0;2,0}} + M^{-r}\big\|\partial^r_\eta v\big\|_{\chi^{0,0;r+1,r;2,0}} \\ &+ N^{-s}\big\|\partial^s_\zeta v\big\|_{\chi^{0,0;1,0;s+2,s}}.\end{aligned}$$

Now, we bound the norms of v in the right hand side by the norms of u. By using (2.10), we have

$$\partial^l_\xi v(\xi,\eta,\zeta) = \Big(\frac{(1-\eta)(1-\zeta)}{8}\Big)^l \partial^l_x u(x,y,z), \qquad l \ge 1. \tag{B.1}$$

Further, a recursive use of (2.10) gives

$$
\begin{aligned}
\partial_\eta^l v(\xi,\eta,\zeta) &= \partial_\eta^{l-1}\Big(\frac{(1-\xi)(1-\zeta)}{8}\partial_y + \frac{(1+\xi)(1-\zeta)}{8}(\partial_y-\partial_x)\Big)u(x,y,z)\\
&=\Big(\frac{(1-\xi)(1-\zeta)}{8}\partial_\eta^{l-1}\partial_y + \frac{(1+\xi)(1-\zeta)}{8}\partial_\eta^{l-1}(\partial_y-\partial_x)\Big)u(x,y,z) = \cdots \\
&=\sum_{j=0}^{l}\binom{l}{j}\Big(\frac{(1-\xi)(1-\zeta)}{8}\Big)^j\Big(\frac{(1+\xi)(1-\zeta)}{8}\Big)^{l-j}\partial_y^j(\partial_y-\partial_x)^{l-j}u(x,y,z),
\end{aligned}
\tag{B.2}
$$

and

$$
\begin{aligned}
\partial_\zeta^l v(\xi,\eta,\zeta) &= \partial_\zeta^{l-1}\Big(\frac{(1-\xi)(1-\eta)}{8}\partial_z + \frac{1+\eta}{4}(\partial_z-\partial_y)\\
&\qquad + \frac{(1+\xi)(1-\eta)}{8}(\partial_z-\partial_x)\Big)u(x,y,z)\\
&=\Big(\frac{(1-\xi)(1-\eta)}{8}\partial_\zeta^{l-1}\partial_z + \frac{1+\eta}{4}\partial_\zeta^{l-1}(\partial_z-\partial_y)\\
&\qquad + \frac{(1+\xi)(1-\eta)}{8}\partial_\zeta^{l-1}(\partial_z-\partial_x)\Big)u(x,y,z)\\
&=\cdots=\sum_{j=0}^{l}\sum_{k=0}^{l-j}\binom{l}{j,k}\Big(\frac{(1-\xi)(1-\eta)}{8}\Big)^j\Big(\frac{1+\eta}{4}\Big)^k\Big(\frac{(1+\xi)(1-\eta)}{8}\Big)^{l-j-k}\\
&\quad\times\partial_z^j(\partial_z-\partial_y)^j(\partial_z-\partial_x)^{l-j-k}u(x,y,z),
\end{aligned}
\tag{B.3}
$$

where $\binom{l}{j,k}=\frac{\Gamma(l+1)}{\Gamma(j+1)\Gamma(k+1)\Gamma(l-j-k+1)}$. Thanks to the above identities and the triangle inequality, we obtain that

$$
\begin{aligned}
\|\Pi_{LMN}u-u\|_{\mathcal{T}} &\lesssim L^{-q}\|\partial_x^q u\|_{\chi^{q,q;2q+1,0;2q+2,0}}\\
&\quad + M^{-r}\sum_{j=0}^{r}\|\partial_y^j(\partial_y-\partial_x)^{r-j}u\|_{\chi^{2j,2r-2j;r+1,r;2r+2,0}}\\
&\quad + N^{-s}\sum_{j=0}^{s}\sum_{k=0}^{s-j}\|\partial_z^j(\partial_z-\partial_y)^k(\partial_z-\partial_x)^{s-j-k}u\|_{\chi^{2j,2s-2j-2k;2s-2k+1,2k;s+2,s}}.
\end{aligned}
$$

