Fast summation techniques for sparse shape functions in tetrahedral *hp*-FEM

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This paper considers the *hp*-finite element discretization of an elliptic boundary value problem using tetrahedral elements. The discretization uses a polynomial basis in which the number of nonzero entries per row is bounded independently of the polynomial degree. The authors present an algorithm which computes the nonzero entries of the stiffness matrix in optimal complexity.

The algorithm is based on sum factorization and makes use of the nonzero pattern of the stiffness matrix.

1 Introduction

hp-finite element methods (*hp*-FEM), see e.g. Schwab [1998], Demkowicz et al. [2008], have become very popular for the approximation of solutions of boundary value problems with more regularity. In order to obtain the approximate finite element solution numerically stable and fast, the functions have to be chosen properly in *hp*-FEM. For quadrilateral and hexahedral elements, tensor products of integrated Legendre polynomials are the prefered basis functions, see Babuška et al. [1989]. For triangular and tetrahedral elements, the element can be considered as collapsed quadrilateral or hexahedron. This allows us to use tensor product functions. In order to obtain sparsity in the element matrices and a moderate increase of the condition number, integrated Jacobi polynomials have to be used, see Beuchler and Pillwein [2007], Beuchler and Schöberl [2006], Karniadakis and Sherwin [2005]. Then, it has been shown that the element stiffness and mass matrix have a bounded num-

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ber of nonzero entries per row, see Beuchler and Pillwein [2007], Beuchler and Schöberl [2006], Beuchler et al. [2010] which results in a total number of $\mathcal{O}(p^d)$, $d = 2, 3$, nonzero entries in two and three space dimensions, respectively. However, the explicit computation of the nonzero entries is very involved.

This paper presents an algorithm which computes the element stiffness and mass matrices in $\mathcal{O}(p^3)$ operations in two and three space dimensions. The algorithm combines ideas based on sum factorization, Melenk et al. [1999], with the sparsity pattern of the matrices. One other important ingredient is the fast evaluation of the Jacobi polynomials.

The outline of this paper is as follows. Section 2 defines defines H^1-conforming, i.e. globally continuous picewise polynomials, basis functions on the tetrahedron. The sum factorization algorithm is presented in section 3. Section 4 is devoted to the evaluation of the Jacobi polynomials. The complexity of the algorithm is estimated in Section 5.

2 Definition of the basis functions

For the definition of our basis functions Jacobi polynomials are required. Let

$$p_n^\alpha(x) = \frac{1}{2^n n! (1-x)^\alpha} \frac{\mathrm{d}^n}{\mathrm{d}x^n} \left((1-x)^\alpha (x^2-1)^n \right) \quad n \in \mathbb{N}_0,\ \alpha, \beta > -1 \tag{1}$$

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

$$\hat{p}_n^\alpha(x) = \int_{-1}^{x} p_{n-1}^\alpha(y)\, \mathrm{d}y \quad n \geq 1, \quad \hat{p}_0^\alpha(x) = 1 \tag{2}$$

be the nth integrated Jacobi polynomial. Several relations are known between the different families of Jacobi polynomials, see e.g. Abramowitz and Stegun [1964]. In this paper, the relations

$$p_n^{\alpha-1}(x) = \frac{1}{\alpha + 2n} \left[(\alpha+n) p_n^\alpha(x) - n p_{n-1}^\alpha(x) \right], \tag{3}$$

$$\begin{aligned} \hat{p}_{n+1}^\alpha(x) = & \frac{2n+\alpha-1}{(2n+2)(n+\alpha)(2n+\alpha-2)} \\ & \times \left((2n+\alpha-2)(2n+\alpha)x + \alpha(\alpha-2) \right) \hat{p}_n^\alpha(x) \\ & - \frac{(n-1)(n+\alpha-2)(2n+\alpha)}{(n+1)(n+\alpha)(2n+\alpha-2)} \hat{p}_{n-1}^\alpha(x), \quad n \geq 1. \end{aligned} \tag{4}$$

are required.

