Sparse shape functions for tetrahedral p-FEM using integrated Jacobi polynomials

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Abstract

In this paper we investigate the discretization of an elliptic boundary value problem in 3D by means of the hp-version of the finite element method using a mesh of tetrahedrons. We present several bases based on integrated Jacobi polynomials in which the element stiffness matrix has $\mathcal{O}(p^3)$ nonzero entries, where p denotes the polynomial degree. The proof of the sparsity requires the assistance of computer algebra software. Several numerical experiments show the efficiency of the proposed bases for higher polynomial degrees p.

AMS-subjects: 65N30, 65N35, 33C45 (primary), 65N22, 65N55, 65Q05 (secondary)
Key words: High order Finite Elements, Orthogonal polynomials, Computer algebra, Solution of discretized equations

1 Introduction

In this paper, we investigate the following boundary value problem: Let $\Omega \subset \mathbb{R}^3$ be a bounded domain and let $\mathcal{A}(x, y, z)$ be a 3×3 matrix which is symmetric and uniformly positive definite in Ω. Find $u \in H^1_{\Gamma_1}(\Omega) = \{u \in H^1(\Omega), u = 0 \text{ on } \Gamma_1\}$, $\Gamma_1 \cap \Gamma_2 = \emptyset$, $\Gamma_1 \cup \Gamma_2 = \partial\Omega$ such that

$$a_\triangle(u, v) := \int_\Omega (\nabla u)^T \mathcal{A}(x, y, z) \nabla v = \int_\Omega f v + \int_{\Gamma_2} f_1 v := \langle f, v\rangle_\Omega + \langle f_1, v\rangle_{\Gamma_2} \tag{1}$$

holds for all $v \in H^1_{\Gamma_1}(\Omega)$. Problem (1) will be discretized by means of the hp-version of the finite element method using tetrahedral elements $\triangle_s$, $s = 1, \ldots, nel$. Let $\hat{\triangle}$ be the reference tetrahedron and $F_s : \hat{\triangle} \to \triangle_s$ be the (possibly nonlinear) isoparametric mapping to the element $\triangle_s$. We define the finite element space $\mathbb{M} := \{u \in H^1_{\Gamma_1}(\Omega), u\mid_{\triangle_s} = \tilde{u}(F_s^{-1}(x, y, z)), \tilde{u} \in \mathbb{P}_p\}$, where $\mathbb{P}_p$ is the space of all polynomials of maximal total degree p.

By $\Psi = (\psi_1, \ldots, \psi_N)$, we denote a basis for $\mathbb{M}$ in which the functions $\psi_1, \ldots, \psi_{n_v}$ are the usual hat functions. The high order functions

$\psi_{n_v+(j-1)(p-1)+1}, \ldots, \psi_{n_v+j(p-1)}$ correspond to the edge e_j of the mesh, and vanish on all other edges, i.e. satisfy the condition $\psi_{n_v+(j-1)(p-1)+k-1} \mid_{e_l}= \delta_{j,l} p_k$, where p_k is a polynomial of degree p, $k = 2, \ldots, p$. The support of an edge function is formed by those elements, which have e_j in common. One defines $\frac{(p-1)(p-2)}{2}$ face shapes which are polynomial on the defining face and vanish on all other faces. The support of these face-based functions is formed by the two elements sharing the defining face. The remaining basis functions are interior bubble functions consisting of a support containing one element only. These functions vanish on each face of the mesh. With this definition, the basis functions ψ_i can be divided into four groups,

- the vertex functions,
- the edge bubble functions,
- face bubble functions,
- the interior bubble functions,

locally on each element $\triangle_s$, and globally on Ω.

The Galerkin projection of (1) onto $\mathbb{M}$ leads to the linear system of algebraic finite element equations

$$\mathcal{K}_\Psi \underline{u} = \underline{f}, \quad \text{where} \quad \mathcal{K}_\Psi = [a_\Delta(\psi_j, \psi_i)]_{i,j=1}^N, \quad \underline{f}_p = [\langle f, \psi_i \rangle + \langle f_1, \psi_i \rangle_{\Gamma_2}]_{i=1}^N. \tag{2}$$

The global stiffness matrix $\mathcal{K}_\Psi$ can be expressed by the local stiffness matrices on the elements, i.e.

$$\mathcal{K}_\Psi = \sum_{s=1}^{nel} R_s^T K_s R_s, \tag{3}$$

where K_s is the stiffness matrix on the element $\triangle_s$ and R_s denotes the connectivity matrix for the numbering of the shape functions on $\triangle_s$ and Ω.

Using the vector $\underline{u}$, an approximation $u_p = \Psi \underline{u}$ of the exact solution u of (1) can be built from the usual finite element isomorphism. In the case of smooth solutions u in parts of the domain Ω, spectral methods, [19], and finite elements of high order (p-version), see e.g. [28], [31], and the references therein, have become more and more popular in the last twenty years. For the h-version of the FEM, the polynomial degree p of the shape functions on the elements is kept constant and the mesh-size h is decreased. This is in contrast to the p-version of the FEM in which the polynomial degree p is increased and the mesh-size h is kept constant. Both ideas, mesh refinement and increasing the polynomial degree, can be combined. This is called the hp-version of the FEM.

The advantage of the p-version in comparison to the h-version is that the solution converges faster to the exact solution with respect to the number of unknowns N. However, the choice of a basis Ψ in which the element stiffness matrix K_s has $\mathcal{O}(N)$ nonzero matrix entries is a difficult question. In the one-dimensional case, e.g. for the differential equation $-u''+u=f$, one can take the primitives of orthogonal polynomials in order to get a sparse system matrix, see e.g. [18]. In the 2D and 3D case, the choice of a basis which is optimal due to condition number and sparsity of $\mathcal{K}_\Psi$ is not so clear. In [7], several bases have been investigated regarding their condition number. In the case of tensor product elements $\triangle_s$ like quadrilaterals and hexahedrons and a constant diffusion matrix $\mathcal{A}$, one can take tensor products of integrated Legendre polynomials, see e.g. [6], [18]. Then, the element stiffness matrix K_s has $\mathcal{O}(N)$ nonzero matrix entries and $\mathcal{K}_\Psi$ can be computed in $\mathcal{O}(N)$ operations via (3). However, in the case of a general quadrilateral (hexahedral in 3D) element $\triangle_s$ with nonparallel opposite edges (faces), most of the orthogonality relations of the reference element case disappear and K_s (and hence $\mathcal{K}_\Psi$) has, in general, $\mathcal{O}(p^6)$ matrix entries. Using a quadrature rule, the cost in order to obtain $\mathcal{K}_\Psi$ is $\mathcal{O}(p^9)$. In [23], tensor products of Lagrangian polynomials on the grid of the Gauss-Lobatto points are proposed. Then, the cost for computing K_s by a quadrature rule is $\mathcal{O}(p^5)$. This approach can be extended to the tetrahedral case by the Duffy transformation, [14], see also [19]. If the diffusion function $\mathcal{A}$ is piecewise constant, the cost for the generation of the stiffness matrix can be reduced to $\mathcal{O}(p^4)$ by the technique of precomputed arrays; see [25], [19]. However, the choice of a basis in which K_s has $\mathcal{O}(N)$ matrix entries for some elements $\triangle_s$ is more difficult. In [30], a new basis for triangular and tetrahedral elements has been proposed. This basis has many nonzero entries, see [29]. A proof for the sparsity of the element stiffness matrix with $\mathcal{O}(p^3)$ nonzero entries is still an open problem in the literature. In [13], another basis for the triangular case is proposed. Moreover, it is proved that the element stiffness matrix has $\mathcal{O}(p^2)$ nonzero entries. In comparison to the basis in [30], the weight of the Jacobi polynomials in y-direction is increased.

In this paper, we investigate several basis functions for tetrahedral elements. On one element, we have to define $\frac{1}{6}(p+1)(p+2)(p+3)$ shape functions. We prove that the element stiffness matrix K_s has $\mathcal{O}(p^3)$ nonzero matrix entries in the case of piecewise constant coefficients $\mathcal{A}(x,y,z)$ on the elements $\triangle_s$ and affine linear mappings F_s. Moreover, each nonzero matrix entry can be computed in $\mathcal{O}(1)$ operations. So, the matrix vector multiplication and the generation of the stiffness matrix can be done in $\mathcal{O}(N)$ arithmetical operations. One example of these bases is the basis proposed in [30]. The proof of the sparsity of the system matrix requires the assistance of a computer algebra system. For another example where computer algebra software (esp. symbolic summation techniques) have been applied to a problem arising in the *hp*-version of FEM see [8]. There the construction of low energy edge and vertex shape functions for triangles is described, for which cheap recurrence relations have been derived applying recently developed computer algebra algorithms for hypergeometric summation. A comment on linking symbolic to numerical computation in the context of *hp*-FEM can be found in [26].

In section 2, we formulate and prove the most important properties of Jacobi polynomials and their primitives. In section 3, the shape functions on the reference tetrahedron $\hat{\triangle}$ are defined and the main result of this paper, Theorem 3.3, is formulated. The computational properties of the element stiffness matrix are summarized in section 4. In section 5, we derive a simple Domain Decomposition (DD) preconditioner for the block of the interior bubbles. In section 6 we describe how Theorem 3.3 can be proved in an algorithmic manner. We have executed this proof by the aid of a program we implemented in the computer algebra system Mathematica. In section 7, we give some remarks for an efficient implementation of the computation of the element stiffness matrix. In the appendix, we give the reader an impression of the computation of the nonzero matrix entries of the element stiffness matrix using our Mathematica program.

Throughout this paper, the reference tetrahedron $\hat{\triangle}$ denotes the tetrahedron with the vertices $(-1,-1,-1)$, $(1,-1,-1)$, $(0,1,-1)$ and $(0,0,1)$. The parameter *nel* denotes the number of elements and p denotes the polynomial degree. By F_s, we denote the isoparametric mapping from $\hat{\triangle}$ to the tetrahedron $\triangle_s$.

2 Properties of Jacobi polynomials with weight $(1-x)^\alpha$

For the definition of our basis functions on the reference element, Jacobi polynomials are required. In this section, we summarize the most important properties of Jacobi polynomials. We refer the reader to the books of Abramowitz and Stegun, [1], Andrews, Askey and Roy, [5], and Tricomi, [32], for more details. Moreover, we state and prove some properties which only hold for polynomials with weight $(1-x)^\alpha(1+x)^0$.

For $n \in \mathbb{N}_0, \alpha, \beta > -1$, let

$$p_n^{\alpha,\beta}(x) = \frac{1}{2^n n!(1-x)^\alpha(1+x)^\beta} \frac{\mathrm{d}^n}{\mathrm{d}x^n} \Big((1-x)^\alpha(1+x)^\beta(x^2-1)^n\Big) \tag{4}$$

be the nth Jacobi polynomial with respect to the weight function $(1-x)^\alpha(1+x)^\beta$. The function $p_n^{\alpha,\beta}(x)$ is a polynomial of degree n, i.e. $p_n^{\alpha,\beta} \in \mathbb{P}_n((-1,1))$, where $\mathbb{P}_n$ is the space of all polynomials of degree n on the interval. In the special case $\alpha = \beta = 0$, the functions $p_n^{0,0}(x)$ are called Legendre polynomials. Moreover, let

$$\hat{p}_n^{\alpha,\beta}(x) = \int_{-1}^{x} p_{n-1}^{\alpha,\beta}(y)\,\mathrm{d}y \quad n \geq 1, \quad \hat{p}_0^{\alpha,\beta}(x) = 1 \tag{5}$$

be the nth integrated Jacobi polynomial.

We would like to mention that the integrated Jacobi polynomial (5) can be expressed in terms of Jacobi polynomials (4) with modified weights, i.e.

$$\hat{p}_n^{\alpha,\beta}(x) = \frac{2}{n+\alpha+\beta-1}\left[p_n^{\alpha-1,\beta-1}(x) - p_n^{\alpha-1,\beta-1}(-1)\right], \tag{6}$$

for $\alpha > 0$ or $\beta > 0$. This is easy to see, since the derivatives of Jacobi polynomials are again Jacobi polynomials with shifted parameters, i.e.

$$\frac{\mathrm{d}}{\mathrm{d}x} p_n^{\alpha,\beta}(x) = \frac{n+\alpha+\beta+1}{2} p_{n-1}^{\alpha+1,\beta+1}(x),$$

see [5].

In the following, we use only the Jacobi and integrated Jacobi polynomials with weight $(1-x)^\alpha$, i.e. $\beta = 0$. Therefore, we omit the second index β in (4), (5). In this case, relation (6) simplifies to

$$\hat{p}_n^{\alpha}(x) = \frac{2}{n+\alpha-1} p_n^{\alpha-1,-1}(x),$$

where Jacobi polynomials with negative index $\beta = -1, \alpha > -1$ are defined as

$$p_n^{\alpha,-1}(x) = \frac{1+x}{2}\frac{n+\alpha}{n} p_{n-1}^{\alpha,1}(x).$$

The orthogonality with respect to the weight function $(1-x)^\alpha/(1+x)$ for $n \geq 1$ is immediate from the corresponding orthogonality relation of Jacobi polynomials $p_n^{\alpha,1}(x)$. For $\alpha = 0$, i.e. integrated Legendre polynomials $\hat{p}_n^0(x) \sim p_n^{-1,-1}(x)$, we are in a limiting case, for which the well known identity $\hat{p}_n^0(x) = \frac{x^2-1}{2(n-1)} p_{n-2}^{1,1}(x)$ exists.