Note that for any $\alpha_1,\beta_1,\alpha_2,\beta_2,\alpha_3,\beta_3\geq 0$,

$$
\big|\chi^{\alpha_1,\beta_1;\alpha_2,\beta_2;\alpha_3,\beta_3}(\xi,\eta,\zeta)\big|\lesssim 1, \qquad \forall\,(\xi,\eta,\zeta)\in\mathcal{Q}. \tag{B.4}
$$

We finally get that

$$
\begin{aligned}
\|\Pi_{LMN}u-u\|_{\mathcal{T}} &\lesssim L^{-q}\|\partial_x^q u\|_{\chi^{q,q;2q+1,0;2q+2,0}}\\
&\quad + M^{-r}\sum_{j=0}^{r}\|\partial_y^j(\partial_y-\partial_x)^{r-j}u\|_{\chi^{j,r-j;r+1,r;2r+2,0}}\\
&\quad + N^{-s}\sum_{j=0}^{s}\sum_{k=0}^{s-j}\|\partial_z^j(\partial_z-\partial_y)^k(\partial_z-\partial_x)^{s-j-k}u\|_{\chi^{j,s-j-k;s-k+1,k;2s+2,s}}\\
&\lesssim L^{-q}\|\partial_x^q u\|_{\omega^{q,q,0,0},\mathcal{T}} + M^{-r}\sum_{j=0}^{r}\|\partial_y^j(\partial_y-\partial_x)^{r-j}u\|_{\omega^{j,r-j,r,0},\mathcal{T}}\\
&\quad + N^{-s}\sum_{j=0}^{s}\sum_{k=0}^{s-j}\|\partial_z^j(\partial_z-\partial_y)^k(\partial_z-\partial_x)^{s-j-k}u\|_{\omega^{j,s-j-k,k,s},\mathcal{T}}.
\end{aligned}
$$

This completes the proof.

Appendix C. The Proof of Theorem 2.2

Let $v(\xi,\eta,\zeta)=u(x,y,z)$. One verifies readily that

$$(\mathit{I\!I}_M u)(x,y,z)=(\mathcal{I}_M^{\xi}\,\mathcal{I}_M^{\eta}\mathcal{I}_M^{\zeta}v)(\xi,\eta,\zeta). \tag{C.1}$$

where $\mathcal{I}_M^{\xi}=\mathcal{I}_{M,\xi}^{L}$ is the Legendre-Gauss-Lobatto interpolation operator in ξ, $\mathcal{I}_M^{\eta}=\mathcal{I}_{M,\eta}^{R,1}$ and $\mathcal{I}_M^{\zeta}=\mathcal{I}_{M,\zeta}^{R,2}$ are the Jacobi-Gauss-Radau interpolation operator in η and ζ, respectively (cf. Appendix A).

We begin the proof with (C.1), (2.7), (A.12), (A.14) and the triangle inequality,

(C.2)

