

Cheap and stable quadrature on polyhedral elements

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February 14, 2025

Abstract

We discuss a cheap tetrahedra-free approach to the numerical integration of polynomials on polyhedral elements, based on hyperinterpolation in a bounding box and Chebyshev moment computation via the divergence theorem. No conditioning issues arise, since no matrix factorization or inversion is needed. The resulting quadrature formula is theoretically stable even in the presence of some negative weights.

2020 AMS subject classification: 65D32.

Keywords: Polyhedral elements, tetrahedra-free quadrature, stable quadrature.

1 Introduction

Within the field of polytopal FEM, which has been constantly growing during the last two decades, one of the main computational bottlenecks, especially for high-order methods in 3D, is the necessity of computing in a fast and stable way the integrals of products of polynomials naturally arising on arbitrary polyhedral elements, avoiding sub-tessellation into tetrahedra.

Indeed, a specific literature on this topic has been emerging, where we may quote for example, with no pretence of exhaustivity, [1, 2, 4, 5, 9, 10, 14, 21, 23, 24] and the references therein. Among them we focus on tetrahedra-free moment-based quadratures, which rely on the divergence theorem, together with the availability of efficient quadrature formulas for the polygonal faces and a possible compression in case of high-cardinality; cf., e.g., [21, 23, 24].

The recent paper [10] proposed an appealing way to reduce the computational cost, that ultimately corresponds to moment-matching with the monomial basis by supporting the quadrature formula on approximate Fekete points of an enclosing box for the polyhedral element, computed by QR factorization with

column pivoting of a large Vandermonde matrix (cf. [20]). In such a way the relevant computations can be made once and for all in a reference box, and the formula weights can be computed by solving relatively small linear systems (whose size is the dimension of the exactness polynomial space). The resulting weights are not all positive, but the sums of their absolute values remains experimentally bounded, ensuring empirical stability.

In the present paper we adopt a similar idea, namely that of supporting the quadrature formula on a low cardinality set, but this time such a set is the support itself of a suitable hyperinterpolation formula in the enclosing box, by a sort of generalized Clenshaw-Curtis approach proposed in [22]. We recall that hyperinterpolation, introduced by Sloan in the seminal paper [17], is a Fourier-like orthogonal projection on a total-degree polynomial space with respect to an absolutely continuous measure, discretized by an algebraic quadrature formula with positive weights.

This approach gives not only a simple explicit and cheap formula for the computation of the quadrature weights, consisting essentially of a single matrix-by-vector product, but also theoretically ensures stability of the quadrature formula. In practice, the computational cost substantially reduces to the mere cost of computing the moments of the orthogonal basis used for hyperinterpolation. Moreover, differently from [10], no conditioning issue can arise by increasing the exactness degree, not only because we can use in a natural way for example the Chebyshev basis instead of the monomial basis, but mainly because no QR factorization or linear system is involved. The theoretical foundation upon hyperinterpolation following [22], with the consequent stability result, make the present approach also quite different from the adaptive scheme recently proposed in [2].

The paper is organized as follows. In Section 2 we describe the theoretical base of the method, while in Section 3 we discuss its implementation and provide some numerical examples.

2 Polyhedral quadrature by hyperinterpolation

The proposed quadrature formula relies on two main results, that were proved in [17] and [22]. We summarize for convenience these results as a single theorem, which concerns product-like formulas obtained via hyperinterpolation, and their stability.

Below, we shall denote by \mathbb{P}_n^d the space of d -variate polynomials with total degree not exceeding n , with dimension $N = \binom{n+d}{n}$.

Theorem 1 *Let $K \subset \mathbb{R}^d$ be a compact subset, μ an absolutely continuous measure on K with respect to the Lebesgue measure. Denote by $\{\phi_j\}_{1 \leq j \leq N}$ an orthonormal polynomial basis of \mathbb{P}_n^d for μ . Moreover, let $(X, \mathbf{u}) = (\{P_i\}, \{u_i\})$, $1 \leq i \leq \nu = \nu(n)$, be the nodes and positive weights of a quadrature formula for integration in $d\mu$, exact on \mathbb{P}_{2n}^d (the polynomials with total degree not exceeding $2n$), and $h \in L_\mu^2(K)$.*

Then, the following algebraic product-like formula holds

$$\int_K h(P) f(P) d\mu = \sum_{i=1}^{\nu} w_i f(P_i), \quad \forall f \in \mathbb{P}_n^d, \quad (1)$$

where the quadrature weights $\{w_i\}$ are defined by the product-like moments

$$w_i = u_i \sum_{j=1}^N \phi_j(P_i) m_j, \quad 1 \leq i \leq \nu, \quad m_j = \int_K \phi_j(P) h(P) d\mu. \quad (2)$$

Moreover, the formula is stable, since

$$\lim_{n \rightarrow \infty} \sum_{i=1}^{\nu} |w_i| = \int_K |h(P)| d\mu. \quad (3)$$

For the proof of this theorem, we refer the reader to [17] and [22]. We recall that $\nu \geq N$, and that when $\nu = N$ the quadrature formula for μ is called minimal; cf. [13]. Concerning stability, though there could be some negative weights, (3) clearly implies that $\sum_{i=1}^{\nu} |w_i|$ is bounded. Moreover, notice that if h is almost everywhere nonnegative, then the stability parameter of the quadrature formula, namely $\sum_i |w_i| / |\sum_i w_i| = \sum_i |w_i| / \|h\|_{L^1(K)}$, tends to 1 as $n \rightarrow \infty$.