The following two lemmas summarize the properties of Jacobi and integrated Jacobi polynomials which have been proved in [13].

Lemma 2.1. *Let* p_n^α *be defined via* (4). *Moreover, let* $j, l \in \mathbb{N}_0$ *and* $\alpha > -1$. *Then, we have*

$$p_n^{\alpha-1}(x) = \frac{1}{\alpha+2n}\left[(\alpha+n)p_n^\alpha(x) - n p_{n-1}^\alpha(x)\right], \tag{7}$$

$$\begin{aligned} p_{n+1}^\alpha(x) = {} & \frac{2n+\alpha+1}{(2n+2)(n+\alpha+1)(2n+\alpha)} \\ & \times \left((2n+\alpha+2)(2n+\alpha)x + \alpha^2\right) p_n^\alpha(x) \\ & - \frac{n(n+\alpha)(2n+\alpha+2)}{(n+1)(n+\alpha+1)(2n+\alpha)} p_{n-1}^\alpha(x), \quad n \geq 1. \end{aligned} \tag{8}$$

Moreover, the integral relations

$$\int_{-1}^{1} (1-x)^\alpha p_j^\alpha(x) p_l^\alpha(x)\,\mathrm{d}x = \rho_j^\alpha \delta_{jl}, \quad \textit{where } \rho_j^\alpha = \frac{2^{\alpha+1}}{2j+\alpha+1}, \tag{9}$$

$$\int_{-1}^{1} (1-x)^\alpha p_j^\beta(x) q_l(x)\,\mathrm{d}x = 0 \tag{10}$$

$$\forall q_l \in \mathbb{P}_l, \alpha - \beta \in \mathbb{N}_0, j > l + \alpha - \beta$$

hold.

Lemma 2.2. *Let $l, j \in \mathbb{N}_0$. Let p_n^α and $\hat{p}_n^\alpha$ be defined via (4) and (5). Then, the identities*

$$
\begin{aligned}
\hat{p}_n^\alpha(-1) &= 0, \quad n \geq 1, && (11)\\
\hat{p}_n^\alpha(x) &= \frac{2n+2\alpha}{(2n+\alpha-1)(2n+\alpha)} p_n^\alpha(x) + \frac{2\alpha}{(2n+\alpha-2)(2n+\alpha)} p_{n-1}^\alpha(x) \\
&\quad - \frac{2n-2}{(2n+\alpha-1)(2n+\alpha-2)} p_{n-2}^\alpha(x), \quad n \geq 2, && (12)\\
\hat{p}_{n+1}^\alpha(x) &= \frac{2n+\alpha-1}{(2n+2)(n+\alpha)(2n+\alpha-2)} \\
&\quad \times \left((2n+\alpha-2)(2n+\alpha)x + \alpha(\alpha-2)\right) \hat{p}_n^\alpha(x) \\
&\quad - \frac{(n-1)(n+\alpha-2)(2n+\alpha)}{(n+1)(n+\alpha)(2n+\alpha-2)} \hat{p}_{n-1}^\alpha(x), \quad n \geq 1, && (13)\\
\hat{p}_n^\alpha(x) &= \frac{2}{2n+\alpha-1} \left(p_n^{\alpha-1}(x) + p_{n-1}^{\alpha-1}(x)\right), \quad n \geq 1, && (14)
\end{aligned}
$$

and the integral relations

$$
\begin{aligned}
\int_{-1}^{1} (1-x)^\alpha \hat{p}_j^\alpha(x) \hat{p}_l^\alpha(x) \,\mathrm{d}x &= 0 \quad \text{if } |j-l| > 2, && (15)\\
\int_{-1}^{1} (1-x)^\alpha \hat{p}_j^{\beta+1}(x) q_l(x) \,\mathrm{d}x &= 0 && (16)\\
&\qquad \forall q_l \in \mathbb{P}_l, \alpha - \beta \in \mathbb{N}_0, j > l + 1 + \alpha - \beta
\end{aligned}
$$

hold.

The most important results are the formulas (12) and (8). With relation (8), we are recursively able to compute function values of the Jacobi polynomials. Relation (12) gives a simple connection between the Jacobi and the integrated Jacobi polynomials.

Finally, we prove three properties of the Jacobi polynomials which have not been presented in [13].

Lemma 2.3. *Let $j \in \mathbb{N}$. Let p_n^α and $\hat{p}_n^\alpha$ be defined via (4) and (5). Then,*

$$
\begin{aligned}
(\alpha-1)\hat{p}_j^\alpha(y) &= (1-y)p_{j-1}^\alpha(y) + 2p_j^{\alpha-2}(y), \quad \alpha > 1, && (17)\\
4(\alpha+j-2)p_{j-1}^{\alpha-2}(y) + {} & \\
(2\alpha-4)p_j^{\alpha-2}(y) &= (1-y)\left((2-2j)p_{j-2}^\alpha(y) + \alpha p_{j-1}^\alpha(y)\right) && (18)\\
&\quad + (\alpha+2j-2)(\alpha-1)\hat{p}_j^\alpha(y), \quad \alpha > 1,\\
y p_{j-1}^\alpha(y) - j\hat{p}_j^\alpha(y) &= \frac{1}{2j+\alpha-2}\left(-\alpha p_{j-1}^\alpha(y) + (2j-2)p_{j-2}^\alpha(y)\right),\\
&\qquad \alpha > -1 && (19)
\end{aligned}
$$

with $p_{-1}^\alpha(y) = 0$.

Proof. We start with the proof of (17). Using (8), we can represent

$$\begin{aligned}(1-y)p_{j-1}^{\alpha}(y) &= -\frac{2j(j+\alpha)}{(2j+\alpha-1)(2j+\alpha)}p_j^{\alpha}(y)\\ &\quad -\frac{(2j-2)(j+\alpha-1)}{(2j+\alpha-2)(2j+\alpha-1)}p_{j-2}^{\alpha}(y)\\ &\quad +\frac{(2j+\alpha-2)(2j+\alpha)+\alpha^2}{(2j+\alpha-2)(2j+\alpha)}p_{j-1}^{\alpha}(y).\end{aligned} \tag{20}$$

Using (7) twice, we conclude that

$$\begin{aligned}2p_j^{\alpha-2}(y) &= 2\frac{\alpha-1+j}{\alpha+2j-1}\cdot\frac{\alpha+j}{\alpha+2j}p_j^{\alpha}(y)\\ &\quad -4\frac{\alpha-1+j}{\alpha+2j-2}\cdot\frac{j}{\alpha+2j}p_{j-1}^{\alpha}(y)\\ &\quad +2\frac{j}{\alpha+2j-1}\frac{j-1}{\alpha+2j-2}p_{j-2}^{\alpha}(y).\end{aligned} \tag{21}$$

Adding (20) and (21) and using (12), we obtain

$$\begin{aligned}(1-y)p_{j-1}^{\alpha}(y)+2p_j^{\alpha-2}(y) &= \frac{(2j+2\alpha)(\alpha-1)}{(2j+\alpha-1)(2j+\alpha)}p_j^{\alpha}(y)\\ &\quad +\frac{2(\alpha-1)\alpha}{(2j+\alpha-2)(2j+\alpha)}p_{j-1}^{\alpha}(y)\\ &\quad -\frac{(2j-2)(\alpha-1)}{(2j+\alpha-1)(2j+\alpha-2)}p_{j-2}^{\alpha}(y)\\ &= (\alpha-1)\hat{p}_j^{\alpha}(y).\end{aligned}$$

This proves (17). Next, we prove (18). Using (17) for p_{j-2}^{α} and p_{j-1}^{α}, we have

$$\begin{aligned}&(1-y)\left((2-2j)p_{j-2}^{\alpha}(y)+\alpha p_{j-1}^{\alpha}(y)\right)\\ &\qquad +(\alpha+2j-2)(\alpha-1)\hat{p}_j^{\alpha}(y) = (\alpha-1)\left(-(2j-2)\hat{p}_{j-1}^{\alpha}(y)\right.\\ &\qquad\qquad \left.+\,(2\alpha+2j-2)\hat{p}_j^{\alpha}(y)\right)\\ &\qquad\qquad +(4j-4)p_{j-1}^{\alpha-2}(y)-2\alpha p_j^{\alpha-2}(y).\end{aligned} \tag{22}$$

Next, we simplify the right hand side of the previous equation. Using (14) and (7), we obtain

$$\begin{aligned}
-(2j-2)\hat{p}^{\alpha}_{j-1}(y)+ & \\
+(2\alpha+2j-2)\hat{p}^{\alpha}_{j}(y) &= \frac{4(j+\alpha-1)}{2j+\alpha-1}(p^{\alpha-1}_{j}(y)+p^{\alpha-1}_{j-1}(y)) \\
&\quad -\frac{4(j-1)}{2j+\alpha-3}(p^{\alpha-1}_{j-1}(y)+p^{\alpha-1}_{j-2}(y)) \\
&= \frac{4(j+\alpha-1)}{2j+\alpha-1}p^{\alpha-1}_{j}(y)-\frac{4j}{2j+\alpha-1}p^{\alpha-1}_{j-1}(y) \\
&\quad +\frac{4(j+\alpha-2)}{2j+\alpha-3}p^{\alpha-1}_{j-1}(y)-\frac{4(j-1)}{2j+\alpha-3}p^{\alpha-1}_{j-2} \\
&= 4(p^{\alpha-2}_{j}(y)+p^{\alpha-2}_{j-1}(y)). \qquad (23)
\end{aligned}$$

Now, we insert (23) into (22) which proves (18).

Finally, we prove (19). First, we obtain from (12) that

$$\begin{aligned}
yp^{\alpha}_{j-1}(y) &= 2j\frac{\alpha+j}{(2j+\alpha-1)(2j+\alpha)}p^{\alpha}_{j}(y) \qquad (24) \\
&\quad -\frac{\alpha^2}{(2j+\alpha)(2j+\alpha-2)}p^{\alpha}_{j-1}(y) \\
&\quad +(2j-2)\frac{j+\alpha-1}{(2j+\alpha-1)(2j+\alpha-2)}p^{\alpha}_{j-2}(y).
\end{aligned}$$

Secondly, using (8) we get

$$\begin{aligned}
j\hat{p}^{\alpha}_{j-1}(y) &= 2j\frac{\alpha+j}{(2j+\alpha-1)(2j+\alpha)}p^{\alpha}_{j}(y) \qquad (25) \\
&\quad +2j\frac{\alpha}{(2j+\alpha)(2j+\alpha-2)}p^{\alpha}_{j-1}(y) \\
&\quad -(2j-2)\frac{j}{(2j+\alpha-1)(2j+\alpha-2)}p^{\alpha}_{j-2}(y).
\end{aligned}$$

Subtracting (25) from (24), we conclude that

$$yp^{\alpha}_{j-1}(y)-j\hat{p}^{\alpha}_{j}(y)=\frac{1}{2j+\alpha-2}\left(-\alpha p^{\alpha}_{j-1}(y)+(2j-2)p^{\alpha}_{j-2}(y)\right).$$

This is (19) and completes the proof. □

Remark 2.4. *The relations* (7)-(19) *can also be generated and proven with the RISC-summation packages, e.g. [20, 27, 33].*

3 Element stiffness matrix

In this section, we define the shape functions on the reference element $\hat{\triangle}$. Then, we formulate our main theorem stating that the element stiffness matrix has $\mathcal{O}(p^3)$ nonzero matrix entries. The parameter p denotes the polynomial degree.

3.1 Definition of the shape functions

Let $\hat{\triangle}$ be the reference tetrahedron with the vertices A, B, C, and D, the edges $e1, \ldots, e6$, and the faces $F1, \ldots, F4$, see Figure 1.

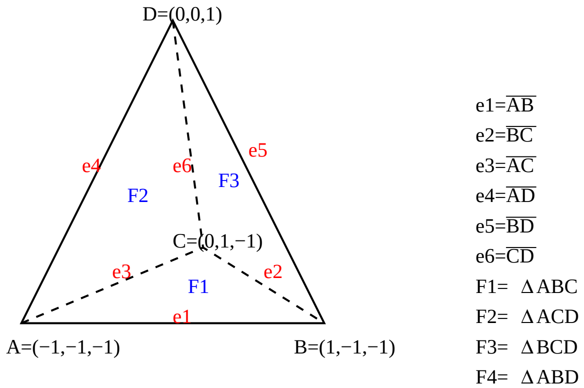

Figure 1: Notation of the faces, edges and vertices on the reference element $\hat{\triangle}$.

Now, we split the definition of the shape functions into the vertex, edge bubble, face bubble and interior bubble functions:

- The vertex functions are defined as the usual hat functions, i.e.

$$\phi_{A/B}(x,y,z) = \frac{1-2y-z\pm 4x}{4}, \qquad \phi_C(x,y,z) = \frac{1+2y-z}{2}, \tag{26}$$
$$\phi_D(x,y,z) = \frac{1+z}{2}.$$

  Let $\Phi_V = [\phi_A, \phi_B, \phi_C, \phi_D]$ denote the basis of the hat functions.