$$\begin{aligned}
\big\|(\mathit{I\!I}_M-\mathbb{I})u\big\|_{\mathcal{T}} &= \frac{1}{8}\big\|(\mathcal{I}_M^{\xi}\,\mathcal{I}_M^{\eta}\mathcal{I}_M^{\zeta}-\mathbb{I})v\big\|_{\chi^{0,0;1,0;2,0}}\\
&\lesssim \big\|(\mathcal{I}_M^{\xi}-\mathbb{I})v\big\|_{\chi^{-1,-1;1,0;2,0}}+\big\|(\mathcal{I}_M^{\eta}-\mathbb{I})v\big\|_{\chi^{0,0;1,0;2,0}}+\big\|(\mathcal{I}_M^{\zeta}-\mathbb{I})v\big\|_{\chi^{0,0;1,0;2,0}}\\
&\quad+\big\|(\mathcal{I}_M^{\xi}-\mathbb{I})(\mathcal{I}_M^{\eta}-\mathbb{I})v\big\|_{\chi^{-1,-1;1,0;2,0}}+\big\|(\mathcal{I}_M^{\xi}-\mathbb{I})(\mathcal{I}_M^{\zeta}-\mathbb{I})v\big\|_{\chi^{-1,-1;1,0;2,0}}\\
&\quad+\big\|(\mathcal{I}_M^{\eta}-\mathbb{I})(\mathcal{I}_M^{\zeta}-\mathbb{I})v\big\|_{\chi^{0,0;1,0;2,0}}+\big\|(\mathcal{I}_M^{\xi}-\mathbb{I})(\mathcal{I}_M^{\eta}-\mathbb{I})(\mathcal{I}_M^{\zeta}-\mathbb{I})v\big\|_{\chi^{-1,-1;1,0;2,0}}\\
&\lesssim M^{-r}\big\|\partial_\xi^r v\big\|_{\chi^{r-1,r-1;1,0;2,0}}+\big\|(\mathcal{I}_M^{\eta}-\mathbb{I})v\big\|_{\chi^{0,0;1,0;2,0}}+\big\|(\mathcal{I}_M^{\zeta}-\mathbb{I})v\big\|_{\chi^{0,0;1,0;2,0}}\\
&\quad+M^{-1}\big\|(\mathcal{I}_M^{\eta}-\mathbb{I})\partial_\xi v\big\|_{\chi^{0,0;1,0;2,0}}+M^{-1}\big\|(\mathcal{I}_M^{\zeta}-\mathbb{I})\partial_\xi v\big\|_{\chi^{0,0;1,0;2,0}}\\
&\quad+\big\|(\mathcal{I}_M^{\eta}-\mathbb{I})(\mathcal{I}_M^{\zeta}-\mathbb{I})v\big\|_{\chi^{0,0;1,0;2,0}}+M^{-1}\big\|(\mathcal{I}_M^{\eta}-\mathbb{I})(\mathcal{I}_M^{\zeta}-\mathbb{I})\partial_\xi v\big\|_{\chi^{0,0;1,0;2,0}}\\
&\lesssim M^{-r}\big\|\partial_\xi^r v\big\|_{\chi^{r-1,r-1;1,0;2,0}}+M^{-r}\big\|\partial_\eta^r v\big\|_{\chi^{0,0;r+1,r;2,0}}+\big\|(\mathcal{I}_M^{\zeta}-\mathbb{I})v\big\|_{\chi^{0,0;1,0;2,0}}\\
&\quad+M^{-r}\big\|(\pi_{M-r+1,\eta}^{r,r-1}-\mathbb{I})\partial_\eta^{r-1}\partial_\xi v\big\|_{\chi^{0,0;r,r-1;2,0}}+M^{-1}\big\|(\mathcal{I}_M^{\zeta}-\mathbb{I})\partial_\xi v\big\|_{\chi^{0,0;1,0;2,0}}\\
&\quad+M^{-1}\big\|(\mathcal{I}_M^{\zeta}-\mathbb{I})\partial_\eta v\big\|_{\chi^{0,0;2,1;2,0}}+M^{-2}\big\|(\mathcal{I}_M^{\zeta}-\mathbb{I})\partial_\eta\partial_\xi v\big\|_{\chi^{0,0;2,1;2,0}}\\
&\lesssim M^{-r}\Big(\big\|\partial_\xi^r v\big\|_{\chi^{r-1,r-1;1,0;2,0}}+\big\|\partial_\eta^r v\big\|_{\chi^{0,0;r+1,r;2,0}}+\big\|\partial_\zeta^r v\big\|_{\chi^{0,0;1,0;r+2,r}}\\
&\quad+\big\|(\pi_{M-r+1,\eta}^{r,r-1}-\mathbb{I})\partial_\eta^{r-1}\partial_\xi v\big\|_{\chi^{0,0;r,r-1;2,0}}\\
&\quad+\big\|(\pi_{M-r+1,\zeta}^{r+1,r-1}-\mathbb{I})\partial_\zeta^{r-1}\partial_\xi v\big\|_{\chi^{0,0;1,0;r+1,r-1}}\\
&\quad+\big\|(\pi_{M-r+1,\zeta}^{r+1,r-1}-\mathbb{I})\partial_\zeta^{r-1}\partial_\eta v\big\|_{\chi^{0,0;2,1;r+1,r-1}}\\
&\quad+\big\|(\pi_{M-r+2,\zeta}^{r,r-2}-\mathbb{I})\partial_\zeta^{r-2}\partial_\eta\partial_\xi v\big\|_{\chi^{0,0;2,1;r,r-2}}\Big).
\end{aligned}$$

