

Efficient Matrix Computation for Tensor-Product Isogeometric Analysis: The use of Sum Factorization

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Abstract

In this paper we discuss the use of the sum-factorization for the calculation of the integrals arising in Galerkin isogeometric analysis. While introducing very little change in an isogeometric code based on element-by-element quadrature and assembling, the sum-factorization approach, taking advantage of the tensor-product structure of splines or NURBS shape functions, significantly reduces the quadrature computational cost.

Keywords: Numerical integration, Isogeometric analysis, Splines, NURBS, Sum-factorization

1. Introduction

Isogeometric analysis (IGA) is a computational technique for the solution of boundary value problems. It is recent and at the same time well known in the computational engineering academic community, as an extension of the classical Finite Element Method (FEM). IGA was proposed in the seminal paper [17], based on the idea of using the functions adopted in Computer Aided Design (CAD), that is, splines and Non-Uniform Rational B-Splines (NURBS), not only to describe the domain geometry, but also to represent the numerical solution of the problem, in the isoparametric framework. For the interested reader, we refer to the book on IGA [12]. A recent overview on the mathematical aspects of IGA is [6], that covers the known mathematical theory of IGA but also contains an updated bibliography with references to the major contributions and applications of IGA in various engineering fields.

One of the interesting features of IGA, compared to high order FEM, is that it allows for higher global regularity of the shape functions, up to C^{p-1} inter-element continuity for p -degree splines and NURBS. This leads to a higher accuracy per degree-of-freedom (see [14, 5]), improved spectrum properties of the discrete

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operators (see [18]), and the possibility of constructing smooth discretizations of the fundamental structures of the differential operators (such as De Rham diagrams, see e.g. [7, 15]).

IGA can be implemented re-using the existing finite element technology. This may be not the most efficient way to use IGA but surely is one key reason of its fast diffusion and the easiest way to apply IGA on complex problems. In particular, the construction of the matrix of the linear system arising in a Galerkin isogeometric method is typically made by the element-by-element quadrature and assembling as in FEMs. However for high regular and high degree ($p \geq 3$) splines and NURBS, it is experienced that most of the CPU time goes in the quadrature and assembling itself. This may be understood comparing IGA with C^0 to C^{p-1} p -degree splines (or, equivalently, FEM and typical IGA) on the same mesh: element-wise quadrature has the same computational cost in the two cases, even though the C^{p-1} case results in a much smaller linear system. The high cost of quadrature has motivated the research on quadrature rules that keep into account the interelement regularity of IGA functions, see [19, 3, 27], improving efficiency w.r.t. Gauss quadrature. In this paper we consider another significant improvement: one can exploit the tensor-product structure of multivariate splines by adopting the so called *sum-factorization*, a well-known technique for spectral elements or some high-degree finite elements (see e.g. [13, 23, 1]), but never used with IGA, at our knowledge.

The aim of this paper is to discuss and benchmark the use of sum-factorization in IGA. We show that there is a clear advantage versus the standard quadrature approach, and show that the cost of quadrature (by sum-factorization) is balanced with the cost of the linear solver for high degree IGA. We also discuss the implementation of the proposed sum-factorization within our isogeometric library **igatools** [25]. We do not consider parallel implementation though this is clearly a key ingredient for a modern and efficient isogeometric code (see for example [20]).

There are other possibilities to circumvent the element-by-element quadrature issue that however require a change of paradigm. For example, if the mesh is uniform, one can efficiently and directly compute the entries of the linear system matrix (see [8, 9] and [21, 22]) or switch from Galerkin to a collocation formulation [2, 26].

The outline of the paper is as follows. In Section 2 we set up the notation and briefly describe the setting of an academic problem. Section 3 introduces the sum-factorization algorithm and discuss its computational cost in terms of the degree p . Section 4 is devoted to the numerical testing and comparison with other strategies. Finally, we draw conclusions in Section 5. An Appendix is included in order to describe the treatment of the linear elasticity stiffness matrix.

2. Preliminaries

We consider the elliptic problem

$$\begin{cases} -\mu \nabla^2 u + \sigma u = f & \text{in } \Omega \\ u = 0 & \text{on } \partial\Omega \end{cases} \quad (2.1)$$

as a model problem. Its Galerkin approximation on a discrete space V requires the computation of the following matrix entries:

- the mass matrix (or mass integrals)

$$M_{i,j} = \int_{\Omega} \sigma(\mathbf{x}) R_i(\mathbf{x}) R_j(\mathbf{x}) \, d\mathbf{x}; \quad (2.2)$$

- the stiffness matrix (or stiffness integrals)

$$S_{i,j} = \int_{\Omega} \mu(\mathbf{x}) \nabla R_i(\mathbf{x}) \cdot \nabla R_j(\mathbf{x}) \, d\mathbf{x}; \quad (2.3)$$

where R_i and R_j denote two basis function in V , $\mu : \Omega \rightarrow \mathbb{R}$ and $\sigma : \Omega \rightarrow \mathbb{R}$.

In IGA, Ω is given by a spline or NURBS parametrization. For the sake of simplicity, we assume Ω is given by a d -dimensional single patch spline representation:

$$\Omega = \mathbf{F}([0, 1]^d), \text{ with } \mathbf{F}(\hat{\mathbf{x}}) = \sum_i \mathbf{C}_i \hat{B}_i(\hat{\mathbf{x}}),$$

where \mathbf{C}_i are the control points and \hat{B}_i are p -degree tensor-product B-spline basis functions defined on the parametric patch $[0, 1]^d$.

Being IGA based on the isoparametric paradigm, the basis functions R_i are defined as $R_i = \hat{B}_i \circ \mathbf{F}^{-1}$. The integrals above are then computed by change of variable and element-by-element assembling. For more details, see [12].

Then, we consider the computation of the local matrices related to a parametric element $\hat{\Omega} \subset [0, 1]^d$, $\hat{\Omega} := [a_1, b_1] \times \dots \times [a_d, b_d]$. With an abuse of notation, we denote by \hat{B}_{α} the B-splines that are non-zero on $\hat{\Omega}$ and index them by the local multi-index $\alpha = (\alpha_1, \dots, \alpha_d)$, $\alpha_j \in \{1, \dots, p+1\} \, \forall j = 1, \dots, d$, and set $\hat{\mathbf{x}} = (\hat{x}_1, \dots, \hat{x}_d)$. The total number of local basis functions is $(p+1)^d$, i.e. $\#\{\alpha\} = (p+1)^d$.

The local mass matrix, that corresponds to the global one (2.2) after change of variable $\hat{\mathbf{x}} = \mathbf{F}^{-1}(\mathbf{x})$, is $\mathbb{M} = \{m_{\alpha,\beta}\} \in \mathbb{R}^{(p+1)^d \times (p+1)^d}$ where:

$$m_{\alpha,\beta} = \int_{\hat{\Omega}} \hat{B}_{\alpha}(\hat{\mathbf{x}}) \hat{B}_{\beta}(\hat{\mathbf{x}}) c(\hat{\mathbf{x}}) \, d\hat{\mathbf{x}}, \quad (2.4)$$

with $c(\hat{\mathbf{x}}) = \hat{\sigma}(\hat{\mathbf{x}}) |\hat{\mathbf{D}}\mathbf{F}(\hat{\mathbf{x}})|$.