- The edge bubbles are defined as

$$\begin{aligned}
\phi_{e1,i}(x,y,z) &= \hat{p}_i^0\left(\frac{4x}{1-2y-z}\right)\left(\frac{1-2y-z}{4}\right)^i, \quad i=2,\ldots,p,\\
\phi_{e2/e3,j}(x,y,z) &= \frac{1-2y-z\pm 4x}{4}\hat{p}_j^0\left(\frac{2y}{1-z}\right)\left(\frac{1-z}{2}\right)^j,\\
&\quad j=1,\ldots,p-1,\\
\phi_{e4/e5,k}(x,y,z) &= \frac{1-2y-z\mp 4x}{4}\hat{p}_k^0(z), \quad k=1,\ldots,p-1,\\
\phi_{e6,k}(x,y,z) &= \frac{1+2y-z}{2}\hat{p}_k^0(z), \quad k=1,\ldots,p-1.
\end{aligned} \tag{27}$$

  We denote by

$$\begin{aligned}
\Phi_e &= \Big[\{\phi_{e1,i}\}_{i=2}^{p}, \{\phi_{e2,j}\}_{j=1}^{p-1}, \{\phi_{e3,j}\}_{j=1}^{p-1},\\
&\quad \{\phi_{e4,k}\}_{k=1}^{p-1}, \{\phi_{e5,k}\}_{k=1}^{p-1}, \{\phi_{e6,k}\}_{k=1}^{p-1}\Big]
\end{aligned}$$

the basis of all edge bubble functions.

- The face bubble functions are

$$
\begin{aligned}
\phi_{F1,i,j}(x,y,z) &= \hat{p}_i^0\left(\frac{4x}{1-2y-z}\right)\left(\frac{1-2y-z}{4}\right)^i \\
&\quad \times \hat{p}_j^{2i-a}\left(\frac{2y}{1-z}\right)\left(\frac{1-y}{2}\right)^j \\
&\quad\quad i\geq 2, j\geq 1, i+j\leq p, \\
\phi_{F2/3,j,k}(x,y,z) &= \frac{1-2y-z\mp 4x}{4}\hat{p}_j^0\left(\frac{2y}{1-z}\right)\left(\frac{1-y}{2}\right)^j \qquad (28)\\
&\quad \times \hat{p}_k^{2j+2-b}(z), \quad j,k\geq 1, j+k\leq p-1, \\
\phi_{F4,i,k}(x,y,z) &= \hat{p}_i^0\left(\frac{4x}{1-2y-z}\right)\left(\frac{1-2y-z}{4}\right)^i \hat{p}_k^{2i-b}(z), \\
&\quad\quad i\geq 2, k\geq 1, i+k\leq p.
\end{aligned}
$$

  We denote by

$$
\begin{aligned}
\Phi_F &= \Big[\{\phi_{F1,i,j}\}_{i=2,j=1}^{i+j=p}, \{\phi_{F2,j,k}\}_{j,k=1}^{j+k=p-1}, \\
&\quad \{\phi_{F3,j,k}\}_{j,k=1}^{j+k=p-1}, \{\phi_{F4,i,k}\}_{i=2,k=1}^{i+k=p}\Big]
\end{aligned}
$$

  the basis of all face bubble functions.

- The interior bubbles read as

$$
\begin{aligned}
\phi_{ijk}(x,y,z) &= \hat{p}_i^0\left(\frac{4x}{1-2y-z}\right)\left(\frac{1-2y-z}{4}\right)^i \\
&\quad \times \hat{p}_j^{2i-a}\left(\frac{2y}{1-z}\right)\left(\frac{1-y}{2}\right)^j \hat{p}_k^{2i+2j-b}(z), \\
&\quad\quad i+j+k\leq p, i\geq 2, j,k\geq 1. \qquad (29)
\end{aligned}
$$

  The parameters $a, b \in \mathbb{N}_0$ satisfy the following assumptions

$$
0\leq a\leq 4, \quad a\leq b\leq 6. \qquad (30)
$$

  Moreover, $\Phi_I = [\phi_{ijk}]_{i\geq 2, j\geq 1, k\geq 1}^{i+j+k\leq p}$ denotes the basis of the interior bubbles.

Let

$$
\Phi = [\Phi_V, \Phi_e, \Phi_F, \Phi_I]
$$

be the basis of all shape functions. The interior bubbles coincide with the functions given in [30], see also [19], if $a = b = 0$.

Remark 3.1. *With the same arguments as presented in [13], it can be proved that the edge bubbles* (27) *corresponding to the edge e vanish on all other edges. The face bubbles* (28) *corresponding to the face F vanish on all other faces. The interior bubbles are zero on all faces. Hence, the functions are linearly independent and* $\mathrm{span}\Phi = \mathbb{P}_p$.

Remark 3.2. *To define the global shape functions, we adapt the numbering method developed in [2], i.e. the mapping F_s transforms the vertices $V1, \ldots, V4$ on $\hat{\triangle}$ to the vertices $v1, \ldots, v4$ of the FE mesh on $\triangle_s$ with $\sharp v1 < \sharp v2 < \sharp v3 < \sharp v4$. The construction of our face bubbles* (28) *requires a characteristic vertex on each face. Due to our construction, the vertex with the largest number is the characteristic vertex on each face. Moreover, the face bubbles are*

$$\begin{aligned}
\phi_{F2/3,i,k}(r,s) &= \frac{1-\frac{2r}{1-s}}{2}\hat{p}^0_{i-1}\left(\frac{2r}{1-s}\right)\left(\frac{1-s}{2}\right)^i \hat{p}^{2i-b}_k(s), \\
&\qquad r-1 \le 2s \le 1-r, -1 \le r \le 1 \\
\phi_{F1/4,i,k}(r,s) &= \hat{p}^0_i\left(\frac{2r}{1-s}\right)\left(\frac{1-s}{2}\right)^i \hat{p}^{2i-a}_k(s), \\
&\qquad r-1 \le 2s \le 1-r, -1 \le r \le 1.
\end{aligned}$$

There exists a simple basis transformation matrix W between the two bases $\left[\hat{p}^0_i(t)\right]_{i=2}^p$ and $\left[(1-t)\hat{p}^0_{i-1}(t)\right]_{i=2}^p$, [13]. This matrix W is a pentadiagonal and upper triangular matrix. Using the arguments proposed in [13], the continuity of the face bubbles along element boundaries can be enforced. With the same arguments, the continuity of the edge bubbles can be enforced as well.

Let

$$\hat{\mathcal{A}} = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{12} & a_{22} & a_{23} \\ a_{13} & a_{23} & a_{33} \end{bmatrix} \in \mathbb{R}^{3\times 3}$$

be a diffusion matrix with constant coefficients. We introduce

$$\hat{K}_{\hat{\mathcal{A}}} = \int_{\hat{\triangle}} (\nabla\Phi)^T \hat{\mathcal{A}} \nabla\Phi \tag{31}$$

as the stiffness matrix with respect to the functions (26)-(29) on the reference tetrahedron. Moreover, let

$$\begin{aligned}
\hat{K}_{\hat{\mathcal{A}},I} &= \left[a^{\hat{\mathcal{A}}}_{ijk,i'j'k'}\right]_{i,i'=2,j,j',k,k'=1}^{i+j+k=p,i'+j'+k'=p} \\
&= \left[\int_{\hat{\triangle}} (\nabla\phi_{ijk})^T \hat{\mathcal{A}} \nabla\phi_{i'j'k'}\right]_{i,i'=2,j,j',k,k'=1}^{i+j+k=p,i'+j'+k'=p}
\end{aligned} \tag{32}$$

be the block of $\hat{K}_{\hat{\mathcal{A}}}$ which corresponds to the interior bubbles.

Now, we are in the position to formulate the main theorem of this paper.

Theorem 3.3. *Let $\hat{K}_{\hat{\mathcal{A}}}$ be defined via equation* (31)*. Then, this matrix has* $\frac{(p+1)(p+2)(p+3)}{6}$ *rows and columns. If condition* (30) *is satisfied, each row has a bounded number of nonzero entries and the number of total nonzero entries is* $\mathcal{O}(p^3)$*. Moreover, the entry* $a^I_{ijk,i'j'k'}$ *of the matrix* $\hat{K}_{I,I}$ (32) *is zero if* $|i-i'| \notin \{0,2\}$*, or* $|i+j-i'-j'| > 3+a$*, or* $|i+j+k-i'-j'-k'| > 2+b$*.*

Proof. The proof is given in section 6. □

Remark 3.4. *As presented in [13, Theorem 3.2], the result can be extended to the case of a general tetrahedron.*

4 Properties of the interior block of the element stiffness matrix

In this section, we present the most important computational properties for the matrix $\hat{K}_{I,I}$ (32) which corresponds to the interior block of the element stiffness matrix. In several numerical experiments, we investigate the nonzero pattern, the number of nonzero entries and the condition number for the bases (29) for several values of a and b. Finally, the time for the generation of the matrix $\hat{K}_{I,I}$ and the matrix vector multiplication $\hat{K}_{I,I}\underline{x}$ is measured. All computations are performed on a 2 GHz workstation.

Figure 2 displays the nonzero pattern of the matrix $\hat{K}_{I,I}$, i.e. the block of the interior bubbles for the Laplacian, using the basis functions

$$\begin{aligned}\phi_{ijk}(x,y,z) \quad &= \quad \hat{p}_i^0\left(\frac{4x}{1-2y-z}\right)\left(\frac{1-2y-z}{4}\right)^i \\ &\qquad \hat{p}_j^{2i}\left(\frac{2y}{1-z}\right)\left(\frac{1-z}{2}\right)^j \hat{p}_k^{2i+2j}(z),\end{aligned}$$

$i+j+k \leq p, i \geq 2, j, k \geq 1$, i.e. the functions (29) with $a = b = 0$. A typical stencil like structure of the nonzero entries can be observed.

Figure 3 displays the averaged numbers of nonzero entries for the matrix $\hat{K}_{I,I}$ for several values of a and b. If $0 \leq a \leq b \leq 6$, the averaged number of nonzero entries per row are bounded by a constant $c_{a,b}$ which is independent of the polynomial degree p. This constant depends on the special choice of a and b and is the lowest one for $a = b = 0$. The optimality of the number of nonzero entries per row for $a = b = 0$ is a consequence of the proof of Theorem 3.3. In general, one obtains $c_{a,b} = 3(7 + 2a)(5 + 2b)$. In the case $b < a$, our assumption (30) is violated. Since the averaged number of nonzero entries per row increases with p, this assumption is necessary to prove Theorem 3.3.

Figure 4 displays the maximal and the inverse of the minimal eigenvalue of the diagonally preconditioned matrix $\hat{K}_{I,I}$. In all cases, the maximal

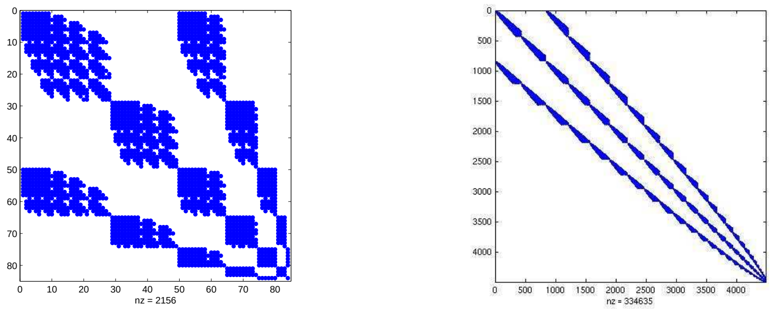

Figure 2: Nonzero pattern of the interior bubbles for $p = 10$ (left) and $p = 32$ (right) with $a = b = 0$.

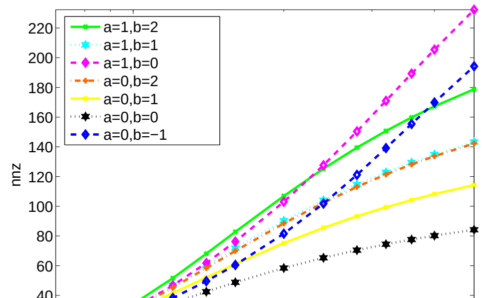

Figure 3: Averaged number of nonzero entries for the interior bubbles per row.

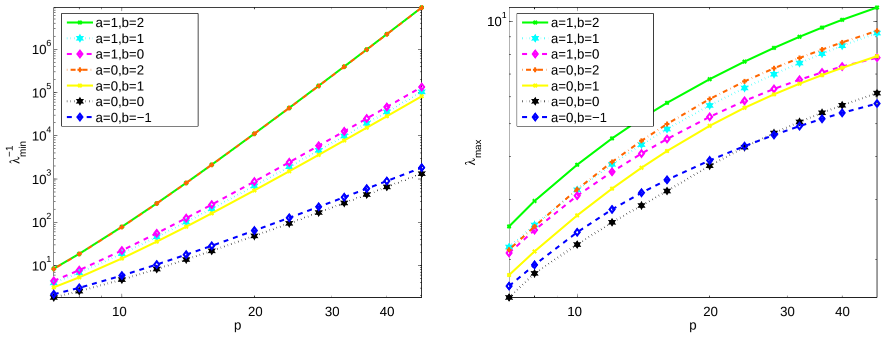

Figure 4: Maximal and minimal eigenvalue of the diagonally preconditioned matrix $\hat{K}_{I,I}$.