For further simplification, we note that

$$\begin{aligned}
8\partial_\eta^{r-1}\partial_\xi v &= \partial_\eta^{r-1}\big((1-\eta)(1-\zeta)\partial_x u\big)\\
&=(1-\eta)(1-\zeta)\partial_\eta^{r-1}(\partial_x u)-(r-1)(1-\zeta)\partial_\eta^{r-2}(\partial_x u),\\
8\partial_\zeta^{r-1}\partial_\xi v &= \partial_\zeta^{r-1}\big((1-\eta)(1-\zeta)\partial_x u\big)\\
&=(1-\eta)(1-\zeta)\partial_\zeta^{r-1}(\partial_x u)-(r-1)(1-\eta)\partial_\zeta^{r-2}(\partial_x u),
\end{aligned}$$

and

$$\begin{aligned}
8\partial_\zeta^{r-1}\partial_\eta v &= \partial_\zeta^{r-1}\big(2(1-\zeta)\partial_y u-(1+\xi)(1-\zeta)\partial_x u\big)\\
&=2(1-\zeta)\partial_\zeta^{r-1}\partial_y u-(1+\xi)(1-\zeta)\partial_\zeta^{r-1}\partial_x u-2(r-1)\partial_\zeta^{r-2}\partial_y u\\
&\quad+(r-1)(1+\xi)\partial_\zeta^{r-2}\partial_x u.
\end{aligned}$$

Thus by (A.8) and the triangle inequality, we have

$$
\begin{aligned}
&\big\|\big(\pi^{r,r-1}_{M-r+1,\eta}-\mathbb{I}\big)\partial_\eta^{r-1}\partial_\xi v\big\|_{\chi^{0,0;r,r-1;2,0}}\\
&\quad\lesssim \big\|\big(\pi^{r,r-1}_{M-r+1,\eta}-\mathbb{I}\big)\big((1-\zeta)\partial_\eta^{r-2}(\partial_x u)\big)\big\|_{\chi^{0,0;r,r-1;2,0}}\\
&\qquad+\big\|\big(\pi^{r,r-1}_{M-r+1,\eta}-\mathbb{I}\big)\big((1-\eta)(1-\zeta)\partial_\eta^{r-1}(\partial_x u)\big)\big\|_{\chi^{0,0;r,r-1;2,0}}\\
&\quad\lesssim \big\|\partial_\eta\big((1-\zeta)\partial_\eta^{r-2}(\partial_x u)\big)\big\|_{\chi^{0,0;r+2,r+1;2,0}}\\
&\qquad+\big\|(1-\eta)(1-\zeta)\partial_\eta^{r-1}(\partial_x u)\big\|_{\chi^{0,0;r,r-1;2,0}}\\
&\quad\lesssim \big\|\partial_\eta^{r-1}(\partial_x u)\big\|_{\chi^{0,0;r+2,r+1;4,0}}+\big\|\partial_\eta^{r-1}(\partial_x u)\big\|_{\chi^{0,0;r+2,r-1;4,0}}\\
&\quad\lesssim \big\|\partial_\eta^{r-1}(\partial_x u)\big\|_{\chi^{0,0;r+2,r-1;4,0}},
\end{aligned}\tag{C.3}
$$

$$
\begin{aligned}
&\big\|\big(\pi^{r+1,r-1}_{M-r+1,\zeta}-\mathbb{I}\big)\partial_\zeta^{r-1}\partial_\xi v\big\|_{\chi^{0,0;1,0;r+1,r-1}}\\
&\quad\lesssim \big\|\big(\pi^{r+1,r-1}_{M-r+1,\zeta}-\mathbb{I}\big)\big((1-\eta)\partial_\zeta^{r-2}(\partial_x u)\big)\big\|_{\chi^{0,0;1,0;r+1,r-1}}\\
&\qquad+\big\|\big(\pi^{r+1,r-1}_{M-r+1,\zeta}-\mathbb{I}\big)\big((1-\eta)(1-\zeta)\partial_\zeta^{r-1}(\partial_x u)\big)\big\|_{\chi^{0,0;1,0;r+1,r-1}}\\
&\quad\lesssim \big\|\partial_\zeta\big((1-\eta)\partial_\zeta^{r-2}(\partial_x u)\big)\big\|_{\chi^{0,0;1,0;r+3,r+1}}\\
&\qquad+\big\|(1-\eta)(1-\zeta)\partial_\zeta^{r-1}(\partial_x u)\big\|_{\chi^{0,0;1,0;r+1,r-1}}\\
&\quad\lesssim \big\|\partial_\zeta^{r-1}(\partial_x u)\big\|_{\chi^{0,0;3,0;r+3,r+1}}+\big\|\partial_\zeta^{r-1}(\partial_x u)\big\|_{\chi^{0,0;3,0;r+3,r-1}}\\
&\quad\lesssim \big\|\partial_\zeta^{r-1}(\partial_x u)\big\|_{\chi^{0,0;3,0;r+3,r-1}},
\end{aligned}\tag{C.4}
$$