Let $\hat{\triangle}$ be the reference tetrahedron with the four vertices at $(-1,-1,-1)$, $(1,-1,-1)$, $(0,1,-1)$ and $(0,0,1)$. On this element, the interior bubble functions

$$\phi_{ijk}(x,y,z) = u_i(x,y,z)v_{ij}(y,z)w_{ijk}(z), \quad i \geq 2, \;\; j,k \geq 1, i+j+k \leq p \quad (5)$$

are proposed for H^1 elliptic problems in [Beuchler and Pillwein, 2007, (29)], where the auxiliary functions are

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

In addition, there are vertex, face and edge based basis functions which can be regarded as special cases of the above functions (5) for limiting cases of the indices i, j and k, see Beuchler and Pillwein [2007] for more details.

Then, the element stiffness matrix for the Laplacian on the reference element $\hat{\triangle}$ with respect to the interior bubbles reads as

$$\mathcal{K} = \left[\int_{\hat{\triangle}} \nabla\phi_{ijk}(x,y,z) \cdot \nabla\phi_{i'j'k'}(x,y,z)\,\mathrm{d}(x,y,z)\right]_{i,j,k\leq p, i'+j'+k'\leq p}. \quad (6)$$

The transformation to the unit cube $(-1,1)^3$ (Duffy trick) and the evaluation of the nabla operation results in the integration of 21 different summands. More precisely,

$$\mathcal{K} = \sum_{m=1}^{21} \kappa_m \hat{\mathcal{I}}^{(m)}$$

with known numbers $\kappa_m \in \mathbb{R}$ and

$$\begin{aligned} \hat{\mathcal{I}}^{(m)} = &\left[\int_{-1}^{1} p_{x,1}(x)p_{x,2}(x)\,\mathrm{d}x \right. \\ &\times \int_{-1}^{1}\left(\frac{1-y}{2}\right)^{\gamma_y} p_{y,1}(y)p_{y,2}(y)\,\mathrm{d}y \\ &\left.\times \int_{-1}^{1}\left(\frac{1-z}{2}\right)^{\gamma_z} p_{z,1}(z)p_{z,2}(z)\,\mathrm{d}z\right]_{i+j+k<p; i'+j'+k'<p}. \end{aligned}$$

The structure of the functions and coefficients is displayed in Table 1.

One summand is the term

$$\hat{\mathcal{I}}^{(6)} = (m_{ijk,i'j'k'})_{i+j+k\leq p, i'+j'+k'\leq p} \quad (7)$$

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

Table 1 Integrands for $\mathcal{K}$, where $\beta = i + j$, $\beta' = i' + j'$

which corresponds (before the Duffy trick) to

$$\begin{aligned} m_{ijk,i'j'k'} = \int_{\hat{\triangle}} & \hat{p}_i^0\left(\frac{4x}{1-2y-z}\right)\hat{p}_{i'}^0\left(\frac{4x}{1-2y-z}\right)\left(\frac{1-2y-z}{4}\right)^{i+i'} \\ & \times \hat{p}_j^{2i-1}\left(\frac{2y}{1-z}\right)\hat{p}_{j'}^{2i'-1}\left(\frac{2y}{1-z}\right)\left(\frac{1-z}{2}\right)^{j+j'} \\ & \times p_{k-1}^{2i+2j-2}(z)p_{k'-1}^{2i'+2j'-2}(z)\,\mathrm{d}(x,y,z). \end{aligned}$$

The Duffy transformation applied to (7) gives

$$\begin{aligned} m_{ijk,i'j'k'} = & \int_{-1}^{1}\hat{p}_i^0(x)\hat{p}_{i'}^0(x)\,\mathrm{d}x\int_{-1}^{1}\left(\frac{1-y}{2}\right)^{i+i'+1}\hat{p}_{j'}^{2i'-1}(y)\hat{p}_j^{2i-1}(y)\,\mathrm{d}y \\ & \times\int_{-1}^{1}\left(\frac{1-z}{2}\right)^{i+j+i'+j'+2}p_{k-1}^{2i+2j-2}(z)p_{k'-1}^{2i'+2j'-2}(z)\,\mathrm{d}z. \end{aligned} \tag{8}$$