Moreover, for the local stiffness matrix $\mathbb{S} = \{s_{\alpha,\beta}\} \in \mathbb{R}^{(p+1)^d \times (p+1)^d}$ we have:

$$s_{\alpha,\beta} = \int_{\hat{\Omega}} \left(\hat{\mathbf{D}}\mathbf{F}^{-T} \hat{\nabla} \hat{B}_{\alpha} \right)^T \left(\hat{\mathbf{D}}\mathbf{F}^{-T} \hat{\nabla} \hat{B}_{\beta} \right) \hat{\mu} |\hat{\mathbf{D}}\mathbf{F}| d\hat{\mathbf{x}} = \int_{\hat{\Omega}} \hat{\nabla} \hat{B}_{\alpha}^T \left([\hat{\mathbf{D}}\mathbf{F}^{-1} \hat{\mathbf{D}}\mathbf{F}^{-T}] \hat{\mu} |\hat{\mathbf{D}}\mathbf{F}| \right) \hat{\nabla} \hat{B}_{\beta} d\hat{\mathbf{x}} .$$

Also in this case we change notations and we write:

$$s_{\alpha,\beta} = \sum_{i,j=1}^d \int_{\hat{\Omega}} \frac{\partial \hat{B}_{\alpha}}{\partial \hat{x}_i}(\hat{\mathbf{x}}) c_{i,j}(\hat{\mathbf{x}}) \frac{\partial \hat{B}_{\beta}}{\partial \hat{x}_j}(\hat{\mathbf{x}}) d\hat{\mathbf{x}} , \quad (2.5)$$

so that $C(\hat{\mathbf{x}}) := \{c_{i,j}(\hat{\mathbf{x}})\}_{i,j=1,\dots,d}$ is the matrix:

$$C(\hat{\mathbf{x}}) = [\hat{\mathbf{D}}\mathbf{F}^{-1}(\hat{\mathbf{x}}) \hat{\mathbf{D}}\mathbf{F}^{-T}(\hat{\mathbf{x}})] \hat{\mu}(\hat{\mathbf{x}}) |\hat{\mathbf{D}}\mathbf{F}(\hat{\mathbf{x}})| .$$

Finally, we express the tensor-product structure of the B-splines basis functions writing:

$$\hat{B}_{\alpha}(\hat{\mathbf{x}}) = \hat{B}_{\alpha_1,\dots,\alpha_d}(\hat{x}_1,\dots,\hat{x}_d) = \prod_{k=1}^d \hat{B}_{\alpha_k}(\hat{x}_k). \quad (2.6)$$

Remark 2.1. *If NURBS are used instead of splines, the situation is similar. Writing NURBS in terms of B-splines then sum-factorization can be used to integrate the B-splines that form the basis. For the mass matrix, the use of NURBS only affects the coefficient $c(\hat{\mathbf{x}})$, that takes into account the NURBS weight function, and the structure is still the one in (2.4). For the stiffness matrix instead, the derivation rule will produce a few terms, similar to (2.4) or (2.5).*

3. Computation of the local matrices by quadrature

The elements of the local matrices are multidimensional integrals in a d -rectangular domain so that in order to calculate the integrals we need a multidimensional quadrature rule. For the sake of simplicity we consider a quadrature formula constructed via the same univariate quadrature rule in each direction (properly scaled) but everything can be straightforwardly replaced by any tensor-product quadrature scheme. With this aim we introduce a r -points univariate quadrature rule in the reference domain $[0, 1]$: we will denote by ζ_{γ} , $\gamma = 1, \dots, r$ the quadrature nodes and with ω_{γ} the relative weights. This formula, then, will be rescaled to be used in the domains $[a_i, b_i]$: $\zeta_{\gamma}^{(i)} = (b_i - a_i)\zeta_{\gamma} + a_i$, $\omega_{\gamma}^{(i)} = (b_i - a_i)\omega_{\gamma}$. In the d -dimensional domain $\hat{\Omega}$ we will have the set of r^d quadrature points $\zeta_{\gamma} = (\zeta_{\gamma_1}^{(1)}, \dots, \zeta_{\gamma_d}^{(d)})$ and relative weights $\omega_{\gamma} = \prod_{i=1}^d \omega_{\gamma_i}^{(i)}$.

In order to recover the expected convergence rates we take a quadrature rule of degree of exactness $2p + 1$, see [10, Theorem 4.1.6]. In the following we will use r -points gaussian quadrature. In this case the usual choice is $r = p + 1$, which ensures exact integration of (2.4)-(2.5) when the coefficients $c(\hat{\mathbf{x}})$ and $\{c_{i,j}(\hat{\mathbf{x}})\}_{i,j=1,\dots,d}$ are element-wise constant. For non-constant but regular (element-by-element) coefficients, the choice $r = p + 1$ is proved to guarantee optimality of the Galerkin formulation with numerical quadrature (see, e.g., [10, Section

4.1]).

The entries of the local mass and stiffness matrices are $(p+1)^{2d}$ thus if the quadrature procedure is applied directly one obtains that the overall cost for the local matrix construction results in $r^d(p+1)^{2d}$. Because $r = O(p)$, one expects to have an overall cost of $O(p^{3d})$ for the construction of each local matrix, as usually reported. Aim of this paper is to reduce this cost to $O(p^{2d+1})$ by exploiting the tensor product structure via the so-called sum factorization approach [24]. This technique is widely employed in spectral methods, and has also been applied also for high order FEMs [13, 23]. We will discuss in this paper its' application to the case of IGA, maintaining the element-by-element assembly procedure.

In order to clarify the use of the sum factorization algorithm in our framework, we will now present a general application in the 3D case for the calculation of the integral $\int_{\hat{\Omega}} \hat{B}_{\alpha}(\hat{\mathbf{x}}) \hat{B}_{\beta}(\hat{\mathbf{x}}) c(\hat{\mathbf{x}}) d\hat{\mathbf{x}}$. Simple application of the quadrature rule leads to:

$$\int_{\hat{\Omega}} \hat{B}_{\alpha}(\hat{\mathbf{x}}) \hat{B}_{\beta}(\hat{\mathbf{x}}) c(\hat{\mathbf{x}}) d\hat{\mathbf{x}} \approx \sum_{\gamma \in \{1, \dots, r\}^3} \omega_{\gamma} \hat{B}_{\alpha}(\zeta_{\gamma}) \hat{B}_{\beta}(\zeta_{\gamma}) c(\zeta_{\gamma}) = \mathbb{I}_M(\alpha, \beta). \quad (3.1)$$