and

$$
\begin{aligned}
&\big\|\big(\pi^{r+1,r-1}_{M-r+1,\zeta}-\mathbb{I}\big)\partial_\zeta^{r-1}\partial_\eta v\big\|_{\chi^{0,0;2,1;r+1,r-1}}\\
&\quad\lesssim \big\|\big(\pi^{r+1,r-1}_{M-r+1,\zeta}-\mathbb{I}\big)\big(2\partial_\zeta^{r-2}\partial_y u-(1+\xi)\partial_\zeta^{r-2}\partial_x u\big)\big\|_{\chi^{0,0;2,1;r+1,r-1}}\\
&\qquad+\big\|\big(\pi^{r+1,r-1}_{M-r+1,\zeta}-\mathbb{I}\big)\big(2(1-\zeta)\partial_\zeta^{r-1}\partial_y u-(1+\xi)(1-\zeta)\partial_\zeta^{r-1}\partial_x u\big)\big\|_{\chi^{0,0;2,1;r+1,r-1}}\\
&\quad\lesssim \big\|\partial_\zeta\big((1-\xi)\partial_\zeta^{r-2}\partial_y u+(1+\xi)\partial_\zeta^{r-2}(\partial_y-\partial_x)u\big)\big\|_{\chi^{0,0;2,1;r+3,r+1}}\\
&\qquad+\big\|(1-\xi)(1-\zeta)\partial_\zeta^{r-1}\partial_y u-(1+\xi)(1-\zeta)\partial_\zeta^{r-1}(\partial_y u-\partial_x)u\big\|_{\chi^{0,0;2,1;r+1,r-1}}\\
&\quad\lesssim \big\|\partial_\zeta^{r-1}\partial_y u\big\|_{\chi^{2,0;2,1;r+3,r+1}}+\big\|\partial_\zeta^{r-1}(\partial_y-\partial_x)u\big\|_{\chi^{0,2;2,1;r+3,r+1}}\\
&\qquad+\big\|\partial_\zeta^{r-1}\partial_y u\big\|_{\chi^{2,0;2,1;r+3,r-1}}+\big\|\partial_\zeta^{r-1}(\partial_y-\partial_x)u\big\|_{\chi^{0,2;2,1;r+3,r-1}}\\
&\quad\lesssim \big\|\partial_\zeta^{r-1}\partial_y u\big\|_{\chi^{2,0;2,1;r+3,r-1}}+\big\|\partial_\zeta^{r-1}(\partial_y-\partial_x)u\big\|_{\chi^{0,2;2,1;r+3,r-1}}.
\end{aligned}\tag{C.5}
$$

Meanwhile, one verifies that

$$
\begin{aligned}
64\partial_\zeta^{r-2}\partial_\eta\partial_\xi v &= 8\partial_\zeta^{r-2}\partial_\eta\big((1-\eta)(1-\zeta)\partial_x u\big)\\
&= 8\partial_\zeta^{r-2}\big((1-\eta)(1-\zeta)\partial_\eta\partial_x-(1-\zeta)\partial_x\big)u\\
&= \partial_\zeta^{r-2}\big((1-\eta)(1-\zeta)^2(2\partial_y\partial_x u-(1+\xi)\partial_x^2 u)\big)-8\partial_\zeta^{r-2}\big((1-\zeta)\partial_x u\big)\\
&= (1-\eta)(1-\zeta)^2\partial_\zeta^{r-2}\big(2\partial_y\partial_x u-(1+\xi)\partial_x^2 u\big)-8((1-\zeta)\partial_\zeta^{r-2}+\partial_\zeta^{r-3})\partial_x u\\
&\quad-2(r-2)(1-\eta)\big((1-\zeta)\partial_\zeta^{r-3}+\partial_\zeta^{r-4}\big)\big(2\partial_y\partial_x u-(1+\xi)\partial_x^2 u)\big)\\
&\quad+8(r-1)\partial_\zeta^{r-3}\partial_x u+(r-2)(r-1)(1-\eta)\partial_\zeta^{r-4}(2\partial_y\partial_x u-(1+\xi)\partial_x^2 u)\big).
\end{aligned}
$$