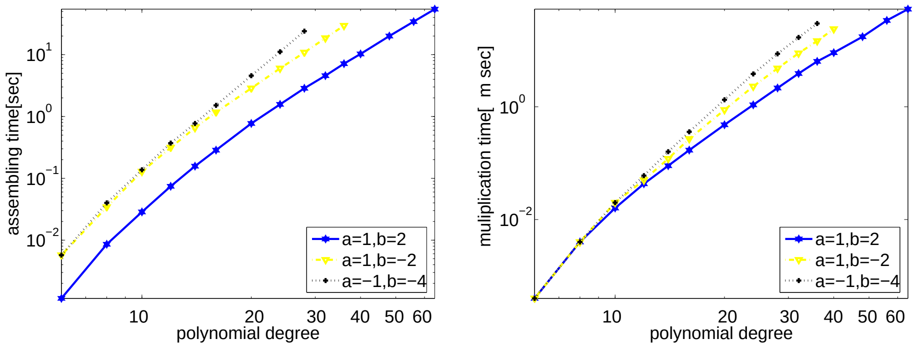

Figure 5: Time for assembling $\hat{K}_{I,I}$ (left) and for $\hat{K}_{I,I}\underline{x}$ (right) for several polynomial degrees.

eigenvalue is bounded by a constant of about $7 \dots 15$. The minimal eigenvalue λ_{min} depends strongly on the choice of a and b. From the numerical results, one can conclude that λ_{min}^{-1} grows as $\mathcal{O}(p^{\max\{4,4+2a,4+2b,4+2a+2b\}})$. So, the condition number grows at least with p^4. The optimal order for the condition number can be achieved if $a, b \leq 0$. In combination with Theorem 3.3, the basis with $a = b = 0$ should be preferred since it yields to the lowest number of nonzero entries and the best condition number.

A last example shows the significance of the usage of sparse shape functions. Figure 5 displays the time for the generation of the matrix $\hat{K}_{I,I}$ and the multiplication $\hat{K}_{I,I}\underline{x}$ for several polynomial degrees and the parameter choices $(a, b) \in \{(1, 2), (1, -2), (-1, -4)\}$. Due to Theorem 3.3, the number of nonzero entries is $\mathcal{O}(p^3)$, $\mathcal{O}(p^4)$ and $\mathcal{O}(p^5)$, respectively. In the experiments, we computed the nonzero matrix entries with a sum-factorization algorithm. The remaining one-dimensional integrals are computed recursively using (7) and (13) using the product recurrence given in [26]. From the results one can see that an assembling time of about three seconds is required for $p = 36$ if $a = 1, b = 2$. In the same time, the matrix for $p = 24$

can be generated if $a = 1$, $b = -2$, or, the matrix for $p = 20$ can be generated if $a = -1$ and $b = -4$. For all polynomial degrees the sparse basis with $a = 1$ and $b = 2$ should be preferred against the two another ones.

5 Application: A preconditioner for the interior bubbles

In this section, we derive a simple preconditioner for the block of the interior bubbles. It is well known from the literature that preconditioned gradient methods (pcg-methods) with DD preconditioners of Dirichlet-Dirichlet-type are among the most efficient iterative solvers for systems of type (2), cf. [6], [4], [18], [21]. Corresponding to the partition of basis functions $\Psi = [\Psi_V, \Psi_E, \Psi_F, \Psi_I] = [\Psi_C, \Psi_I]$, i.e. $C = V \cup E \cup F$, let

$$\mathcal{K}_\Psi = \begin{bmatrix} \mathcal{K}_C & \mathcal{K}_{CI} \\ \mathcal{K}_{IC} & \mathcal{K}_I \end{bmatrix} = \begin{bmatrix} I & \mathcal{K}_{CI}\mathcal{K}_I^{-1} \\ \mathbf{0} & I \end{bmatrix} \begin{bmatrix} \mathcal{S} & \mathbf{0} \\ \mathbf{0} & \mathcal{K}_I \end{bmatrix} \begin{bmatrix} I & \mathbf{0} \\ \mathcal{K}_I^{-1}\mathcal{K}_{IC} & I \end{bmatrix} \tag{33}$$

be the block structure of the stiffness matrix with the Schur-complement $\mathcal{S} = \mathcal{K}_C - \mathcal{K}_{CI}\mathcal{K}_I^{-1}\mathcal{K}_{IC}$. Our domain decomposition preconditioner for the matrix $\mathcal{K}_\Psi$ will be of the form

$$\mathcal{C} = \begin{bmatrix} I & -E^T \\ \mathbf{0} & I \end{bmatrix} \begin{bmatrix} C_S & \mathbf{0} \\ \mathbf{0} & C_I \end{bmatrix} \begin{bmatrix} I & \mathbf{0} \\ -E & I \end{bmatrix}, \tag{34}$$

where

- C_I is a preconditioner for $\mathcal{K}_I$,
- C_S is a preconditioner for the Schur-complement $\mathcal{S} = \mathcal{K}_C - \mathcal{K}_{CI}\mathcal{K}_I^{-1}\mathcal{K}_{IC}$ and
- E is the matrix representation of an extension operator acting from the edges of the elements into the interior.

Preconditioners for the Schur-complement have been proposed in [16] and [21]. For C_I, a wavelet preconditioner has been developed for hexahedral elements in [12]. The papers [6], [3] and [24] deal with the extension operator for the p-version of the FEM using triangular or tetrahedral elements. In [9], see also [17], an algebraic analysis of a preconditioner of type (34) is given.

Now, we propose a relatively simple preconditioner C_I for $\mathcal{K}_I$ and (based on this) a matrix representation E for the extension operator of the form (34). By (3), the global stiffness matrix is the result of assembling local stiffness matrices $\tilde{K}_s$, i.e. $\mathcal{K}_\Psi = \sum_{s=1}^{nel} R_s^T \tilde{K}_s R_s$. Let

$$\mathcal{C}_0 = \sum_{s=1}^{nel} R_s C_0 R_s^T, \quad \text{where} \quad C_0 = \int_{\hat{\triangle}} (\nabla\tilde{\Phi}(x,y,z))^T \nabla\tilde{\Phi}(x,y,z) \, \mathrm{d}(x,y,z). \tag{35}$$

In this matrix, the stiffness matrix for the Laplacian on the reference element is assembled on each element. According to (33), (34), we consider a block decomposition of $\mathcal{C}_0$, i.e.

$$\mathcal{C}_0 = \begin{bmatrix} \mathcal{C}_C & \mathcal{C}_{CI} \\ \mathcal{C}_{IC} & \mathcal{C}_I \end{bmatrix}. \tag{36}$$

and define the preconditioner

$$\mathcal{C}_1 = \begin{bmatrix} I & \mathcal{C}_{CI}\mathcal{C}_I^{-1} \\ \mathbf{0} & I \end{bmatrix} \begin{bmatrix} C_S & \mathbf{0} \\ \mathbf{0} & \mathcal{C}_I \end{bmatrix} \begin{bmatrix} I & \mathbf{0} \\ \mathcal{C}_I^{-1}\mathcal{C}_{IC} & I \end{bmatrix} \tag{37}$$

for $\mathcal{K}_\Psi$, where C_S is a preconditioner for the Schur complement and $\mathcal{C}_I$ and $\mathcal{C}_{IC}$ are taken from (36). Now, we formulate

Theorem 5.1. *Let $\mathcal{C}_1$ be defined via (37). Moreover, let C_S be a preconditioner for the Schur complement such that $C_S^{-1}\underline{v}$ requires not more than $\mathcal{O}(p^6)$ operations and*

$$c_1\,(C_S\underline{v},\underline{v}) \leq (S\underline{v},\underline{v}) \leq c_2\,(C_S\underline{v},\underline{v}) \quad \forall \underline{v} \tag{38}$$

and some constants c_1, c_2. Then, $\kappa({\mathcal{C}_1}^{-\frac{1}{2}}\mathcal{K}_\Psi{\mathcal{C}_1}^{-\frac{1}{2}}) = \mathcal{O}(\frac{c_2}{c_1})$. The operation $\mathcal{C}_1^{-1}\underline{u}$ requires $\mathcal{O}(p^6)$ operations.

Proof. The proof is similar to the proof of Theorem 4.2 in [13]. Using [18], we can prove that $\kappa({\mathcal{C}_0}^{-\frac{1}{2}}\mathcal{K}_\Psi{\mathcal{C}_0}^{-\frac{1}{2}}) = \mathcal{O}(1)$. Hence, the first assertion $\kappa({\mathcal{C}_1}^{-\frac{1}{2}}\mathcal{K}_\Psi{\mathcal{C}_1}^{-\frac{1}{2}}) = \mathcal{O}(\frac{c_2}{c_1})$ follows from (38) immediately.

To prove the complexity argument for $\mathcal{C}_1^{-1}\underline{u}$, we investigate the nonzero pattern for the matrix $\hat{K}_{I,I}$. Due to Theorem 3.3, see also Figure 2, the nonzero pattern has the structure of a 3D-finite difference stencil. Let $(\mathbb{V},\mathbb{E})$ be the corresponding graph of the matrix $\hat{K}_{I,I}$. $(\mathbb{V},\mathbb{E})$ has an $\mathcal{O}(N^{2/3})$ separator property and therefore the method of nested dissection, [15], yields a total cost of $\mathcal{O}(N^2) = \mathcal{O}(p^6)$, see [22]. □

6 Proof of Theorem 3.3.

In this section, we prove the main theorem of this paper using several auxiliary results. In a first step, we give a formula for the gradient of the interior bubble functions (29). Before we formulate an auxiliary result which simplifies the computation of the gradient.

We start be formulating a lemma that simplifies the computation of the gradient of the interior bubble functions (29). Let $g_{a(x),b,c,\alpha,j} : \mathbb{R} \mapsto \mathbb{R}$ be defined via

$$g_{a(x),b,c,\alpha,j}(y) = \hat{p}_j^\alpha\left(\frac{ax}{b-cy}\right)\left(\frac{b-cy}{a}\right)^j. \tag{39}$$

Lemma 6.1. *Let* $\hat{p}_j^\alpha$ *be the integrated Jacobi polynomial* (5) *and let the function* $g_{a(x),b,c,\alpha,j} : \mathbb{R} \mapsto \mathbb{R}$ *be defined via* (39). *Then,*

$$\begin{aligned} g'_{a(x),b,c,\alpha,j}(y) &= \frac{c}{a(2j+\alpha-2)} \left(\frac{b-cy}{a}\right)^{j-1} \\ &\times \left(-\alpha p_{j-1}^\alpha \left(\frac{ax}{b-cy}\right) + (2j-2) p_{j-2}^\alpha \left(\frac{ax}{b-cy}\right)\right). \end{aligned} \tag{40}$$

Proof. Let $w = \left(\frac{ax}{b-cy}\right)$. Using the chain and the product rule, we get

$$g'_{a(x),b,c,\alpha,j}(y) = \frac{c}{a}\left(\frac{b-cy}{a}\right)^{j-1} \left(w p_{j-1}^\alpha(w) - j\hat{p}_j^\alpha(w)\right). \tag{41}$$

Next, we insert (19) into (41) and obtain

$$\begin{aligned} g'_{a(x),b,c,\alpha,j}(y) &= \frac{c}{a(2j+\alpha-2)} \left(\frac{b-cy}{a}\right)^{j-1} \\ &\times \left(-\alpha p_{j-1}^\alpha \left(\frac{ax}{b-cy}\right) + (2j-2) p_{j-2}^\alpha \left(\frac{ax}{b-cy}\right)\right) \end{aligned}$$

which proves the lemma. □

The following lemma gives a formula for the gradient of the interior bubble functions (29).

Lemma 6.2. *Let* $\phi_{ijk}(x,y,z)$ *be defined via* (29). *With the abbreviations* $r = \frac{1-2y-z}{4}$ *and* $s = \frac{1-z}{2}$ *the following relations hold.*

$$\frac{\partial \phi_{ijk}}{\partial x}(x,y,z) = p_{i-1}^0\left(\frac{x}{r}\right) r^{i-1}\, \hat{p}_j^{2i-a}\left(\frac{y}{s}\right) s^j\, \hat{p}_k^{2i+2j-b}(z), \tag{42}$$

$$\begin{aligned} \frac{\partial \phi_{ijk}}{\partial y}(x,y,z) &= \frac{1}{2} p_{i-2}^0\left(\frac{x}{r}\right) r^{i-1}\, \hat{p}_j^{2i-a}\left(\frac{y}{s}\right) s^j\, \hat{p}_k^{2i+2j-b}(z) \\ &+ \hat{p}_i^0\left(\frac{x}{r}\right) r^i\, p_{j-1}^{2i-a}\left(\frac{y}{s}\right) s^j\, \hat{p}_k^{2i+2j-b}(z), \end{aligned} \tag{43}$$

$$\begin{aligned} \frac{\partial \phi_{ijk}}{\partial z}(x,y,z) &= -\frac{2i-a}{4j+4i-4-2a} \hat{p}_i^0\left(\frac{x}{r}\right) r^i\, p_{j-1}^{2i-a}\left(\frac{y}{s}\right) s^{j-1}\, \hat{p}_k^{2i+2j-b}(z) \\ &+ \frac{2j-2}{4j+4i-4-2a} \hat{p}_i^0\left(\frac{x}{r}\right) r^i\, p_{j-2}^{2i-a}\left(\frac{y}{s}\right) s^{j-1}\, \hat{p}_k^{2i+2j-b}(z) \\ &+ p_{i-2}^0\left(\frac{x}{r}\right) r^{i-1}\, \hat{p}_j^{2i-a}\left(\frac{y}{s}\right) s^j\, \hat{p}_k^{2i+2j-b}(z) \\ &+ \hat{p}_i^0\left(\frac{x}{r}\right) r^i\, \hat{p}_j^{2i-a}\left(\frac{y}{s}\right) s^j\, p_{k-1}^{2i+2j-b}(z) \end{aligned} \tag{44}$$

Proof. The relations (42) and (43) have been proved in [13].