Due to Beuchler and Pillwein [2007], this matrix has the sparsity pattern

$$m_{ijk,i'j'k'} = 0 \quad \text{if } (i,j,k,i',j',k') \in \mathfrak{S}^p(ijk,i'j'k') \tag{9}$$

where

$$\begin{aligned} \mathfrak{S}^p(ijk,i'j'k') = \{ i+j+k \le p, i'+j'+k' \le p, |i-i'| > 2 \\ \vee \quad |i-i'+j-j'| > 4 \qquad \vee \quad |i-i'+j-j'+k-k'| > 4 \} \end{aligned} \tag{10}$$

cf. [Beuchler and Pillwein, 2007, Theorem 3.3].

All 21 integrals give rise to a similar band structure as detailed above for $\hat{\mathcal{I}}^{(6)}$ and can thus be treated in the same way as explained below for the particular case of $\hat{\mathcal{I}}^{(6)}$. The only difference are shifts in the weights α of the Jacobi polynomials or changes of the weight functions.

3 Sum Factorization

In this section, we present an algorithm for the fast numerical generation of the local element matrices (6) for tetrahedra. The methods are based on fast summation techniques presented in Melenk et al. [1999], Karniadakis and Sherwin [2005] and are carried out in detail for the example of the matrix $\hat{\mathcal{I}}^{(6)}$ (8).

All one dimensional integrals in (8) are computed numerically by a Gaussian quadrature rule with points x_k, $k = 1, \ldots, p+1$ and corresponding weights ω_k. The points and weights are chosen such that

$$\int_{-1}^{1} f(x)\,\mathrm{d}x = \sum_{l=1}^{p+1} \omega_l f(x_l) \quad \forall f \in \mathcal{P}_{2p}. \tag{11}$$

Since only polynomials of maximal degree $2p$ are integrated in (8), these integrals are evaluated exactly. Therefore, we have to compute

$$\begin{aligned} m_{ijk,i'j'k'} = &\sum_{l=1}^{p+1} \omega_l \hat{p}_i^0(x_l) \hat{p}_{i'}^0(x_l) \\ &\times \sum_{m=1}^{p+1} \omega_m \left(\frac{1-x_m}{2}\right)^{i+i'+1} \hat{p}_{j'}^{2i'-1}(x_m) \hat{p}_j^{2i-1}(x_m) \\ &\times \sum_{n=1}^{p+1} \omega_n \left(\frac{1-x_n}{2}\right)^{i+j+i'+j'+2} p_k^{2i+2j-2}(x_n) p_{k'}^{2i'+2j'-2}(x_n), \end{aligned}$$

i.e., for all $(i,j,k,i',j',k') \notin \mathfrak{S}^p(ijk,i'j'k')$, cf. (10), (9). This is done by the following algorithm.

Algorithm 3.1 *1. Compute*

$$h^{(1)}_{i;i'} = \sum_{l=1}^{p+1} \omega_l \hat{p}^0_i(x_l)\hat{p}^0_{i'}(x_l)$$

for all $i, i' \in \mathbb{N}$ satisfying $|i - i'| \leq 2$ and $i, i' \leq p$.

2. Compute

$$h^{(2)}_{i,j;i',j'} = \sum_{m=1}^{p+1} \omega_m \left(\frac{1-x_m}{2}\right)^{i+i'+1} \hat{p}^{2i-1}_j(x_m)\hat{p}^{2i'-1}_{j'}(x_m)$$

for all $i, j, i', j' \in \mathbb{N}$ satisfying $|i - i'| \leq 2$, $|i + j - i' - j'| \leq 4$, $i + j \leq p$ and $i' + j' \leq p$.