As a result, we get, by (A.8) and the triangle inequality, that

(C.6)
$$\begin{aligned}
&\big\|\big(\pi^{r,r-2}_{M-r+2,\zeta}-\mathbb{I}\big)\partial_\zeta^{r-2}\partial_\eta\partial_\xi v\big\|_{\chi^{0,0;2,1;r,r-2}}\\
&\quad\lesssim \big\|\big(\pi^{r,r-2}_{M-r+2,\zeta}-\mathbb{I}\big)\big((1-\eta)(1-\zeta)^2\partial_\zeta^{r-2}(2\partial_y\partial_x u-(1+\xi)\partial_x^2 u)\big)\big\|_{\chi^{0,0;2,1;r,r-2}}\\
&\qquad+\big\|\big(\pi^{r,r-2}_{M-r+2,\zeta}-\mathbb{I}\big)\big((1-\eta)((1-\zeta)\partial_\zeta^{r-3}+\partial_\zeta^{r-4})\\
&\qquad\qquad(2\partial_y\partial_x u-(1+\xi)\partial_x^2 u)\big)\big\|_{\chi^{0,0;2,1;r,r-2}}\\
&\qquad+\big\|\big(\pi^{r,r-2}_{M-r+2,\zeta}-\mathbb{I}\big)\big((1-\eta)\partial_\zeta^{r-4}(2\partial_y\partial_x u-(1+\xi)\partial_x^2 u)\big)\big\|_{\chi^{0,0;2,1;r,r-2}}\\
&\qquad+\big\|\big(\pi^{r,r-2}_{M-r+2,\zeta}-\mathbb{I}\big)\big(((1-\zeta)\partial_\zeta^{r-2}+\partial_\zeta^{r-3})\partial_x u\big)\big\|_{\chi^{0,0;2,1;r,r-2}}\\
&\qquad+\big\|\big(\pi^{r,r-2}_{M-r+2,\zeta}-\mathbb{I}\big)\big(\partial_\zeta^{r-3}\partial_x u\big)\big\|_{\chi^{0,0;2,1;r,r-2}}\\
&\quad\lesssim \big\|(1-\eta)(1-\zeta)^2\partial_\zeta^{r-2}(2\partial_y\partial_x u-(1+\xi)\partial_x^2 u)\big\|_{\chi^{0,0;2,1;r,r-2}}\\
&\qquad+\big\|\partial_\zeta\big((1-\eta)((1-\zeta)\partial_\zeta^{r-3}+\partial_\zeta^{r-4})(2\partial_y\partial_x u-(1+\xi)\partial_x^2 u)\big)\big\|_{\chi^{0,0;2,1;r+2,r}}\\
&\qquad+\big\|\partial_\zeta^2\big((1-\eta)\partial_\zeta^{r-4}(2\partial_y\partial_x u-(1+\xi)\partial_x^2 u)\big)\big\|_{\chi^{0,0;2,1;r+4,r+2}}\\
&\qquad+\big\|\partial_\zeta\big(((1-\zeta)\partial_\zeta^{r-2}+\partial_\zeta^{r-3})\partial_x u\big)\big\|_{\chi^{0,0;2,1;r+2,r}}+\big\|\partial_\zeta^2\big(\partial_\zeta^{r-3}\partial_x u\big)\big\|_{\chi^{0,0;2,1;r+4,r+2}}\\
&\quad\lesssim \big\|(1-\eta)(1-\zeta)^2\big((1-\xi)\partial_\zeta^{r-2}\partial_y\partial_x u+(1+\xi)\partial_\zeta^{r-2}(\partial_y-\partial_x)\partial_x u\big)\big\|_{\chi^{0,0;2,1;r,r-2}}\\
&\qquad+\big\|(1-\eta)(1-\zeta)\big((1-\xi)\partial_\zeta^{r-2}\partial_y\partial_x u+(1+\xi)\partial_\zeta^{r-2}(\partial_y-\partial_x)\partial_x u\big)\big\|_{\chi^{0,0;2,1;r+2,r}}\\
&\qquad+\big\|(1-\eta)\big((1-\xi)\partial_\zeta^{r-2}\partial_y\partial_x u+(1+\xi)\partial_\zeta^{r-2}(\partial_y-\partial_x)\partial_x u\big)\big\|_{\chi^{0,0;2,1;r+4,r+2}}\\
&\qquad+\big\|(1-\zeta)\partial_\zeta^{r-1}\partial_x u\big\|_{\chi^{0,0;2,1;r+2,r}}+\big\|\partial_\zeta^{r-1}\partial_x u\big\|_{\chi^{0,0;2,1;r+4,r+2}}\\
&\quad\lesssim \big\|(1-\xi)\partial_\zeta^{r-2}\partial_y\partial_x u+(1+\xi)\partial_\zeta^{r-2}(\partial_y-\partial_x)\partial_x u\big\|_{\chi^{0,0;4,1;r+4,r-2}}\\
&\qquad+\big\|\partial_\zeta^{r-1}\partial_x u\big\|_{\chi^{0,0;2,1;r+4,r}}\\
&\quad\lesssim \big\|\partial_\zeta^{r-2}\partial_y\partial_x u\big\|_{\chi^{2,0;4,1;r+4,r-2}}+\big\|\partial_\zeta^{r-2}(\partial_y-\partial_x)\partial_x u\big\|_{\chi^{0,2;4,1;r+4,r-2}}\\
&\qquad+\big\|\partial_\zeta^{r-1}\partial_x u\big\|_{\chi^{0,0;2,1;r+4,r}}.
\end{aligned}$$