To prove (44), we write the dependence in z direction in the following way:

$$\phi_{ijk}(x,y,z) = g_{2(y),1,1,2i-a,j}(z)\ g_{4(x),1-2y,1,0,i}(z)\ \hat{p}_k^{2i+2j-b}(z)$$

with the function g defined via (39). Using the product rule, we obtain

$$\begin{aligned}\frac{\partial\phi_{ijk}}{\partial z} &= g'_{2(y),1,1,2i-a,j}(z)g_{4(x),1-2y,1,0,i}(z)\hat{p}_k^{2i+2j-b}(z)\\ &\quad+g_{2(y),1,1,2i-a,j}(z)g'_{4(x),1-2y,1,0,i}(z)\hat{p}_k^{2i+2j-b}(z)\\ &\quad+g_{2(y),1,1,2i-a,j}(z)g_{4(x),1-2y,1,0,i}(z)p_{k-1}^{2i+2j-b}(z).\end{aligned}$$

Now, we insert (40) and obtain

$$\begin{aligned}\frac{\partial\phi_{ijk}}{\partial z} &= \frac{1}{4j+4i-4-a}\left(\frac{1-z}{2}\right)^{j-1} g_{4(x),1-2y,1,0,i}(z)\hat{p}_k^{2i+2j-b}(z)\\ &\quad\times\left(-(2i-a)p_{j-1}^{2i-a}\left(\frac{2y}{1-z}\right)+(2j-2)p_{j-2}^{2i-a}\left(\frac{2y}{1-z}\right)\right)\\ &\quad+g_{2(y),1,1,2i-a,j}(z)\frac{1}{4}\left(\frac{1-2y-z}{4}\right)^{j-1}\\ &\quad\times p_{j-2}^{0}\left(\frac{4x}{1-2y-z}\right)\hat{p}_k^{2i+2j-b}(z)\\ &\quad+g_{2(y),1,1,2i-a,j}(z)g_{4(x),1-2y,1,0,i}(z)p_{k-1}^{2i+2j-b}(z),\end{aligned}$$

or with the abbreviations $r = \dfrac{1-2y-z}{4}$ and $s = \dfrac{1-z}{2}$,

$$\begin{aligned}\frac{\partial\phi_{ijk}}{\partial z} &= -\frac{2i-a}{4j+4i-4-a}\hat{p}_i^0\left(\frac{x}{r}\right)\ r^i\ p_{j-1}^{2i-a}\left(\frac{y}{s}\right)\ s^{j-1}\ \hat{p}_k^{2i+2j-b}(z)\\ &\quad+\frac{2j-2}{4j+4i-4-a}\hat{p}_i^0\left(\frac{x}{r}\right)\ r^i\ p_{j-2}^{2i-a}\left(\frac{y}{s}\right)\ s^{j-1}\ \hat{p}_k^{2i+2j-b}(z)\\ &\quad+\frac{1}{4}p_{i-2}^0\left(\frac{x}{r}\right)\ r^{i-1}\ \hat{p}_j^{2i-a}\left(\frac{y}{s}\right)\ s^j\ \hat{p}_k^{2i+2j-b}(z)\\ &\quad+\hat{p}_i^0\left(\frac{x}{r}\right)\ r^i\ \hat{p}_j^{2i-a}\left(\frac{y}{s}\right)\ s^j\ p_{k-1}^{2i+2j-b}(z).\end{aligned}$$

This proves the lemma. □

Now, we are able to prove Theorem 3.3.

Proof. We present only a proof for the block of interior bubbles. The face, edge and vertex bubbles can be interpreted as special cases of the interior bubbles for $i = 0, 1$, $j = 0$, or, $k = 0$. More precisely, we have

$\phi_{F1,i,j}(x,y,z) = \phi_{ij0}(x,y,z)$ and $\phi_{F4,i,k}(x,y,z) = \phi_{i0k}(x,y,z)$ with $\hat{p}_0^\alpha(\xi) = 1$. For $\phi_{F2/3,j,k}$, the situation is similar. Let $\hat{p}_1^0(x) = \frac{1\pm x}{2}$. Then, one obtains

$$\phi_{1,j,k}(x,y,z) = \frac{1-2y-z\mp 4x}{4}\hat{p}_j^{2-a}\left(\frac{2y}{1-z}\right)\left(\frac{1-z}{2}\right)^j \hat{p}_k^{2j+2-b}(z).$$

So, the only difference to the functions (28) is the choice of the weight parameter in $\hat{p}_j^{2-a}\left(\frac{2y}{1-z}\right)$, which is 0 in (28). Using (7), we can represent each polynomial $\hat{p}_i^0(\xi)$ as the sum of not so many polynomials $\hat{p}_i^{2-a}(\xi)$, where $a \leq 2$. This proves a sparsity with $\mathcal{O}(p^2)$ nonzero matrix entries for the block between the interior bubbles and the face bubbles. In the case $a \geq 3$, a direct computation shows that the integrals in x-direction are zero for $i \geq 4$, whereas integrals of the type $\int_{-1}^{1}(1-y)^\gamma \hat{p}_j^0(y)\hat{p}_{j'}^0(y)\ \mathrm{d}y$ have to be investigated in y-direction. Using (16), the sparsity can be shown.

Now, let us focus on the block of the interior bubbles. Since all zero entries base on the orthogonality relation (9) the result can easily be extended to the remaining blocks.

In order to compute the entries of the inner block of the stiffness matrix $\hat{K}_{I,I}$ we have to evaluate integrals of the form

$$\int_{\hat{\triangle}} \frac{\partial}{\partial\zeta}\phi_{i,j,k}\frac{\partial}{\partial\zeta}\phi_{i',j',k'}\ \mathrm{d}(x,y,z), \qquad \zeta = x,y,z. \tag{45}$$

Note that if the coefficient matrix $\mathcal{A}$ is not a diagonal matrix then we also have to consider the mixed terms $\frac{\partial}{\partial\zeta}\phi_{i,j,k}\frac{\partial}{\partial\eta}\phi_{i',j',k'}$, with $(\zeta,\eta) \in \{(x,y),(x,z),(y,z)\}$. They are treated in complete analogy to the following and we will comment below on the nonzero pattern of these blocks.

We transform the integration domain from the reference tetrahedron to the cube $(-1,1)^3$ using the Duffy transformation

$$w = \frac{4x}{1-2y-z}, \qquad \mathrm{d}x = \frac{1-2y-z}{4}\mathrm{d}w,$$

and

$$w = \frac{2y}{1-z}, \qquad \mathrm{d}y = \frac{1-z}{2}\mathrm{d}w.$$

After applying this Duffy transformation (45) has the form

$$\int_{\hat{\triangle}} \frac{\partial}{\partial\zeta}\phi_{i,j,k}\frac{\partial}{\partial\zeta}\phi_{i',j',k'}\ \mathrm{d}(x,y,z) =: \int_{-1}^{1}\int_{-1}^{1}\int_{-1}^{1}\hat{\mathcal{I}}(r,s,z)\ \mathrm{d}r\ \mathrm{d}s\ \mathrm{d}z, \tag{46}$$

where $r = \frac{x(1-y)(1-z)}{4}$ and $s = \frac{y(1-z)}{2}$. Due to the tensor product like structure of the basis functions we have thereby decoupled the integrals over x, y

and z. Now we use the results of Lemma 6.2 to compute the partial derivatives and perform the above substitution. Thus we obtain 21 integrands adding up to

$$\hat{\mathcal{I}}(r,s,z) = \hat{\mathcal{I}}^{(1)}(r,s,z) + \sum_{l=2}^{5} \hat{\mathcal{I}}^{(l)}(r,s,z) + \sum_{l=6}^{21} \hat{\mathcal{I}}^{(l)}(r,s,z).$$

The first integrand stems from the product of the x-partial derivatives, the next four from the product of the y-partial derivatives and the last 16 from the product of the z-partial derivatives. The integrands

$$\begin{aligned} \hat{\mathcal{I}}^{(l)}(r,s,z) &= c_l p_{x,1}(r) p_{x,2}(r) \left(\frac{1-s}{2}\right)^{i+i'+\gamma_y} \\ &\quad \times p_{y,1}(s) p_{y,2}(s) \left(\frac{1-z}{2}\right)^{i+i'+j+j'+\gamma_z} p_{z,1}(z) p_{z,2}(z), \end{aligned}$$

$l = 1, \dots, 21$, for $\hat{K}_{I,I}$ in the indicated order are listed in Table 1 omitting the constants.

These integrands already illustrate the complexity of the problem of determining the nonzero pattern of the system matrix. We have tackled this problem with a program we implemented in the computer algebra software Mathematica. This program explicitly computes the entries of $\hat{K}_{I,I}$ using the identities stated in section 2 for all parameters a, b in the valid range, i.e. with $0 \leq a \leq 4, a \leq b \leq 6$. The intermediate steps can be documented and checked via output, yet the formulae do not posses a nice closed form, which is why they are not stated here. The program can also be used for solving the subproblem of determining the nonzero pattern for the analogue family of interior bubbles for triangles.

Our Mathematica program evaluates the integrals from left to right, starting by integrating with respect to x, which is clear from the dependence of the parameters. To determine the values of the integrals the orthogonality relation (9) is used. Hence the polynomials under the integral have to be rewritten as Jacobi polynomials p_n^α where α corresponds to the appearing weights $i + i' + \gamma_y$ and $i + j + i' + j' + \gamma_z$. This concept follows the lines of the proof described in [13].
We present now our algorithm for the simplification of the integral

$$\int_{-1}^{1} (1-\zeta)^\gamma q_{n_1}(\zeta) q_{n_2}(\zeta)\, \mathrm{d}\zeta, \tag{47}$$

where $q_{n_1}(\zeta)$ and $q_{n_2}(\zeta)$ can be either Jacobi or integrated Jacobi polynomials of degree n_1 and n_2 respectively, and γ is the appearing weight.

Algorithm.

Input: Integrand (47).
Output: Mass matrix entries with band structure.