In order to exploit the tensor product structure we start from (2.6) and notice that:

$$\int_{\hat{\Omega}} \hat{B}_{\alpha}(\hat{\mathbf{x}}) \hat{B}_{\beta}(\hat{\mathbf{x}}) c(\hat{\mathbf{x}}) d\hat{\mathbf{x}} = \int_{a_1}^{b_1} \hat{B}_{\alpha_1}(\hat{x}_1) \hat{B}_{\beta_1}(\hat{x}_1) \left[\int_{a_2}^{b_2} \hat{B}_{\alpha_2}(\hat{x}_2) \hat{B}_{\beta_2}(\hat{x}_2) \left[\int_{a_3}^{b_3} \hat{B}_{\alpha_3}(\hat{x}_3) \hat{B}_{\beta_3}(\hat{x}_3) c(\hat{x}_1, \hat{x}_2, \hat{x}_3) d\hat{x}_3 \right] d\hat{x}_2 \right] d\hat{x}_1$$

Then, if we apply the univariate quadrature rules in this nested integrals we obtain:

$$\mathbb{I}_M(\alpha, \beta) = \sum_{\gamma_1=1}^r \omega_{\gamma_1}^{(1)} \hat{B}_{\alpha_1}(\zeta_{\gamma_1}^{(1)}) \hat{B}_{\beta_1}(\zeta_{\gamma_1}^{(1)}) \left[\sum_{\gamma_2=1}^r \omega_{\gamma_2}^{(2)} \hat{B}_{\alpha_2}(\zeta_{\gamma_2}^{(2)}) \hat{B}_{\beta_2}(\zeta_{\gamma_2}^{(2)}) \left[\sum_{\gamma_3=1}^r \omega_{\gamma_3}^{(3)} \hat{B}_{\alpha_3}(\zeta_{\gamma_3}^{(3)}) \hat{B}_{\beta_3}(\zeta_{\gamma_3}^{(3)}) c(\zeta_{\gamma_1}^{(1)}, \zeta_{\gamma_2}^{(2)}, \zeta_{\gamma_3}^{(3)}) \right] \right]$$

To calculate this sums $\forall \alpha, \beta$, we introduce the following recursion:

$$\begin{aligned} (i) \quad \mathbb{C}^{(0)}(\zeta_{\gamma_1}^{(1)}, \zeta_{\gamma_2}^{(2)}, \zeta_{\gamma_3}^{(3)}) &= c(\zeta_{\gamma_1}^{(1)}, \zeta_{\gamma_2}^{(2)}, \zeta_{\gamma_3}^{(3)}) \\ (ii) \quad \mathbb{C}^{(1)}(\zeta_{\gamma_1}^{(1)}, \zeta_{\gamma_2}^{(2)}; \alpha_3, \beta_3) &= \sum_{\gamma=1}^r \omega_{\gamma}^{(3)} \hat{B}_{\alpha_3}(\zeta_{\gamma}^{(3)}) \hat{B}_{\beta_3}(\zeta_{\gamma}^{(3)}) \mathbb{C}^{(0)}(\zeta_{\gamma_1}^{(1)}, \zeta_{\gamma_2}^{(2)}, \zeta_{\gamma}^{(3)}) \\ (iii) \quad \mathbb{C}^{(2)}(\zeta_{\gamma_1}^{(1)}; \alpha_2, \beta_2; \alpha_3, \beta_3) &= \sum_{\gamma=1}^r \omega_{\gamma}^{(2)} \hat{B}_{\alpha_2}(\zeta_{\gamma}^{(2)}) \hat{B}_{\beta_2}(\zeta_{\gamma}^{(2)}) \mathbb{C}^{(1)}(\zeta_{\gamma_1}^{(1)}, \zeta_{\gamma}^{(2)}; \alpha_3, \beta_3) \\ (iv) \quad \mathbb{I}_M(\alpha, \beta) = \mathbb{I}_M(\alpha_1, \beta_1; \alpha_2, \beta_2; \alpha_3, \beta_3) &= \sum_{\gamma=1}^r \omega_{\gamma}^{(1)} \hat{B}_{\alpha_1}(\zeta_{\gamma}^{(1)}) \hat{B}_{\beta_1}(\zeta_{\gamma}^{(1)}) \mathbb{C}^{(2)}(\zeta_{\gamma}^{(1)}; \alpha_2, \beta_2; \alpha_3, \beta_3) \end{aligned}$$

Then we can count the operations:

1. Step (i) costs one function evaluation in r^3 quadrature points; these r^3 values have to be stored.
2. Step (ii) costs $3r$ multiplications and $(r-1)$ additions in r^2 quadrature points and for $(p+1)^2$ coefficients α_3, β_3 ; $r^2 \times (p+1)^2$ values have to be stored.
3. Step (iii) costs $3r$ multiplications and $(r-1)$ additions in r quadrature points and for $(p+1)^4$ coefficients $\alpha_3, \beta_3, \alpha_2, \beta_2$; $r \times (p+1)^4$ values have to be stored.
4. Step (iv) costs $3r$ multiplications and $(r-1)$ additions for $(p+1)^6$ coefficients α, β ; the final $(p+1)^6$ values are the requested approximations of the integrals (2.4).

The overall cost is then $O(rp^6)$. We notice also that the symmetries can be exploited in each direction. Indeed:

$$\begin{aligned} \mathbb{C}^{(1)}(\zeta_{\gamma_1}^{(1)}, \zeta_{\gamma_2}^{(2)}; \alpha_3, \beta_3) &= \mathbb{C}^{(1)}(\zeta_{\gamma_1}^{(1)}, \zeta_{\gamma_2}^{(2)}; \beta_3, \alpha_3) \\ \mathbb{C}^{(2)}(\zeta_{\gamma_1}^{(1)}; \alpha_2, \beta_2; \alpha_3, \beta_3) &= \mathbb{C}^{(2)}(\zeta_{\gamma_1}^{(1)}; \alpha_2, \beta_2; \beta_3, \alpha_3) = \mathbb{C}^{(2)}(\zeta_{\gamma_1}^{(1)}; \beta_2, \alpha_2; \alpha_3, \beta_3) \\ \mathbb{I}_M(\alpha_1, \beta_1; \alpha_2, \beta_2; \alpha_3, \beta_3) &= \mathbb{I}_M(\alpha_1, \beta_1; \alpha_2, \beta_2; \beta_3, \alpha_3) = \mathbb{I}_M(\alpha_1, \beta_1; \beta_2, \alpha_2; \alpha_3, \beta_3) = \mathbb{I}_M(\beta_1, \alpha_1; \alpha_2, \beta_2; \alpha_3, \beta_3) \end{aligned}$$

Remark 3.1. *If, instead of gaussian quadrature, one adopts the optimal quadrature proposed in [3, 19], the overall computational cost can be reduced up to a factor 1/2.*

The above procedure is used for the computation of the mass matrix with numerical quadrature:

$$m_{\alpha, \beta} \approx \sum_{\gamma \in \{1, \dots, r\}^d} \omega_\gamma c(\zeta_\gamma) \hat{B}_\alpha(\zeta_\gamma) \hat{B}_\beta(\zeta_\gamma) \quad (3.2)$$

With direct application of the procedure seen before we obtain the requested algorithm, reported in the following box.