Combining (C.2) with (C.3)-(C.6), we derive that

$$\begin{aligned}
\big\|(\mathit{I\!I}_M-\mathbb{I})u\big\|_{\mathcal{T}}\lesssim M^{-r}\Big(&\big\|\partial_\xi^r v\big\|_{\chi^{r-1,r-1;1,0;2,0}}+\big\|\partial_\eta^r v\big\|_{\chi^{0,0;r+1,r;2,0}}\\
&+\big\|\partial_\zeta^r v\big\|_{\chi^{0,0;1,0;r+2,r}}+\big\|\partial_\eta^{r-1}\partial_x u\big\|_{\chi^{0,0;r+2,r-1;4,0}}\\
&+\big\|\partial_\zeta^{r-1}\partial_x u\big\|_{\chi^{0,0;2,0;r+3,r-1}}+\big\|\partial_\zeta^{r-1}\partial_y u\big\|_{\chi^{2,0;2,1;r+3,r-1}}\\
&+\big\|\partial_\zeta^{r-1}(\partial_y-\partial_x)u\big\|_{\chi^{0,2;2,1;r+3,r-1}}+\big\|\partial_\zeta^{r-2}\partial_y\partial_x u\big\|_{\chi^{2,0;4,1;r+4,r-2}}\\
&+\big\|\partial_\zeta^{r-2}(\partial_y-\partial_x)\partial_x u\big\|_{\chi^{0,2;4,1;r+4,r-2}}\Big).
\end{aligned}\tag{C.7}$$

In analogy to (B.2) and (B.3), we have that for integer $l\ge 1$

$$\begin{aligned}
\partial_\eta^l v(\xi,\eta,\zeta)&=\sum_{j=0}^{l}(-1)^{l-j}2^{-3l+j}\binom{l}{j}(1+\xi)^{l-j}(1-\zeta)^l\partial_y^j\partial_x^{l-j}u(x,y,z),\\
\partial_\zeta^l v(\xi,\eta,\zeta)&=\sum_{j=0}^{l}\sum_{k=0}^{l-j}(-1)^{l-j}2^{-3l+2j+k}\binom{l}{j,k}(1+\xi)^{l-j-k}(1-\eta)^{l-j-k}(1+\eta)^k\\
&\quad\times\partial_z^j\partial_y^k\partial_x^{l-j-k}u(x,y,z).
\end{aligned}$$