	$p_{x,1}$	$p_{x,2}$	γ_y	$p_{y,1}$	$p_{y,2}$	γ_z	$p_{z,1}$	$p_{z,2}$
$\hat{\mathcal{I}}^{(1)}$	p^0_{i-1}	$p^0_{i'-1}$	-1	$\hat{p}^{2i-a}_j$	$\hat{p}^{2i'-a}_{j'}$	0	$\hat{p}^{-b+2(i+j)}_k$	$\hat{p}^{-b+2(i'+j')}_{k'}$
$\hat{\mathcal{I}}^{(2)}$	$\hat{p}^0_i$	$\hat{p}^0_{i'}$	1	p^{2i-a}_{j-1}	$p^{2i'-a}_{j'-1}$	0	$\hat{p}^{-b+2(i+j)}_k$	$\hat{p}^{-b+2(i'+j')}_{k'}$
$\hat{\mathcal{I}}^{(3)}$	p^0_{i-2}	$\hat{p}^0_{i'}$	0	$\hat{p}^{2i-a}_j$	$p^{2i'-a}_{j'-1}$	0	$\hat{p}^{-b+2i+2j}_k$	$\hat{p}^{-b+2(i'+j')}_{k'}$
$\hat{\mathcal{I}}^{(4)}$	$\hat{p}^0_i$	$p^0_{i'-2}$	0	p^{2i-a}_{j-1}	$\hat{p}^{2i'-a}_{j'}$	0	$\hat{p}^{-b+2(i+j)}_k$	$\hat{p}^{-b+2(i'+j')}_{k'}$
$\hat{\mathcal{I}}^{(5)}$	p^0_{i-2}	$p^0_{i'-2}$	-1	$\hat{p}^{2i-a}_j$	$\hat{p}^{2i'-a}_{j'}$	0	$\hat{p}^{-b+2(i+j)}_k$	$\hat{p}^{-b+2(i'+j')}_{k'}$
$\hat{\mathcal{I}}^{(6)}$	$\hat{p}^0_i$	$\hat{p}^0_{i'}$	1	$\hat{p}^{2i-a}_j$	$\hat{p}^{2i'-a}_{j'}$	2	$p^{-b+2(i+j)}_{k-1}$	$p^{-b+2(i'+j')}_{k'-1}$
$\hat{\mathcal{I}}^{(7)}$	$\hat{p}^0_i$	$\hat{p}^0_{i'}$	1	p^{2i-a}_{j-2}	$\hat{p}^{2i'-a}_{j'}$	1	$\hat{p}^{-b+2(i+j)}_k$	$p^{-b+2(i'+j')}_{k'-1}$
$\hat{\mathcal{I}}^{(8)}$	$\hat{p}^0_i$	$\hat{p}^0_{i'}$	1	p^{2i-a}_{j-1}	$\hat{p}^{2i'-a}_{j'}$	1	$\hat{p}^{-b+2(i+j)}_k$	$p^{-b+2(i'+j')}_{k'-1}$
$\hat{\mathcal{I}}^{(9)}$	p^0_{i-2}	$\hat{p}^0_{i'}$	0	$\hat{p}^{2i-a}_j$	$\hat{p}^{2i'-a}_{j'}$	1	$\hat{p}^{-b+2(i+j)}_k$	$p^{-b+2(i'+j')}_{k'-1}$
$\hat{\mathcal{I}}^{(10)}$	$\hat{p}^0_i$	$\hat{p}^0_{i'}$	1	$\hat{p}^{2i-a}_j$	$p^{2i'-a}_{j'-2}$	1	$p^{-b+2(i+j)}_{k-1}$	$\hat{p}^{-b+2(i'+j')}_{k'}$
$\hat{\mathcal{I}}^{(11)}$	$\hat{p}^0_i$	$\hat{p}^0_{i'}$	1	$\hat{p}^{2i-a}_j$	$p^{2i'-a}_{j'-1}$	1	$p^{-b+2(i+j)}_{k-1}$	$\hat{p}^{-b+2(i'+j')}_{k'}$
$\hat{\mathcal{I}}^{(12)}$	$\hat{p}^0_i$	$\hat{p}^0_{i'}$	1	p^{2i-a}_{j-2}	$p^{2i'-a}_{j'-2}$	0	$\hat{p}^{-b+2(i+j)}_k$	$\hat{p}^{-b+2(i'+j')}_{k'}$
$\hat{\mathcal{I}}^{(13)}$	$\hat{p}^0_i$	$\hat{p}^0_{i'}$	1	p^{2i-a}_{j-1}	$p^{2i'-a}_{j'-2}$	0	$\hat{p}^{-b+2(i+j)}_k$	$\hat{p}^{-b+2(i'+j')}_{k'}$
$\hat{\mathcal{I}}^{(14)}$	$\hat{p}^0_i$	$\hat{p}^0_{i'}$	1	p^{2i-a}_{j-2}	$p^{2i'-a}_{j'-1}$	0	$\hat{p}^{-b+2(i+j)}_k$	$\hat{p}^{-b+2(i'+j')}_{k'}$
$\hat{\mathcal{I}}^{(15)}$	$\hat{p}^0_i$	$\hat{p}^0_{i'}$	1	p^{2i-a}_{j-1}	$p^{2i'-a}_{j'-1}$	0	$\hat{p}^{-b+2(i+j)}_k$	$\hat{p}^{-b+2(i'+j')}_{k'}$
$\hat{\mathcal{I}}^{(16)}$	p^0_{i-2}	$\hat{p}^0_{i'}$	0	$\hat{p}^{2i-a}_j$	$p^{2i'-a}_{j'-2}$	0	$\hat{p}^{-b+2(i+j)}_k$	$\hat{p}^{-b+2(i'+j')}_{k'}$
$\hat{\mathcal{I}}^{(17)}$	p^0_{i-2}	$\hat{p}^0_{i'}$	0	$\hat{p}^{2i-a}_j$	$p^{2i'-a}_{j'-1}$	0	$\hat{p}^{-b+2(i+j)}_k$	$\hat{p}^{-b+2(i'+j')}_{k'}$
$\hat{\mathcal{I}}^{(18)}$	$\hat{p}^0_i$	$p^0_{i'-2}$	0	$\hat{p}^{2i-a}_j$	$\hat{p}^{2i'-a}_{j'}$	1	$p^{-b+2i+2j}_{k-1}$	$\hat{p}^{-b+2(i'+j')}_{k'}$
$\hat{\mathcal{I}}^{(19)}$	$\hat{p}^0_i$	$p^0_{i'-2}$	0	p^{2i-a}_{j-2}	$\hat{p}^{2i'-a}_{j'}$	0	$\hat{p}^{-b+2(i+j)}_k$	$\hat{p}^{-b+2(i'+j')}_{k'}$
$\hat{\mathcal{I}}^{(20)}$	$\hat{p}^0_i$	$p^0_{i'-2}$	0	p^{2i-a}_{j-1}	$\hat{p}^{2i'-a}_{j'}$	0	$\hat{p}^{-b+2(i+j)}_k$	$\hat{p}^{-b+2(i'+j')}_{k'}$
$\hat{\mathcal{I}}^{(21)}$	p^0_{i-2}	$p^0_{i'-2}$	-1	$\hat{p}^{2i-a}_j$	$\hat{p}^{2i'-a}_{j'}$	0	$\hat{p}^{-b+2(i+j)}_k$	$\hat{p}^{-b+2(i'+j')}_{k'}$

Table 1: Integrands for $\hat{K}_{I,I}$, where $\beta = i + j$, $(i' + j') = i' + j'$

1. FOR i=1 to 2 DO

2. IF (q_{n_i} is integrated Jacobi polynomial) THEN
   Transform integrated Jacobi polynomials to Jacobi polynomials using relations (12), (14) or (17) depending on the relation between the polynomial parameter α and the weight parameter γ,

   (a) $(1-\zeta)^\gamma \hat{p}_n^\alpha(\zeta),\ \gamma-\alpha \geq 0$: transform integrated Jacobi polynomials to Jacobi polynomials with same parameter α using (12).

   (b) $(1-\zeta)^\gamma \hat{p}_n^\alpha(\zeta),\ \alpha = \gamma+1$: transform $\hat{p}_n^\alpha(\zeta)$ to Jacobi polynomials with parameter $\alpha - 1$ using relation (14).

   (c) $(1-\zeta)^\gamma \hat{p}_n^\alpha(\zeta),\ \alpha = \gamma+2$: Use the mixed relation (17) to obtain

$$\hat{p}_n^{\gamma+2}(\zeta) = \frac{1}{\gamma+1}\left(2p_n^\gamma(\zeta) + (1-\zeta)p_{n-1}^{\gamma+2}(\zeta)\right).$$

- ENDIF

3. Rewrite the Jacobi polynomials $p_n^\alpha(\zeta)$ in terms of Jacobi polynomials fitting to the appearing weights $(1-\zeta)^\gamma$ $(\gamma - \alpha > 0)$ by lifting the polynomial parameter α using (7) $(\gamma-\alpha)$-times, i.e.

$$\begin{aligned} p_n^\alpha(\zeta) &= \sum_{m=0}^{\gamma-\alpha}(-1)^k \binom{\gamma-\alpha}{m} \frac{(n+\gamma-m)^{\underline{\gamma-\alpha-m}}\, n^{\underline{m}}}{(2n+\gamma-m+1)^{\underline{\gamma-\alpha+1}}} \\ &\quad \times (2n-2m+\gamma+1)p_{n-m}^\gamma(\zeta), \end{aligned}$$

   where $a^{\underline{k}} = a(a-1)\cdot\ldots\cdot(a-k+1)$ denotes the falling factorial.

- ENDFOR

4. Evaluate the integrals using the orthogonality relation (9).

The algorithm interrupts, if $\alpha > \gamma+2$ in step 2 or $\alpha > \gamma$ in step 3. The output of the program are the rational functions to which the original integrals evaluate. Thereby also the maximal bandwidth for each of these integrals is returned.

Our Mathematica program is executed with the integrand $\hat{\mathcal{I}}^{(l)}(r,s,z)$ as input and applies the above algorithm to all possible integrals. Evaluating the x-integrals gives a bounded number of candidates b_x with $i - i' = b_x$, in which at least one integral can be nonzero. Then, for all candidates b_x, the algorithm is applied to evaluate the y-integrals. This gives a bounded number of candidates b_y with $j - j' = b_y$, in which at least one integral can be nonzero. Finally, the algorithm is applied to the z-integrals for all candidates b_x and b_y. Again, the algorithm gives a bounded number of candidates b_z with $k - k' = b_z$, in which at least one integral can be nonzero. We point out that for the integrand $\hat{\mathcal{I}}^{(l)}(r,s,z)$ the algorithm never interrupts, i.e. never runs into the cases $\alpha > \gamma + 2$ in step 2 or $\alpha > \gamma$ in step 3. This is due to our assumption $b \geq a \geq 0$.

For $a = 1$ and $b = 2$ the output of the program is summarized in Table 2. Since $|i-i'| \in \{0,2\}$, $|i+j-i'-j'| \leq 4$ and $|i+j+k-i'-j'-k'| \leq 4$ for each of the integrands $\hat{\mathcal{I}}^{(l)}$, $l = 1,\dots,21$, the maximal number of nonzero entries per row is bounded by $3 \cdot 9 \cdot 9 = 243$. This proves the sparsity for $a = 1$ and $b = 2$.

For the remaining 24 cases satisfying $0 \leq a \leq b \leq 6$, $a \leq 4$, each of the terms $|i-i'|$, $|i+j-i'-j'|$ and $|i+j+k-i'-j'-k'|$ is bounded by a constant, which depends on a and b, too.

In the appendix A, we present an example how the algorithm proceeds for $a = 1, b = 2$ and the integrand $\hat{\mathcal{I}}^{(7)}$.

We close this proof by stating the nonzero pattern of the blocks containing the mixed terms $\frac{\partial}{\partial \zeta}\phi_{i,j,k}\frac{\partial}{\partial \eta}\phi_{i',j',k'}$, $(\zeta,\eta) \in \{(x,y),(x,z),(y,z)\}$.

	$i-i'$	$i-i'+j-j'$	$i-i'+j-j'+k-k'$
$\hat{\mathcal{I}}^{(1)}$	$\{0\}$	$\{-2,\dots,2\}$	$\{-4,\dots,4\}$
$\hat{\mathcal{I}}^{(2)}$	$\{-2,0,2\}$	$\{-2,\dots,2\}$	$\{-4,\dots,4\}$
$\hat{\mathcal{I}}^{(3)}$	$\{0,2\}$	$\{-2,\dots,2\}$	$\{-4,\dots,4\}$
$\hat{\mathcal{I}}^{(4)}$	$\{-2,0\}$	$\{-2,\dots,2\}$	$\{-4,\dots,4\}$
$\hat{\mathcal{I}}^{(5)}$	$\{0\}$	$\{-2,\dots,2\}$	$\{-4,\dots,4\}$
$\hat{\mathcal{I}}^{(6)}$	$\{-2,0,2\}$	$\{-4,\dots,4\}$	$\{-4,\dots,4\}$
$\hat{\mathcal{I}}^{(7)}$	$\{-2,0,2\}$	$\{-2,\dots,4\}$	$\{-4,\dots,4\}$
$\hat{\mathcal{I}}^{(8)}$	$\{-2,0,2\}$	$\{-3,\dots,3\}$	$\{-4,\dots,4\}$
$\hat{\mathcal{I}}^{(9)}$	$\{0,2\}$	$\{-3,\dots,3\}$	$\{-4,\dots,4\}$
$\hat{\mathcal{I}}^{(10)}$	$\{-2,0,2\}$	$\{-4,\dots,2\}$	$\{-4,\dots,4\}$
$\hat{\mathcal{I}}^{(11)}$	$\{-2,0,2\}$	$\{-3,\dots,3\}$	$\{-4,\dots,4\}$
$\hat{\mathcal{I}}^{(12)}$	$\{-2,0,2\}$	$\{-2,\dots,2\}$	$\{-4,\dots,4\}$
$\hat{\mathcal{I}}^{(13)}$	$\{-2,0,2\}$	$\{-3,\dots,1\}$	$\{-4,\dots,4\}$
$\hat{\mathcal{I}}^{(14)}$	$\{-2,0,2\}$	$\{-1,\dots,3\}$	$\{-4,\dots,4\}$
$\hat{\mathcal{I}}^{(15)}$	$\{-2,0,2\}$	$\{-2,\dots,2\}$	$\{-4,\dots,4\}$
$\hat{\mathcal{I}}^{(16)}$	$\{0,2\}$	$\{-3,\dots,1\}$	$\{-4,\dots,4\}$
$\hat{\mathcal{I}}^{(17)}$	$\{0,2\}$	$\{-2,\dots,2\}$	$\{-4,\dots,4\}$
$\hat{\mathcal{I}}^{(18)}$	$\{-2,0\}$	$\{-3,\dots,3\}$	$\{-4,\dots,4\}$
$\hat{\mathcal{I}}^{(19)}$	$\{-2,0\}$	$\{-1,\dots,3\}$	$\{-4,\dots,4\}$
$\hat{\mathcal{I}}^{(20)}$	$\{-2,0\}$	$\{-2,\dots,2\}$	$\{-4,\dots,4\}$
$\hat{\mathcal{I}}^{(21)}$	$\{0\}$	$\{-2,\dots,2\}$	$\{-4,\dots,4\}$

Table 2: Nonzero pattern for integrals $\hat{\mathcal{I}}^{(1)},\dots,\hat{\mathcal{I}}^{(21)},\ a=1,\ b=2$.