Input: $p + 1$ number of basis functions \hat{B} ; r = number of quadrature points;

Input: $\hat{\Omega} := [a_1, b_1] \times \dots \times [a_d, b_d]$ = element in the reference domain ;

Input: $(\zeta_\gamma, \omega_\gamma)$ r -points quadrature in the domain $[0, 1]$;

{Computation of the function evaluations}

Calculate quadrature nodes and weights along directions $i = 1, \dots, d$:

$$\zeta_\gamma^{(i)} = (b_i - a_i)\zeta_\gamma + a_i; \quad \omega_\gamma^{(i)} = (b_i - a_i)\omega_\gamma .$$

Pre-calculate the basis functions at the quadrature nodes (for re-use purpose):

$$\hat{B}_\alpha(\zeta_\gamma^{(i)}) \quad \forall i \in \{1, \dots, d\}, \forall \gamma \in \{1, \dots, r\}, \forall \alpha \in \{1, \dots, p + 1\}$$

Calculate the function $c(\hat{\mathbf{x}})$ on the nodes:

$$\mathbb{C}^{(0)}(\zeta_{\gamma_1}^{(1)}, \dots, \zeta_{\gamma_d}^{(d)}) = c(\zeta_{\gamma_1}^{(1)}, \dots, \zeta_{\gamma_d}^{(d)}), \quad \mathbb{C}^{(0)} \in \mathbb{R}^{r^d} .$$

{Computation of the mass terms via sum factorization}

for $i = 1, \dots, d$ **do**

Calculate $\mathbb{C}^{(i)} \in \mathbb{R}^{r^{d-i} \times (p+1)^{2i}}$:

$$\begin{aligned} \mathbb{C}^{(i)} \left(\zeta_{\gamma_1}^{(1)}, \dots, \zeta_{\gamma_{d-i}}^{(d-i)}; \alpha_{d-i+1}, \beta_{d-i+1}; \dots; \alpha_d, \beta_d \right) = \\ = \sum_{\gamma=1}^r \left[\omega_\gamma^{(d-i+1)} \hat{B}_{\alpha_{d-i+1}}(\zeta_\gamma^{(d-i+1)}) \hat{B}_{\beta_{d-i+1}}(\zeta_\gamma^{(d-i+1)}) \cdot \right. \\ \left. \mathbb{C}^{(i-1)} \left(\zeta_{\gamma_1}^{(1)}, \dots, \zeta_{\gamma_{d-i}}^{(d-i)}, \zeta_\gamma^{(d-i+1)}; \alpha_{d+i+2}, \beta_{d+i+2}; \dots; \alpha_d, \beta_d \right) \right] \end{aligned}$$

end for [i]

Output:

$$m_{\alpha, \beta} \approx \mathbb{I}_M(\alpha, \beta) = \mathbb{C}^{(d)}(\alpha_1, \beta_1; \dots; \alpha_d, \beta_d)$$

For the calculation of the stiffness matrix, we need to apply the procedure to all the d^2 integrals appearing in equation (2.5). Exploiting the tensor product structure of the gradient we can write the following:

$$\frac{\partial \hat{B}_\alpha}{\partial \hat{x}_i} = \prod_{k=1}^d D^{\delta_{ik}} \hat{B}_{\alpha_k}(\hat{x}_k), \quad (3.3)$$

where we have denoted by:

$$D^{\delta_{ik}} f(\hat{x}) \equiv \begin{cases} f'(\hat{x}) & \text{if } i = k \\ f(\hat{x}) & \text{otherwise} \end{cases} .$$

Then the elements of the stiffness matrix can be written as:

$$s_{\alpha, \beta} = \sum_{i, j=1}^d \int_{\hat{\Omega}} \left[\prod_{k=1}^d D^{\delta_{ik}} \hat{B}_{\alpha_k}(\hat{x}_k) D^{\delta_{jk}} \hat{B}_{\beta_k}(\hat{x}_k) \right] c_{i, j}(\hat{\mathbf{x}}) d\hat{\mathbf{x}} . \quad (3.4)$$

The integrals above are then treated by gaussian quadrature, for example when $d = 3$:

$$s_{\alpha, \beta} \approx \sum_{i, j=1}^3 \left\{ \sum_{\gamma_1=1}^r \omega_{\gamma_1}^{(1)} D^{\delta_{i1}} \hat{B}_{\alpha_1}(\zeta_{\gamma_1}^{(1)}) D^{\delta_{j1}} \hat{B}_{\beta_1}(\zeta_{\gamma_1}^{(1)}) \cdot \left[\sum_{\gamma_2=1}^r \omega_{\gamma_2}^{(2)} D^{\delta_{i2}} \hat{B}_{\alpha_2}(\zeta_{\gamma_2}^{(2)}) D^{\delta_{j2}} \hat{B}_{\beta_2}(\zeta_{\gamma_2}^{(2)}) \cdot \left(\sum_{\gamma_3=1}^r \omega_{\gamma_3}^{(3)} D^{\delta_{i3}} \hat{B}_{\alpha_3}(\zeta_{\gamma_3}^{(3)}) D^{\delta_{j3}} \hat{B}_{\beta_3}(\zeta_{\gamma_3}^{(3)}) c(\zeta_{\gamma_1}^{(1)}, \zeta_{\gamma_2}^{(2)}, \zeta_{\gamma_3}^{(3)}) \right) \right] \right\} = \mathbb{I}_S(\boldsymbol{\alpha}, \boldsymbol{\beta}) \quad (3.5)$$

The sum factorization procedure to compute the quantity in Eq. (3.5) is summarized in the following box.

Input: $p + 1$ number of basis functions \hat{B} ; r = number of quadrature points;

Input: $\hat{\Omega} := [a_1, b_1] \times \dots \times [a_d, b_d]$ = element in the reference domain ;

Input: $(\zeta_\gamma, \omega_\gamma)$ r -points quadrature in the domain $[0, 1]$;

{Computation of the function evaluations}

Calculate quadrature nodes and weights along directions:

$$\zeta_\gamma^{(i)} = (b_i - a_i)\zeta_\gamma + a_i; \quad \omega_\gamma^{(i)} = (b_i - a_i)\omega_\gamma .$$

Pre-calculate the basis functions and derivatives at the quadrature nodes (for re-use purpose):

$$D^0 \hat{B}_\alpha(\zeta_\gamma^{(i)}) \equiv \hat{B}_\alpha(\zeta_\gamma^{(i)}) \quad , \quad D^1 \hat{B}_\alpha(\zeta_\gamma^{(i)}) \equiv \hat{B}'_\alpha(\zeta_\gamma^{(i)}) \\ \forall i \in \{1, \dots, d\}, \forall \gamma \in \{1, \dots, r\}, \forall \alpha \in \{1, \dots, p + 1\}$$