3. Compute

$$h^{(3)}_{\beta,k;\beta,'k'} = \sum_{n=1}^{p+1} \omega_n \left(\frac{1-x_n}{2}\right)^{\beta+\beta'+2} p^{2\beta-2}_k(x_n)p^{2\beta'-2}_{k'}(x_n)$$

for all $k, k', \beta, \beta' \in \mathbb{N}$ satisfying $|\beta-\beta'| \leq 4$, $|\beta+k-\beta'-k'| \leq 4$, $\beta+k \leq p$ and $\beta' + k' \leq p$.

4. For all $(i, j, k, i', j', k') \notin \mathfrak{S}^p(ijk, i'j'k')$, set

$$m_{ijk,i'j'k'} = h^{(1)}_{i;i'} h^{(2)}_{i,j;i',j'} h^{(3)}_{i+j,k;i'+j',k'}.$$

The algorithm requires the numerical evaluation of Jacobi and integrated Jacobi polynomials at the Gaussian points x_l, $l = 1, \ldots, p+1$. In the next subsection, we present an algorithm which computes the required values $\hat{p}^\alpha_k(x_l)$, $m = 1, \ldots, p+1$, $k = 1, \ldots, p$, $\alpha = 1, \ldots, 2p$ in $\mathcal{O}(p^3)$ operations.

4 Fast Evaluation of integrated Jacobi polynomials

The integrated Jacobi polynomials needed in the computation of $m_{ijk,i'j'k'}$ (7) are $\hat{p}^0_i(x), \hat{p}^{2i-1}_j(x)$ (progressing in odd steps with respect to the parameter α) and $\hat{p}^{2i+2j-2}_k(x)$ (progressing in even steps with respect to the parameter α). For $i + j + k \leq p$ with $i \geq 2$ and $j, k \geq 1$ this means that

$$\left[\hat{p}^0_i(x)\right]_{2\leq i\leq p}, [\hat{p}^3_j(x)]_{1\leq j\leq p}, \ldots, [\hat{p}^{2p-3}_j(x)]_{1\leq j\leq p},$$
$$[\hat{p}^4_k(x)]_{1\leq k\leq p}, \ldots, [\hat{p}^{2p-4}_k(x)]_{1\leq k\leq p}$$

are needed. Since one group proceeds in even, the other one in odd steps, the total of integrated Jacobi polynomials that are needed is

$$\hat{p}_n^a(x), \qquad 1 \le n \le p-3, \quad 3 \le a \le 2p-3,$$

if we consider the integrated Legendre polynomials separately. However, integrating over identity (3) yields

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

valid for all $n \ge 0$. Using this relation starting from the integrated Jacobi polynomials of highest degree, i.e., $\alpha = 2i-1 = 2p-3$, the remaining Jacobi polynomials can be computed using only two elements of the previous row. Note that for the initial values $n = 1$ we have $\hat{p}_1^{\alpha}(x) = 1 + x$ for all α. For assembling the polynomials of highest degree the three term recurrence (4) is used. Summarizing, the evaluation of the functions at the Gaussian points can be done in $\mathcal{O}(p^3)$ operations. This is optimal in the three-dimensional case, but not in the two-dimensional case.

5 Complexity of the Algorithm

The cost of the last three steps is $\mathcal{O}(p^3)$, the first step requires $\mathcal{O}(p^2)$ operations. Together with the evaluation of the Jacobi polynomials, the algorithm requires in total $\mathcal{O}(p^3)$ flops.

This algorithm uses only the sparsity structure (10). Since all matrices $\hat{\mathcal{I}}^{(m)}$, $m = 1, \ldots, 21$, have a similar sparsity structure of the form (10), this algorithm can be extended to all ingredients which are required for assembling/computing the element stiffness matrix (6) for the Laplacian, see Beuchler and Pillwein [2007]. The algorithm can also be extended to mass matrices or matrices arising from the discretization of elliptic problems in $H(\mathrm{curl})$ and $H(\mathrm{div})$, see Beuchler et al. [2010]. For two-dimensional problems, the third step of the algorithm is not necessary. However, the values $h^{(2)}_{i,j;i',j'}$ have to be computed. Since this requires $\mathcal{O}(p^3)$ floating point operations, the total cost in 2D is also $\mathcal{O}(p^3)$.

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