We compute the partial derivatives again using the result of Lemma 6.2 and perform the Duffy transformation $r = \frac{x(1-y)(1-z)}{4}$ and $s = \frac{y(1-z)}{2}$ to obtain the integrals,

$$\int_{\hat{\triangle}} \frac{\partial}{\partial x}\phi_{i,j,k}\frac{\partial}{\partial y}\phi_{i',j',k'} \;\mathrm{d}(x,y,z) := \sum_{l=22}^{23}\int_{-1}^{1}\int_{-1}^{1}\int_{-1}^{1}\hat{\mathcal{I}}^{(l)}(r,s,z)\;\mathrm{d}r\;\mathrm{d}s\;\mathrm{d}z$$

$$\int_{\hat{\triangle}} \frac{\partial}{\partial x}\phi_{i,j,k}\frac{\partial}{\partial z}\phi_{i',j',k'} \;\mathrm{d}(x,y,z) := \sum_{l=24}^{27}\int_{-1}^{1}\int_{-1}^{1}\int_{-1}^{1}\hat{\mathcal{I}}^{(l)}(r,s,z)\;\mathrm{d}r\;\mathrm{d}s\;\mathrm{d}z$$

$$\int_{\hat{\triangle}} \frac{\partial}{\partial y}\phi_{i,j,k}\frac{\partial}{\partial z}\phi_{i',j',k'} \;\mathrm{d}(x,y,z) := \sum_{l=28}^{35}\int_{-1}^{1}\int_{-1}^{1}\int_{-1}^{1}\hat{\mathcal{I}}^{(l)}(r,s,z)\;\mathrm{d}r\;\mathrm{d}s\;\mathrm{d}z$$

with the integrands

$$\begin{aligned}\hat{\mathcal{I}}^{(l)}(r,s,z) \;&=\; c_l p_{x,1}(r)p_{x,2}(r)\left(\frac{1-s}{2}\right)^{\gamma_y+i+i'} p_{y,1}(s)p_{y,2}(s)\\ &\quad\times\left(\frac{1-z}{2}\right)^{\gamma_z+i+i'+j+j'} p_{z,1}(z)p_{z,2}(z).\end{aligned}$$

The correct structure of the integrands is listed in Table 3. Applying our

	$p_{x,1}$	$p_{x,2}$	γ_y	$p_{y,1}$	$p_{y,2}$	γ_z	$p_{z,1}$	$p_{z,2}$
$\hat{\mathcal{I}}^{(22)}$	p^0_{i-1}	$p^0_{i'-2}$	-1	$\hat{p}^{2i-a}_j$	$\hat{p}^{2i'-a}_{j'}$	0	$\hat{p}^{-b+2(i+j)}_k$	$\hat{p}^{-b+2(i'+j')}_{k'}$
$\hat{\mathcal{I}}^{(23)}$	p^0_{i-1}	$\hat{p}^0_{i'}$	0	$\hat{p}^{2i-a}_j$	$p^{2i'-a}_{j'-1}$	0	$\hat{p}^{-b+2(i+j)}_k$	$\hat{p}^{-b+2(i'+j')}_{k'}$
$\hat{\mathcal{I}}^{(24)}$	p^0_{i-1}	$\hat{p}^0_{i'}$	0	$\hat{p}^{2i-a}_j$	$\hat{p}^{2i'-a}_{j'}$	1	$\hat{p}^{-b+2(i+j)}_k$	$p^{-b+2(i'+j')}_{k'-1}$
$\hat{\mathcal{I}}^{(25)}$	p^0_{i-1}	$\hat{p}^0_{i'}$	0	$\hat{p}^{2i-a}_j$	$p^{2i'-a}_{j'-2}$	0	$\hat{p}^{-b+2(i+j)}_k$	$\hat{p}^{-b+2(i'+j')}_{k'}$
$\hat{\mathcal{I}}^{(26)}$	p^0_{i-1}	$\hat{p}^0_{i'}$	0	$\hat{p}^{2i-a}_j$	$p^{2i'-a}_{j'-1}$	0	$\hat{p}^{-b+2(i+j)}_k$	$\hat{p}^{-b+2(i'+j')}_{k'}$
$\hat{\mathcal{I}}^{(27)}$	p^0_{i-1}	$p^0_{i'-2}$	-1	$\hat{p}^{2i-a}_j$	$\hat{p}^{2i'-a}_{j'}$	0	$\hat{p}^{-b+2(i+j)}_k$	$\hat{p}^{-b+2(i'+j')}_{k'}$
$\hat{\mathcal{I}}^{(28)}$	$\hat{p}^0_i$	$\hat{p}^0_{i'}$	1	p^{2i-a}_{j-1}	$\hat{p}^{2i'-a}_{j'}$	1	$\hat{p}^{-b+2(i+j)}_k$	$p^{-b+2(i'+j')}_{k'-1}$
$\hat{\mathcal{I}}^{(29)}$	p^0_{i-2}	$\hat{p}^0_{i'}$	0	$\hat{p}^{2i-a}_j$	$\hat{p}^{2i'-a}_{j'}$	1	$\hat{p}^{-b+2(i+j)}_k$	$p^{-b+2(i'+j')}_{k'-1}$
$\hat{\mathcal{I}}^{(30)}$	$\hat{p}^0_i$	$\hat{p}^0_{i'}$	1	p^{2i-a}_{j-1}	$p^{2i'-a}_{j'-2}$	0	$\hat{p}^{-b+2(i+j)}_k$	$\hat{p}^{-b+2(i'+j')}_{k'}$
$\hat{\mathcal{I}}^{(31)}$	$\hat{p}^0_i$	$\hat{p}^0_{i'}$	1	p^{2i-a}_{j-1}	$p^{2i'-a}_{j'-1}$	0	$\hat{p}^{-b+2(i+j)}_k$	$\hat{p}^{-b+2(i'+j')}_{k'}$
$\hat{\mathcal{I}}^{(32)}$	p^0_{i-2}	$\hat{p}^0_{i'}$	0	$\hat{p}^{2i-a}_j$	$p^{2i'-a}_{j'-2}$	0	$\hat{p}^{-b+2(i+j)}_k$	$\hat{p}^{-b+2(i'+j')}_{k'}$
$\hat{\mathcal{I}}^{(33)}$	p^0_{i-2}	$\hat{p}^0_{i'}$	0	$\hat{p}^{2i-a}_j$	$p^{2i'-a}_{j'-1}$	0	$\hat{p}^{-b+2(i+j)}_k$	$\hat{p}^{-b+2(i'+j')}_{k'}$
$\hat{\mathcal{I}}^{(34)}$	$\hat{p}^0_i$	$p^0_{i'-2}$	0	p^{2i-a}_{j-1}	$\hat{p}^{2i'-a}_{j'}$	0	$\hat{p}^{-b+2(i+j)}_k$	$\hat{p}^{-b+2(i'+j')}_{k'}$
$\hat{\mathcal{I}}^{(35)}$	p^0_{i-2}	$p^0_{i'-2}$	-1	$\hat{p}^{2i-a}_j$	$\hat{p}^{2i'-a}_{j'}$	0	$\hat{p}^{-b+2(i+j)}_k$	$\hat{p}^{-b+2(i'+j')}_{k'}$

Table 3: Integrands for the mixed terms $\frac{\partial}{\partial\zeta}\phi_{i,j,k}\frac{\partial}{\partial\eta}\phi_{i',j',k'}$,.

program to evaluate these integrals we obtain the following results,

- $$\int_{\hat{\triangle}} \frac{\partial}{\partial x}\phi_{i,j,k}\frac{\partial}{\partial y}\phi_{i',j',k'}\ \mathrm{d}(x,y,z) \neq 0$$

  if $|i-i'|=1$, $|i-i'+j-j'|\le 1+a$ and $|i-i'+j-j'+k-k'|\le 2+b$.

- $$\int_{\hat{\triangle}} \frac{\partial}{\partial x}\phi_{i,j,k}\frac{\partial}{\partial z}\phi_{i',j',k'}\ \mathrm{d}(x,y,z) \neq 0$$

  if $|i-i'|=1$, $\quad |i-i'+j-j'|\le 2+a$ and $|i-i'+j-j'+k-k'|\le 2+b$.

- $$\int_{\hat{\triangle}} \frac{\partial}{\partial y}\phi_{i,j,k}\frac{\partial}{\partial z}\phi_{i',j',k'}\ \mathrm{d}(x,y,z) \neq 0$$

  if $|i-i'|\in\{0,2\}$, $\quad |i-i'+j-j'|\le 2+a$ and $|i-i'+j-j'+k-k'|\le 2+b$.

This completes the proof of Theorem 3.3. □

We close this section with the following three technical remarks on the proof of Theorem 3.3.

Remark 6.3. *The proof shows that this result can easily be extended to the case of a convection reaction diffusion equation of the form*

$$-\nabla\cdot\mathcal{A}\nabla u+\vec{b}\cdot\nabla u+cu=f$$

with piecewise constant coefficients $\vec{b}$ and c. This result is a direct consequence of the representation

$$\phi_{ijk}(x,y,z)=\sum_{m=k-2}^{k}\kappa_m\hat{p}_i^0\left(\frac{x}{r}\right)\ r^i\ \hat{p}_j^{2i-a}\left(\frac{y}{s}\right)\ s^{j-1}\ p_m^{2i+2j-b}(z)$$

with the abbreviations $r=\dfrac{1-2y-z}{4}$ and $s=\dfrac{1-z}{2}$ and some real numbers κ_m, cf. (12). *This structure is similar to the last summand of $\frac{\partial\phi_{ijk}}{\partial z}(x,y,z)$ in* (44). *With the same arguments as in the proof of Theorem 3.3, the sparsity for the parts of the stiffness matrix corresponding to the integrals $\int_{-1}^{1}\int_{1}^{1}\int_{-1}^{1}\hat{\mathcal{I}}^{(l)}(r,s,z)$, $l=6,7,8,9,10,11,18$, can be shown. This proves the remark.*

Remark 6.4. *In step 3 of this algorithm polynomials down to degree $n-\gamma+\alpha$ are introduced. Hence, this transformation is a costly one as it increases the number of terms significantly, especially if a,b are far from the ideal case $a=b=0$.*

Remark 6.5. *Case (c) in step 2 only occurs if we choose $a=0$ or $a=b$. One example is the y-integration of $\hat{\mathcal{I}}^{(17)}$ for $i'=i-2$. A direct evaluation of the integrand $\hat{\mathcal{I}}^{(17)}$ yields to a dense matrix. However, the y-integration of $\hat{\mathcal{I}}^{(14)}+\hat{\mathcal{I}}^{(15)}+\hat{\mathcal{I}}^{(17)}$ is sparse. Here, the relation* (18) *has to be used. More details on how to handle these exceptions can be found in [10].*

7 Remarks to the efficient implementation

In this section, we present some details concerning the implementation of the basis functions. The implementation of the basis functions within a finite element program requires two steps

- the assembling of the stiffness matrix,
- the evaluation of function values in a postprocessing step.

The evaluation of the function values can be performed with the aid of the recursion formulas (12), (8) and (13). The assembling of the stiffness matrix using our basis functions can be computed in $\mathcal{O}(1)$ flops per nonzero matrix entry by explicit formulas. However, the formulas are quite long. A more efficient way is to use a sum factorization technique. The remaining one-dimensional integrals are computed recursively via (7) and (13) using the product recurrence given in [26].

The algorithm consists of two steps

- the recursive computation of all required one-dimensional integrals of the form
$$M = [m_{n1,n2}]_{n1,n2} = \left[\int_{-1}^{1} (1-\zeta)^\gamma q_{n_1}(\zeta) Q_{n_2}(\zeta)\,\mathrm{d}\zeta\right]_{n1,n2}, \tag{48}$$
where $q_{n_1}(\zeta)$ and $Q_{n_2}(\zeta)$ can be either Jacobi or integrated Jacobi polynomials of degree n_1 and n_2 respectively, and γ is the appearing weight.
- the computation of the element stiffness matrices using sum factorization.

The computation of the matrix entries $m_{n1,n2}$ uses an idea which has been presented in [26]. The product $q_{n_1}(\zeta)Q_{n_2}(\zeta)$ is transformed with the aid of the recursion formulas (8) and (13), i.e.

$$\begin{aligned}
q_{n_1}(\zeta)Q_{n_2}(\zeta) &= (\eta_1\zeta q_{n_1-1}(\zeta) + \eta_2 q_{n_1-1}(\zeta) + \eta_3 q_{n_1-2}(\zeta))\, Q_{n_2}(\zeta)\\
&= \eta_2 m_{n_1-1,n2} + \eta_3 m_{n_1-2,n2} + \eta_1 q_{n_1-1}(\zeta)\zeta Q_{n_2}(\zeta)\\
&= \eta_2 m_{n_1-1,n2} + \eta_3 m_{n_1-2,n2}\\
&\quad +\eta_1 q_{n_1-1}(\zeta)\,(\eta_4 Q_{n_2+1}(\zeta) + \eta_5 Q_{n_2 1}(\zeta) + \eta_6 Q_{n_2-1}(\zeta))\\
&= (\eta_1\eta_5 + \eta_2) m_{n_1-1,n2} + \eta_3 m_{n_1-2,n2}\\
&\quad +\eta_1\eta_4 m_{n_1-1,n2+1} + \eta_1\eta_6 m_{n_1-1,n2-1},
\end{aligned} \tag{49}$$

where η_i, $i = 1,\ldots,6$ are some coefficients depending on n_1, n_2, and the polynomials q and Q. Now, the computation of (48) can be done as follows.

1. Determine the band structure of M using (12), (17), (14), (7) and (9), cf. the Algorithm or the orthogonality relations (16) and (10). Let $m_{n1,n2} = 0$ if $n_1 - n_2 > b_1$ and $n_1 - n_2 < -b_2$.
2. Set $m_{n1,n2} = 0$ for all $0 \le n_1, n_2 \le p$.
3. Compute $m_{n1,n2}$ for $n_1 \in \{0, 1\}$ and $n_2 \le b_2 + 1$ by an explicit formula or numerical integration.
4. `FOR` $n_1 = 2, \dots, p_{max}$ do
   - `FOR` $n_2 = \max\{n_1 - b_1, 1\}, \min\{n_1 + b_2, p_{max}\}$ do
   - Compute $m_{n1,n2}$ via (49)
   - `ENDFOR`

   `ENDFOR`

Now, we are able to compute the element stiffness matrix. In a first step, the element stiffness matrix is transformed into the form (46). Next, for each of the integrands $\hat{\mathcal{I}}^{(l)}(r, s, z)$, $l = 1, \dots, 21$, we compute the element stiffness matrix by the one dimensional integrals for all required combinations of $\{i, i'\}$ and $\{j, j'\}$ due to table 2.