Calculate the functions $\{c_{i,j}(\hat{\boldsymbol{x}})\}_{i,j=1,\dots,d}$ on the nodes:

$$\mathbb{C}_{i,j}^{(0)}(\zeta_{\gamma_1}^{(1)}, \dots, \zeta_{\gamma_d}^{(d)}) = c_{i,j}(\zeta_{\gamma_1}^{(1)}, \dots, \zeta_{\gamma_d}^{(d)}), \quad \mathbb{C}_{i,j}^{(0)} \in \mathbb{R}^{r^d} .$$

{Computation of the stiffness terms via sum factorization}

for $i, j = 1, \dots, d$ **do**

for $l = 1, \dots, d$ **do**

 Calculate $\mathbb{C}_{i,j}^{(l)} \in \mathbb{R}^{r^{d-l} \times (p+1)^{2l}}$:

$$\mathbb{C}_{i,j}^{(l)} \left(\zeta_{\gamma_1}^{(1)}, \dots, \zeta_{\gamma_{d-l}}^{(d-l)}; \alpha_{d-l+1}, \beta_{d-l+1}; \dots; \alpha_d, \beta_d \right) = \\ = \sum_{\gamma=1}^r \left[\omega_\gamma^{(d-l+1)} D^{\delta^{(il)}} \hat{B}_{\alpha_{d-l+1}}(\zeta_\gamma^{(d-l+1)}) D^{\delta^{(jl)}} \hat{B}_{\beta_{d-l+1}}(\zeta_\gamma^{(d-l+1)}) \cdot \right. \\ \left. \mathbb{C}_{i,j}^{(l-1)} \left(\zeta_{\gamma_1}^{(1)}, \dots, \zeta_{\gamma_{d-l}}^{(d-l)}, \zeta_\gamma^{(d-l+1)}; \alpha_{d+l+2}, \beta_{d+l+2}; \dots; \alpha_d, \beta_d \right) \right]$$

end for[l]

end for[i, j]

Output:

$$s_{\boldsymbol{\alpha}, \boldsymbol{\beta}} \approx \mathbb{I}_S(\boldsymbol{\alpha}, \boldsymbol{\beta}) = \sum_{i,j=1}^d \mathbb{C}_{i,j}^{(d)}(\alpha_1, \beta_1 \dots \alpha_d, \beta_d)$$

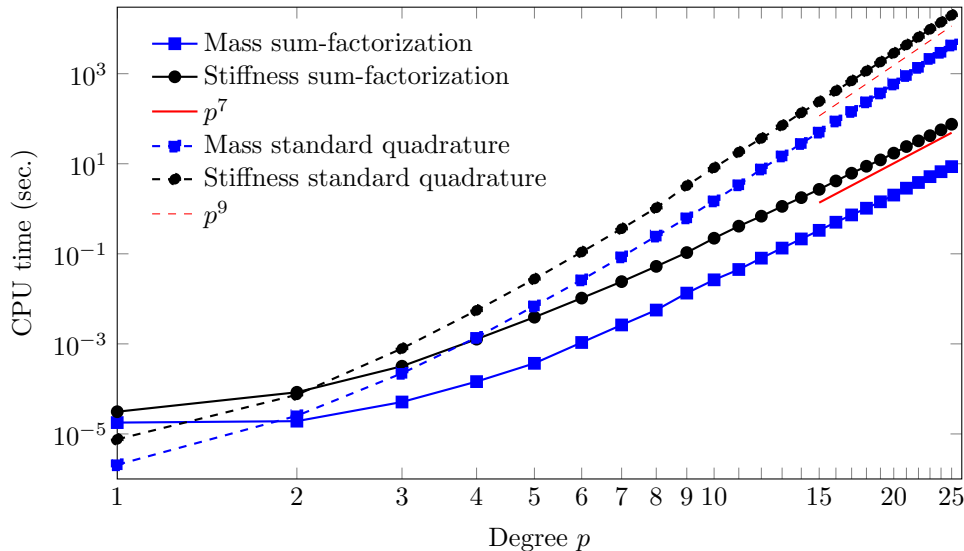


Figure 1: CPU time vs. degree for calculating the local stiffness-matrix and mass-matrix on a single element using sum-factorization and standard quadrature.

4. Numerical results

In this section, in order to evaluate numerically the behaviour of the proposed procedure we present some tests that compare the standard quadrature procedure with the above described sum factorization.

In Section 4.1 we consider the construction of the mass and stiffness matrices in a single mesh element, comparing the CPU costs when the polynomial degree p increases.

In Section 4.2 we compute the solution of a linear elasticity problem on a mesh of $30 \times 15 \times 30$ elements, while in Section 4.3 we compute the solution of an advection-diffusion problem on a mesh of $60 \times 84 \times 12$ elements. For the elasticity problem and the advection-diffusion problem, we have compared the time needed for the computation of the stiffness matrix with the different quadrature strategies and also the time needed by different solver strategies to converge to the solution.

The results for all cases refers to a Linux workstation equipped with Xeon E5-2470 processors (running at 2.3 GHz), where we have used only one core for the simulations in order to avoid any time saving due to parallelization. The previous algorithms have been implemented in the `igatools`, for details see Section 4.4.

4.1. Computation of the local matrices

In Figure 1 we plot the CPU time needed for the calculations on a single 3D element of the mass and stiffness matrices. This test confirms what predicted by the general results in Section 3: the time increases as p^{3d} if no

attention is paid to the tensor product structure, while the sum factorization procedure behaves as p^{2d+1} . Only for $p = 1$ the usual procedure over-performs the sum factorization: this is due to the fact that the complexity of the sum-factorization algorithm is not compensated by the saving due to the smaller number of operations w.r.t. the standard quadrature approach. For degree $p = 2$ the two approaches cost approximatively the same amount of CPU time, while for degree $p \geq 3$ the sum-factorization is less expensive. At degree $p = 4$ one can see that the computational cost with the sum factorization procedure is one order of magnitude below the corresponding one obtained with the standard quadrature.

4.2. Linear elasticity

As a first example it is shown the use of sum factorization technique for a linear elasticity problem:

$$\begin{cases} \nabla \cdot \sigma + f = 0 & \text{in } \Omega, \\ u = g & \text{on } \partial\Omega_D, \\ \sigma \cdot n = t & \text{on } \partial\Omega_N, \end{cases} \quad (4.1)$$

being σ and u the stress and deformation displacement fields. For the linear elasticity case the Cauchy stress tensor σ can be expressed as

$$\sigma(u) = \mathcal{C} : \varepsilon(u), \quad (4.2)$$

where \mathcal{C} is the fourth-order elasticity tensor and ε is the infinitesimal strain tensor, that is the symmetric part of the gradient of u .