Noting that for any $\alpha_1,\beta_1,\alpha_2,\beta_2,\alpha_3,\beta_3 \ge 0$,

$$\left|\chi^{\alpha_1,\beta_1;\alpha_2,\beta_2;\alpha_3,\beta_3}(\xi,\eta,\zeta)\right| \lesssim 1, \qquad \forall\,(\xi,\eta,\zeta)\in\mathcal{Q},$$

we finally find that

$$\begin{aligned}
\left\|(\mathit{I\!I}_M-\mathbb{I})u\right\|_{\mathcal{T}} &\lesssim M^{-r}\Big(\left\|\partial_\xi^r v\right\|_{\chi^{0,0;1,0;2,0}}+\left\|\partial_\eta^r v\right\|_{\chi^{0,0;1,0;2,0}}+\left\|\partial_\eta^{r-1}\partial_x u\right\|_{\chi^{0,0;1,0;2,0}}\\
&\quad+\left\|\partial_\zeta^r v\right\|_{\chi^{0,0;1,0;2,0}}+\left\|\partial_\zeta^{r-1}\partial_x u\right\|_{\chi^{0,0;1,0;2,0}}+\left\|\partial_\zeta^{r-1}\partial_y u\right\|_{\chi^{0,0;1,0;2,0}}\\
&\quad+\left\|\partial_\zeta^{r-2}\partial_y\partial_x u\right\|_{\chi^{0,0;1,0;2,0}}+\left\|\partial_\zeta^{r-2}\partial_x^2 u\right\|_{\chi^{0,0;1,0;2,0}}\Big)\\
&\lesssim M^{-r}\Big(\left\|\partial_x^r u\right\|_{\chi^{0,0;1,0;2,0}}+\sum_{j=0}^{r}\left\|\partial_y^j\partial_x^{r-j}u\right\|_{\chi^{0,0;1,0;2,0}}\\
&\quad+\sum_{j=0}^{r-1}\left\|\partial_y^j\partial_x^{r-j-1}\partial_x u\right\|_{\chi^{0,0;1,0;2,0}}+\sum_{j=0}^{r}\sum_{k=0}^{r-j}\left\|\partial_z^j\partial_y^k\partial_x^{r-j-k}u\right\|_{\chi^{0,0;1,0;2,0}}\\
&\quad+\sum_{j=0}^{r-1}\sum_{k=0}^{r-j-1}\big(\left\|\partial_z^j\partial_y^k\partial_x^{r-j-k-1}\partial_x u\right\|_{\chi^{0,0;1,0;2,0}}+\left\|\partial_z^j\partial_y^k\partial_x^{r-j-k-1}\partial_y u\right\|_{\chi^{0,0;1,0;2,0}}\big)\\
&\quad+\sum_{j=0}^{r-2}\sum_{k=0}^{r-j-2}\left\|\partial_z^j\partial_y^k\partial_x^{r-j-k-2}\partial_y\partial_x u\right\|_{\chi^{0,0;1,0;2,0}}\\
&\quad+\sum_{j=0}^{r-2}\sum_{k=0}^{r-j-2}\left\|\partial_z^j\partial_y^k\partial_x^{r-j-k-1}\partial_x^2 u\right\|_{\chi^{0,0;1,0;2,0}}\Big)\\
&\lesssim M^{-r}\Big(\left\|\partial_x^r u\right\|_{\chi^{0,0;1,0;2,0}}+\sum_{j=0}^{r}\left\|\partial_y^j\partial_x^{r-j}u\right\|_{\chi^{0,0;1,0;2,0}}\\
&\quad+\sum_{j=0}^{r}\sum_{k=0}^{r-j}\left\|\partial_z^j\partial_y^k\partial_x^{r-j-k}u\right\|_{\chi^{0,0;1,0;2,0}}+\sum_{j=0}^{r-1}\sum_{k=0}^{r-j-1}\left\|\partial_z^j\partial_y^{k+1}\partial_x^{r-j-k-1}u\right\|_{\chi^{0,0;1,0;2,0}}\Big)\\
&\lesssim M^{-r}\sum_{j=0}^{r}\sum_{k=0}^{r-j}\left\|\partial_z^j\partial_y^k\partial_x^{r-j-k}u\right\|_{\chi^{0,0;1,0;2,0}}\lesssim M^{-r}\sum_{j=0}^{r}\sum_{k=0}^{r-j}\left\|\partial_z^j\partial_y^k\partial_x^{r-j-k}u\right\|_{\mathcal{T}}.
\end{aligned}$$

This ends the proof.

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