As an example, we explain this sum factorization algorithm for the integrand $\hat{\mathcal{I}}^{(1)}(r, s, z)$ for $a = 1$ and $b = 2$, i.e.

$$\begin{aligned}\hat{\mathcal{I}}^{(1)}(r, s, z) &= p^0_{i-1}(r) p^0_{i'-1}(r)\,(1 - s)^{i+i'-1} \hat{p}^{2i-1}_j(s) \hat{p}^{2i'-1}_{j'}(s) \\ &\quad (1 - z)^{i+i'+j+j'} \hat{p}^{2i+2j-2}_k(z) \hat{p}^{2i'+2j'-2}_{k'}(z).\end{aligned}$$

- `FOR` $i = 2, \dots, p - 2$ do
  - Set $i' = i$
  - Set $h_1 = \int_{-1}^{1} p^0_{i-1}(r) p^0_{i'-1}(r)\, \mathrm{d}r$
  - `FOR` $j = 1, \dots, p - i$ do
    - `FOR` $j' = \max\{j - 2, 1\}, \dots, \min\{p - i', j + 2\}$ do
      - Set $h_2 = \int_{-1}^{1} (1 - s)^{i+i'-1} \hat{p}^{2i-1}_j(s) \hat{p}^{2i'-1}_{j'}(s)\, \mathrm{d}s$
      - `FOR` $k = 1, \dots, p - i$ do
        1. `FOR` $k' = \max\{k - 4, 1\}, \dots, \min\{p - i' - j', k + 4\}$ do
        2. Set $h_3 = \int_{-1}^{1} (1 - z)^{i+i'+j+j'} \hat{p}^{2i+2j-2}_k(z) \hat{p}^{2i'+2j'-2}_{k'}(z)\, \mathrm{d}z$
        3. Set $a_{ijk,i'j'k',I1} = h_1 h_2 h_3$
        4. `ENDFOR`
      - `ENDFOR`
    - `ENDFOR`
  - `ENDFOR`

- ENDFOR

The remaining integrands $\hat{\mathcal{I}}^{(l)}(r,s,z)$, $l=2,\dots,21$ can be performed in the same way with the aid of tables 2 and 1.

8 Concluding Remarks

In this paper, we have proposed several bases for high order FEM on tetrahedral finite element meshes. We have proved that the element stiffness matrix with respect to these bases has $\mathcal{O}(p^3)$ nonzero entries.

The sparsity of the element stiffness matrix has two direct applications,

(a) preconditioning the block of the interior bubbles,

(b) the evaluation of the element stiffness matrix in $\mathcal{O}(p^3)$ operations.

For (b), one can combine the ideas for the recursive evaluation of a matrix $\mathcal{B}$, which have been presented in [26], with the sparsity and the band structure of $\mathcal{B}$. This computes $\mathcal{B}$ in $5(2b+1)(p+1)$ flops where b is the bandwidth of $\mathcal{B}$ and the element stiffness matrix in $\mathcal{O}(p^3)$ flops. As presented in [13], the result can be extended to convection-reaction-diffusion problems with piecewise constant coefficients, or piecewise polynomial coefficients. It is not possible to generalize this construction to problems with arbitrary variable coefficients. However, many practical linear problems, as e.g. problems with different materials in linear elasticity, have piecewise constant coefficients and require high-order finite elements for the discretization in the interior of the domain. Here, one can use affine linear elements in the interior of the domain. Now, one can take one of the proposed bases.

The sparsity has reduced the cost for the computation of the block of interior bubbles from $\mathcal{O}(p^9)$ to $\mathcal{O}(p^6)$. A further reduction to $\mathcal{O}(p^s)$ with $3\le s\le 5$ as presented in [12] for hexahedrons is still a challenging problem. The application (a) works also for an uniformly elliptic second order boundary value problem with arbitrary coefficients.

A Evaluation of the integrand $\hat{\mathcal{I}}^{(7)}$

Now we execute our algorithm on the integrand

$$\hat{\mathcal{I}}^{(7)}(x,y,z) = \frac{(j-1)}{2i+2j-3}\hat{p}_i^0(x)\hat{p}_{i'}^0(x)\left(\frac{1-y}{2}\right)^{i+i'+1} p_{j-2}^{2i-1}(y)\hat{p}_{j'}^{2i'-1}(y) \times\left(\frac{1-z}{2}\right)^{i+j+i'+j'+1}\hat{p}_k^{2i+2j-2}(z)p_{k'-1}^{2i'+2j'-2}(z),$$

that is we want to compute

$$\hat{K}^{(7)} = \int_{-1}^{1}\int_{-1}^{1}\int_{-1}^{1}\hat{\mathcal{I}}^{(7)}(x,y,z)\,\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z$$

for $a = 1$ and $b = 2$. First we evaluate the x-integral, where we only have one integrand at first and start by transforming integrated Jacobi to classical Jacobi polynomials. For the x-integrals we always have $\alpha = \gamma = 0$, i.e. we are in case 2(a) and use (12). Observe that for $\alpha = 0$, $\hat{p}_n^0$ can be expressed using only p_n^0 and p_{n-2}^0. Hence we obtain for the first integral,

$$\int_{-1}^{1} \hat{p}_i^0(x)\hat{p}_{i'}^0(x)\,\mathrm{d}x = \frac{\int_{-1}^{1}(p_{i-2}^0 p_{i'-2}^0 - p_i^0 p_{i'-2}^0 - p_{i-2}^0 p_{i'}^0 + p_i^0 p_{i'}^0)(x)\,\mathrm{d}x}{(2i-1)(2i'-1)}$$

These four integrals are easily evaluated by the orthogonality relation (9) and we obtain

$$\begin{aligned}\int_{-1}^{1} \hat{p}_i^0(x)\hat{p}_{i'}^0(x)\,\mathrm{d}x &= \frac{4\delta_{i,i'}}{(2i-3)(2i-1)(2i+1)} - \frac{2\delta_{i,i'-2}}{(2i-1)(2i+1)(2i+3)} \\ &\quad - \frac{2\delta_{i,i'+2}}{(2i-5)(2i-3)(2i-1)},\end{aligned}$$

see e.g. [18]. So the first integral is nonzero iff $|i - i'| \in \{0, 2\}$. Now we plug in the above result into $\hat{K}^{(7)}$ to obtain the following three integrals,

$$\begin{aligned}\hat{K}^{(7)} = &- \frac{2(j-1)\delta_{i,i'+2}}{(2i-5)(2i-3)(2i-1)(2i+2j-3)} \\ &\times \int_{-1}^{1} \left(\frac{1-y}{2}\right)^{2i-1} p_{j-2}^{2i-1}(y)\hat{p}_{j'}^{2i-5}(y)\,\mathrm{d}y \\ &\times \int_{-1}^{1} \left(\frac{1-z}{2}\right)^{2i+j+j'-1} \hat{p}_k^{2i+2j-2}(z) p_{k'-1}^{2i+2j'-6}(z)\,\mathrm{d}z \\ &+ \frac{4(j-1)\delta_{i,i'}}{(2i-3)(2i-1)(2i+1)(2i+2j-3)} \\ &\times \int_{-1}^{1} \left(\frac{1-y}{2}\right)^{2i+1} p_{j-2}^{2i-1}(y)\hat{p}_{j'}^{2i-1}(y)\,\mathrm{d}y \\ &\times \int_{-1}^{1} \left(\frac{1-z}{2}\right)^{2i+j+j'+1} \hat{p}_k^{2i+2j-2}(z) p_{k'-1}^{2i+2j'-2}(z)\,\mathrm{d}z \\ &- \frac{2(j-1)\delta_{i,i'-2}}{(2i-1)(2i+1)(2i+3)(2i+2j-3)} \\ &\times \int_{-1}^{1} \left(\frac{1-y}{2}\right)^{2i+3} p_{j-2}^{2i-1}(y)\hat{p}_{j'}^{2i+3}(y)\,\mathrm{d}y \\ &\times \int_{-1}^{1} \left(\frac{1-z}{2}\right)^{2i+j+j'+3} \hat{p}_k^{2i+2j-2}(z) p_{k'-1}^{2i+2j'+2}(z)\,\mathrm{d}z\end{aligned}$$

After singling out the y-dependent parts of $\hat{K}^{(7)}$ we see that the first integrand is already a Jacobi polynomial for all three integrals. Moreover, the combination of weight parameter γ and polynomial parameter α is

$(2i-1, 2i-1)$. So, we can omit step 2 for the first polynomial. The second polynomial is an integrated Jacobi polynomial. Hence, we enter step 2 of the algorithm and transform the integrated Jacobi into a classical Jacobi polynomials. The combinations of weight parameter γ and polynomial parameter α occuring are $(\gamma, \alpha) = (2i-1, 2i-5), (2i-1, 2i+1), (2i-1, 2i+3)$. For each of these pairs we have $\gamma - \alpha \geq 0$, i.e. we are in case 2(a) again. Using relation (12) we obtain e.g. for the first y-integrand of $\hat{K}^{(7)}$,

$$\begin{aligned}
&\left(\frac{1-y}{2}\right)^{2i-1} p_{j-2}^{2i-1}(y)\hat{p}_{j'}^{2i-5}(y) = \\
&-\frac{(j'-1)}{(i+j'-3)(2i+2j'-7)}\left(\frac{1-y}{2}\right)^{2i-1} p_{j-2}^{2i-1}(y)p_{j'-2}^{2i-5}(y) \\
&+\frac{2(2i-5)}{(2i+2j'-7)(2i+2j'-5)}\left(\frac{1-y}{2}\right)^{2i-1} p_{j-2}^{2i-1}(y)p_{j'-1}^{2i-5}(y) \\
&+\frac{(2i+j'-5)}{(i+j'-3)(2i+2j'-5)}\left(\frac{1-y}{2}\right)^{2i-1} p_{j-2}^{2i-1}(y)p_{j'}^{2i-5}(y).
\end{aligned}$$

Next we have to adjust the Jacobi polynomials to the weight functions under the integral to be able to exploit their orthogonality, i.e. execute step 3 of the algorithm. After applying (7) four times to $p_{j'-2}^{2i-5}(y), p_{j'-1}^{2i-5}(y)$ and $p_{j'}^{2i-5}(y)$ yields for the above integrand,

$$\begin{aligned}
p_{j-2}^{2i-1}(y)\hat{p}_{j'}^{2i-5}(y) \;=\; & \eta_1 p_{j-2}^{2i-1}(y)p_{j'}^{2i-1}(y) + \eta_2 p_{j-2}^{2i-1}(y)p_{j'-1}^{2i-1}(y) \\
&+\eta_3 p_{j-2}^{2i-1}(y)p_{j'-2}^{2i-1}(y) + \eta_4 p_{j-2}^{2i-1}(y)p_{j'-3}^{2i-1}(y) \\
&+\eta_5 p_{j-2}^{2i-1}(y)p_{j'-4}^{2i-1}(y) + \eta_6 p_{j-2}^{2i-1}(y)p_{j'-5}^{2i-1}(y) \\
&+\eta_7 p_{j-2}^{2i-1}(y)p_{j'-6}^{2i-1}(y)
\end{aligned} \tag{50}$$

with coefficients η_s, $s = 1, \ldots, 7$, which are broken rational functions in i, j, i' and j'. The exact structure can be found in [11].

After executing steps 2 and 3 on all y-integrands of $\hat{K}^{(7)}$ one has to evaluate resulting integrals using orthogonality relation (9). We will now only consider how to proceed with the first summand in the integrand (50), omitting the constants, i.e. the following part of $\hat{K}^{(7)}$,

$$\begin{aligned}
\hat{K}_{\mathrm{pa}}^{(7)} = &\int_{-1}^{1}\left(\frac{1-y}{2}\right)^{2i-1} p_{j-2}^{2i-1}(y)p_{j'}^{2i-1}(y)\,\mathrm{d}y \\
&\times \int_{-1}^{1}\left(\frac{1-z}{2}\right)^{2i+j+j'-1} \hat{p}_{k}^{2i+2j-2}(z)p_{k'-1}^{2i+2j'-6}(z)\,\mathrm{d}z \\
=&\frac{\delta_{j,j'+2}}{i+j-2}\int_{-1}^{1}\left(\frac{1-z}{2}\right)^{2i+2j-3} \hat{p}_{k}^{2i+2j-2}(z)p_{k'-1}^{2i+2j-10}(z)\,\mathrm{d}z.
\end{aligned}$$

In this case the weight parameter $\gamma = 2i+2j-3$ and the polynomial parameter $\alpha = 2i+2j-2$ differ by one. Following step 2(b) of the algorithm we rewrite the integrated Jacobi polynomial $\hat{p}_k^{2i+2j-2}(z)$ using (14),

$$\hat{p}_k^{2i+2j-2}(z) = \frac{2}{2i+2j+2k-3}(p_k^{2i+2j-3}(z) + p_{k-1}^{2i+2j-3}(z)).$$

These polynomials already correspond to the weight function $\left(\frac{1-z}{2}\right)^{2i+2j-3}$, what remains to be done is to apply relation (7) seven times to $p_{k'-1}^{2i+2j-10}(z)$. So finally we have to evaluate $8 \times 2 = 16$ integrals with the orthogonality relation (9) to obtain $\hat{K}_{\mathrm{pa}}^{(7)}$. The default output for the computation of $\hat{K}^{(7)}$ of our Mathematica program is displayed in [11, Figure 6].

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