In this example an isotropic material has been chosen, therefore the components of \mathcal{C} are $C_{ijkl} = \lambda\delta_{ij}\delta_{kl} + \mu(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk})$, $\forall i, j, k, l = 1, \dots, d$. λ and μ are the Lamé parameters, which numerical values for this problem are $\lambda = 576.92$ and $\mu = 384.62$ (the corresponding ones to $E = 1.0 \cdot 10^3$ and $\nu = 0.3$). Homogeneous Dirichlet conditions have been applied to all the components of one of the faces, and non homogeneous Neumann conditions to the opposite face, with $t = \{1, 0, 0\}$. In the other faces homogeneous Neumann conditions are applied and $f = \{0, 0, 0\}$.

The problem domain Ω and the solution of the problem are shown in the Figure 2 for a mesh of $n = 30 \times 15 \times 30$ elements (the second parametric direction corresponds to the thickness of the beam). The quadrature cost for a whole mesh of n elements will be obviously proportional to n . The algorithm for the evaluation of the stiffness matrix of the elasticity problem (4.1) using sum-factorization is described in AppendixA.

In the Figure 3 the CPU times for the evaluation of stiffness matrices for both, sum factorization and standard quadrature, are shown together with the solver time using a direct (Intel MKL PARDISO) and an iterative linear solver (Conjugate Gradient + ILU(0) preconditioner), both provided by the Trilinos library [16]. For the discussion of these and other strategies for the linear solvers we refer to [11].

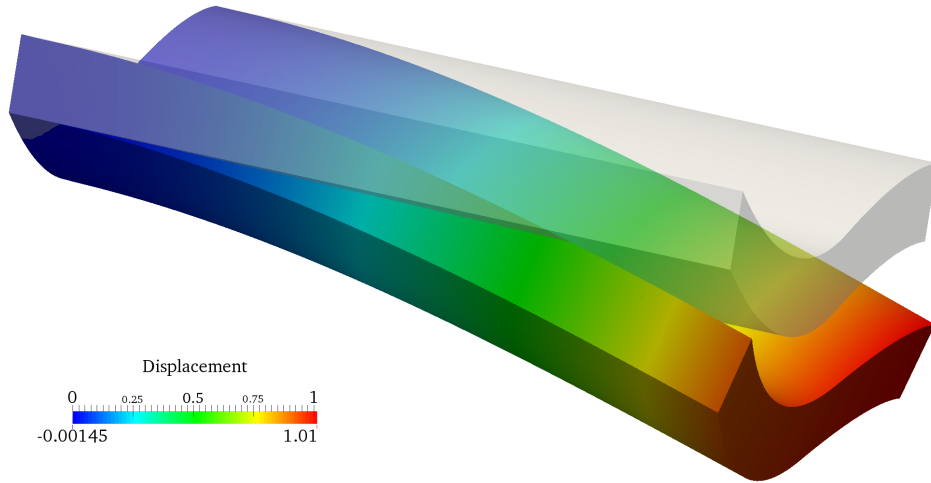


Figure 2: Geometry (before and after deformation) and displacements solution for the linear elasticity problem (4.1).

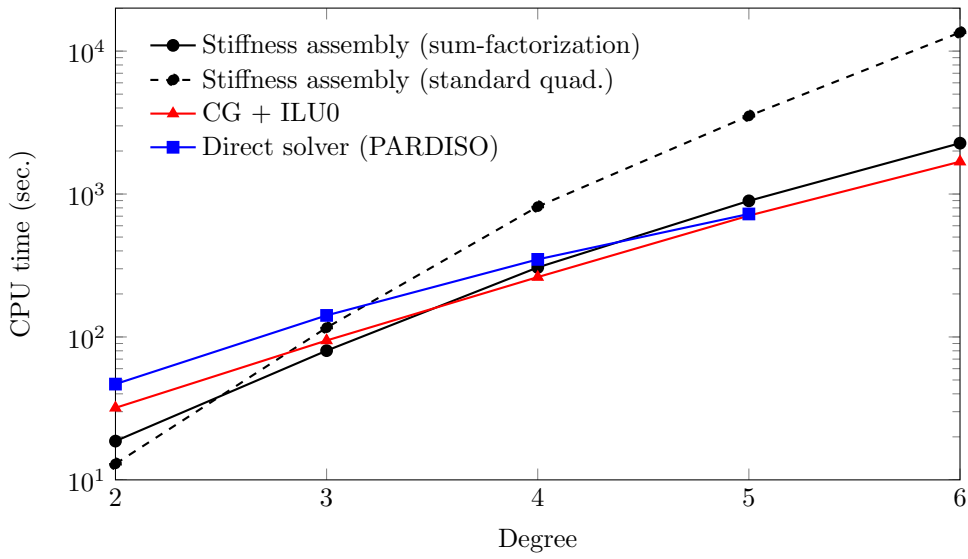


Figure 3: Linear elasticity problem in 3D: comparison of the assembling and solving CPU time vs. degree for a grid of $30 \times 15 \times 30$ elements. The time of the iterative linear solver is the sum of the preconditioner computation (ILU(0)) and the Conjugate Gradient iterations. Both, direct and iterative solvers, are ran using a single thread. The number of degrees of freedom for each degree p are: $\text{ndof}_{p=2} = 52224$, $\text{ndof}_{p=3} = 60588$, $\text{ndof}_{p=4} = 69768$, $\text{ndof}_{p=5} = 79800$ and $\text{ndof}_{p=6} = 90720$.

Some important remarks that arise from the results in Figure 3 are:

- in terms of CPU cost, for $p \geq 3$ the standard quadrature is more demanding than the sum-factorization, and equivalent for $p = 2$, as already noticed and explained in Section 4.1;
- the CPU time ratio between sum-factorization and the iterative solver is constant w.r.t. p ;
- for this problem, the iterative solver outperforms the direct solver for $p < 5$ (for $p > 5$ the memory requirement of the direct solver factorization exceeded the available memory on our system).

For the iterative solver the convergence tolerance considered is 10^{-7} and, in all the cases, the convergence was achieved without any restart of the method.

4.3. Advection-diffusion problem

For the tests we have selected the domain Ω to be the region of space with cylindrical coordinates $1 \leq \rho \leq 4$, $0 \leq \theta \leq \frac{\pi}{2}$ and $0 \leq z \leq 1$ (see Fig. 4), and considered the elliptic problem:

$$\begin{cases} -\mu \nabla^2 u + \mathbf{b} \cdot \nabla u = 0.5 & \text{in } \Omega, \\ u = 0 & \text{on } \partial\Omega. \end{cases} \quad (4.3)$$

with $\mathbf{b} = (1, 0, 0)^T$ and $\mu = 10^{-3}$.

The problem has been solved using a mesh of $n = 60 \times 84 \times 12$ elements, adapted in order to resolve the boundary layer along the side with cylindrical coordinate $\rho = 4$ and avoid spurious oscillations on the numerical IGA solution of (4.3). The CPU times for the simulation are shown in Figure 5.

The curves refer to the CPU time needed for the evaluation of the stiffness matrix using the sum factorization and the standard quadrature approaches and the time needed by some linear solvers to converge to the solution.

The stiffness matrix arising from the discretization of the problem (4.3) is non-symmetric, and for the solution of the associated linear system we have tested different solver strategies: both iterative (GMRES + ILU(k) preconditioner) and direct (Intel MKL PARDISO), provided by the Trilinos library [16].

Regarding the iterative strategy, we have experienced that for this problem is difficult to find a unique combination of GMRES parameters + ILU(k) preconditioner that works well for all degrees p (we have considered $p = 1, \dots, 5$). Increasing the fill-in level k of ILU(k) increases robustness but, at the same time, results in a higher CPU cost for the linear solver.

Regarding the solution of the linear system with a direct solver we experienced that, at least for the degrees we have tested (from 1 to 6), the solution is always obtained, and the CPU cost for $p \geq 4$ was lower than the iterative approaches. We were not able to compute a solution for $p > 6$ because the memory required by the solver during the factorization phase exceeded the memory available on our system.

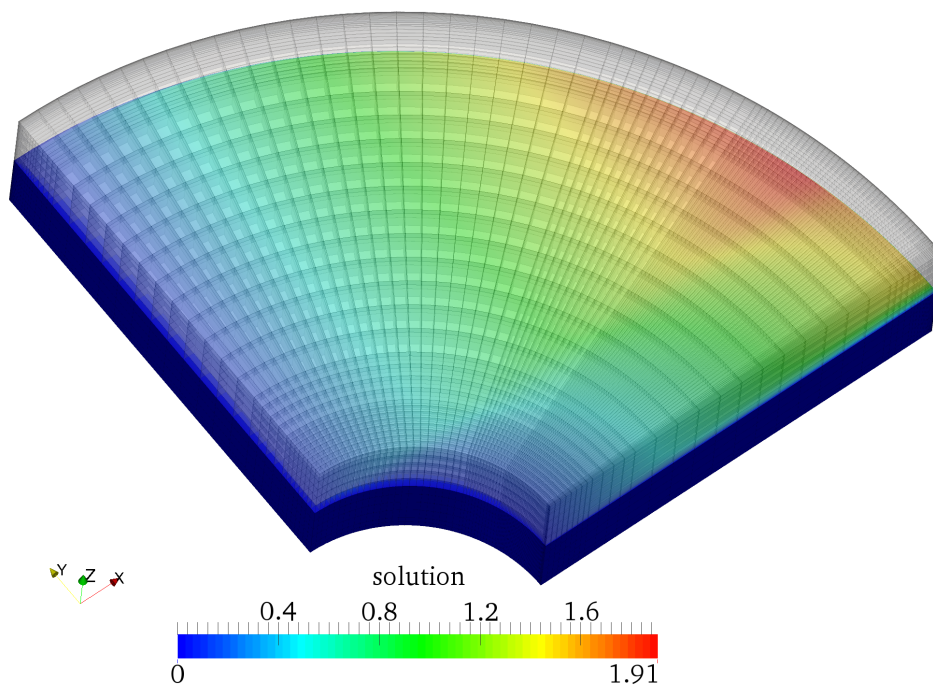


Figure 4: Geometry and solution at the midplane $z = 0.5$ for the advection diffusion problem (4.3).

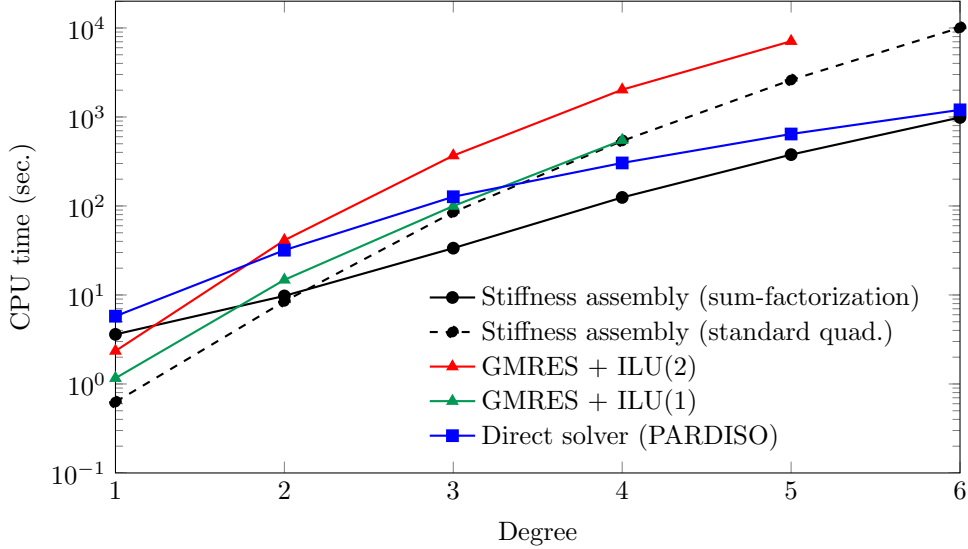


Figure 5: Advection diffusion problem in 3D: comparison of the CPU time vs. degree for a grid of $60 \times 84 \times 12$ elements. The time of the iterative linear solver is the sum of the preconditioner computation with the GMRES iterations. The direct solver (PARDISO) is used with a single thread. Convection/diffusion ratio $\frac{b}{\mu} = 10^3$. The number of degrees of freedom for each degree p are: $\text{ndof}_{p=1} = 67405$, $\text{ndof}_{p=2} = 74648$, $\text{ndof}_{p=3} = 82215$, $\text{ndof}_{p=4} = 90112$, $\text{ndof}_{p=5} = 98345$ and $\text{ndof}_{p=6} = 106920$.

Finally, we have noticed the following on the cost for the computation and assembly of the stiffness matrix:

- analogously to the example above, in terms of CPU cost, for $p \leq 2$ the standard quadrature is less expensive ($p = 1$) or equivalent ($p = 2$) than sum-factorization;
- for $p \geq 3$ the sum-factorization outperform the standard quadrature approach and its CPU cost is always smaller than the CPU cost for the linear solver, while the stiffness matrix computation with standard quadrature costs more than the best linear solver approach when $p \geq 4$ (that is obtained using the the direct solver).

As in the previous example, the convergence tolerance of the iterative solver is 10^{-7} and no restart was applied to the method.

4.4. Implementation details

All the previous algorithms and tests are implemented by the use of the **igatools** library. **igatools** is an open source general purpose isogeometric library, written in C++11 and designed using the object-oriented paradigm. Currently **igatools** provides two classes that group the methods for the computation of the local matrices associated with the elliptic operators

- `EllipticOperatorsStdIntegration` for the computation using the standard quadrature technique;
- `EllipticOperatorsSFIntegration` for the computation using the sum-factorization technique.

For further information on the `igatools` library, see [25] and the official website <http://www.igatools.org>.

5. Summary and Conclusions

We have considered the use of the sum-factorization for the calculation of the integrals arising in Galerkin isogeometric analysis. The minor changes needed in the actual coding in order to implement the proposed technique are presented in general and then detailed in the framework of the `igatools` code. This modification leads to a saving in terms of computational cost that allows high degree computations. The proposed numerical tests confirm the advantage of the sum-factorization when compared to the standard technique.

Appendix A. Sum-factorization for the linear elasticity stiffness matrix

In solid mechanics, it is a common practice the use of Voigt notation for expressing the Galerkin approximation of the strong equation (4.1) as $\mathbb{S} = \{K_{\alpha,\beta}\} \in \mathbb{R}^{d(p+1)^d \times d(p+1)^d}$, being $K_{\alpha,\beta} \in \mathbb{R}^{d \times d}$ such as

$$K_{\alpha,\beta} = \int_{\Omega} \mathbb{B}_{\alpha}^T(\mathbf{x}) \mathbb{D}(\mathbf{x}) \mathbb{B}_{\beta}(\mathbf{x}) d\mathbf{x}, \quad (\text{A.1})$$

see [4] for further details.

For $d = 3$ the matrix \mathbb{D} , that is the Voigt representation of the fourth-order elasticity tensor tensor \mathcal{C} in (4.2), can be expressed as

$$\mathbb{D}(\mathbf{x}) = \begin{bmatrix} \mathcal{C}_{1111}(\mathbf{x}) & \mathcal{C}_{1122}(\mathbf{x}) & \mathcal{C}_{1133}(\mathbf{x}) & \mathcal{C}_{1112}(\mathbf{x}) & \mathcal{C}_{1113}(\mathbf{x}) & \mathcal{C}_{1123}(\mathbf{x}) \\ & \mathcal{C}_{2222}(\mathbf{x}) & \mathcal{C}_{2233}(\mathbf{x}) & \mathcal{C}_{2212}(\mathbf{x}) & \mathcal{C}_{2213}(\mathbf{x}) & \mathcal{C}_{2223}(\mathbf{x}) \\ & & \mathcal{C}_{3333}(\mathbf{x}) & \mathcal{C}_{3312}(\mathbf{x}) & \mathcal{C}_{3313}(\mathbf{x}) & \mathcal{C}_{3323}(\mathbf{x}) \\ & & & \mathcal{C}_{1212}(\mathbf{x}) & \mathcal{C}_{1213}(\mathbf{x}) & \mathcal{C}_{1223}(\mathbf{x}) \\ & \text{sym.} & & & \mathcal{C}_{1313}(\mathbf{x}) & \mathcal{C}_{1323}(\mathbf{x}) \\ & & & & & \mathcal{C}_{2323}(\mathbf{x}) \end{bmatrix}. \quad (\text{A.2})$$

and \mathbb{B}_{α} as

$$\mathbb{B}_{\alpha}(\mathbf{x}) = \begin{bmatrix} \frac{\partial B_{\alpha}}{\partial x_1}(\mathbf{x}) & 0 & 0 \\ 0 & \frac{\partial B_{\alpha}}{\partial x_2}(\mathbf{x}) & 0 \\ 0 & 0 & \frac{\partial B_{\alpha}}{\partial x_3}(\mathbf{x}) \\ \frac{\partial B_{\alpha}}{\partial x_2}(\mathbf{x}) & \frac{\partial B_{\alpha}}{\partial x_1}(\mathbf{x}) & 0 \\ \frac{\partial B_{\alpha}}{\partial x_3}(\mathbf{x}) & 0 & \frac{\partial B_{\alpha}}{\partial x_1}(\mathbf{x}) \\ 0 & \frac{\partial B_{\alpha}}{\partial x_3}(\mathbf{x}) & \frac{\partial B_{\alpha}}{\partial x_2}(\mathbf{x}) \end{bmatrix} = \sum_{i=1}^3 M_i \frac{\partial B_{\alpha}}{\partial x_i}(\mathbf{x}), \quad (\text{A.3})$$

where

$$M_1 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{bmatrix}, \quad M_2 = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \quad M_3 = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix}.$$

Moreover, $\frac{\partial B_\alpha}{\partial x_i}(\mathbf{x}) = \sum_{k=1}^3 (\hat{\mathbf{D}}\mathbf{F}^{-T}(\hat{\mathbf{x}}))_{i,k} \frac{\partial \hat{B}_\alpha}{\partial \hat{x}_k}(\hat{\mathbf{x}})$ for $i = \{1, 2, 3\}$, therefore

$$\mathbb{B}_\alpha(\mathbf{x}) = \sum_{i=1}^3 M_i \frac{\partial B_\alpha}{\partial x_i}(\mathbf{x}) = \sum_{i=1}^3 M_i \sum_{k=1}^3 (\hat{\mathbf{D}}\mathbf{F}^{-T}(\hat{\mathbf{x}}))_{i,k} \frac{\partial \hat{B}_\alpha}{\partial \hat{x}_k}(\hat{\mathbf{x}}) = \sum_{k=1}^3 \hat{M}_k(\hat{\mathbf{x}}) \frac{\partial \hat{B}_\alpha}{\partial \hat{x}_k}(\hat{\mathbf{x}})$$

with $\hat{M}_k(\hat{\mathbf{x}}) = \sum_{i=1}^3 M_i (\hat{\mathbf{D}}\mathbf{F}^{-T}(\hat{\mathbf{x}}))_{i,k}$, $k = \{1, 2, 3\}$.

With these new definitions we can write the integral (A.1) as:

$$\int_{\Omega} \mathbb{B}_\alpha^T(\mathbf{x}) \mathbb{D}(\mathbf{x}) \mathbb{B}_\beta(\mathbf{x}) d\mathbf{x} = \sum_{i=1}^3 \sum_{j=1}^3 \int_Q \frac{\partial \hat{B}_\alpha}{\partial \hat{x}_i}(\hat{\mathbf{x}}) \hat{\mathbb{D}}_{i,j}(\hat{\mathbf{x}}) \frac{\partial \hat{B}_\beta}{\partial \hat{x}_j}(\hat{\mathbf{x}}) d\hat{\mathbf{x}} \quad (\text{A.4})$$

where $\hat{\mathbb{D}}_{i,j}(\hat{\mathbf{x}})$ is the 3×3 matrix defined by $\hat{\mathbb{D}}_{i,j}(\hat{\mathbf{x}}) = \hat{M}_i^T(\hat{\mathbf{x}}) \mathbb{D}(\hat{\mathbf{x}}) | \hat{\mathbf{D}}\mathbf{F}(\hat{\mathbf{x}}) | \hat{M}_j(\hat{\mathbf{x}})$, $i, j = \{1, 2, 3\}$. Using (A.4) we can use the sum-factorization technique in order to exploit the tensor-product structure of the terms $\frac{\partial \hat{B}_\alpha}{\partial \hat{x}_i}(\hat{\mathbf{x}})$ and $\frac{\partial \hat{B}_\beta}{\partial \hat{x}_j}(\hat{\mathbf{x}})$.

An analogous development can be done for $d = 2$.

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