We turn now to the main goal of the present paper, that is constructing a cheap and stable quadrature formula for

$$\int_{\Omega} f(P) dP, \quad \Omega \subset \mathbb{R}^3 \text{ polyhedron}, \quad f \text{ polynomial}. \quad (4)$$

Here and below, $P = (x, y, z)$ and $dP = dx dy dz$.

Now, take $K = B \supseteq \Omega$, where B is a Cartesian bounding box for a polyhedron Ω , that up to an affine change of variables can be taken as the cube $B = [-1, 1]^3$. Given any absolutely continuous measure $d\mu = \sigma(P) dP$, $\sigma \in L_+^1(B)$, for which we know an algebraic quadrature formula with positive weights for total degree $2n$, we can apply Theorem 1 by writing

$$\int_{\Omega} f(P) dP = \int_B h(P) f(P) \sigma(P) dP, \quad h(P) = I_{\Omega}(P) / \sigma(P), \quad (5)$$

provided that $h \in L_{\mu}^2(B)$, that is $1/\sigma \in L_+^1(\Omega)$. We then obtain

$$\begin{aligned} \int_{\Omega} f(P) dP &= \sum_{i=1}^{\nu} w_i f(P_i), \quad \forall f \in \mathbb{P}_n^3, \quad w_i = u_i \sum_{j=1}^N \phi_j(P_i) m_j, \quad 1 \leq i \leq \nu, \\ m_j &= \int_{\Omega} \phi_j(P) dP, \end{aligned} \quad (6)$$

where $N = \dim(\mathbb{P}_n^3) = (n+1)(n+2)(n+3)/6$. Moreover, in this case we have by (3)

$$\lim_{n \rightarrow \infty} \sum_{i=1}^{\nu} |w_i| = \int_B (I_{\Omega}(P)/\sigma(P)) \sigma(P) dP = \text{vol}(\Omega). \quad (7)$$

Observe that this approach to quadrature on polyhedra is quite general, and clearly extendable to any compact set where one is able to compute the Lebesgue measure moments $\{m_j\}$ in (6), for a polynomial basis orthogonal with respect to an absolutely continuous measure in a bounding box. In the case of polyhedra, as we shall see below, this can be effectively done by the divergence theorem.

We have several natural choices for the measure μ . The first that comes to mind is simply $d\mu = dP$, the Lebesgue measure itself. In such a way, the orthogonal basis is the total-degree product Legendre basis (cf. e.g. [8]), and as quadrature formula of exactness degree $2n$ we can choose the tensorial Gauss-Legendre rule with $\nu = (n+1)^3$ nodes, or even a minimal ($\nu = N$) or near-minimal formula for the degrees where it is available in the quadrature literature (cf. e.g. [6]).

It is worth stressing however that the choice of the underlying quadrature formula in the cube is not decisive, because the cardinalities are in any case small enough to make largely predominant the cost of moment computation, via the divergence theorem and algebraic quadrature on the polygonal faces of the polyhedral surface (as we shall see in the numerical section). On the other hand, the computation of the necessary primitives is facilitated by known analytical formulas for the classical univariate orthogonal polynomials.

But we can also choose the product Chebyshev measure. In this case the orthogonal basis is the total-degree product Chebyshev basis, and the tensorial Gauss-Chebyshev or Gauss-Chebyshev-Lobatto rules with $\nu = (n+1)^3$ nodes become a natural choice. A lower cardinality formula could be adopted, for example the formula proposed in [7] with $\nu \approx (n+1)^3/4$, or even a minimal or near-minimal formula at the available degrees in the quadrature literature (cf. e.g. [16]), but again this is not really relevant for a significative reduction of the overall cost.

Remark 1 *We stress that the present approach, like that developed in [10], gives not only a numerical integration method for polynomials, but also a quadrature formula on a polyhedron Ω , applicable to any function that is defined and well-approximated by polynomials in the whole bounding box $B \supseteq \Omega$. Standard estimates in quadrature theory together with (7) allow indeed to write the following error bound for every $f \in C(B)$*

$$\left| \int_{\Omega} f(P) dP - \sum_{i=1}^{\nu} w_i f(P_i) \right| \leq \left(\text{vol}(\Omega) + \sum_{i=1}^{\nu} |w_i| \right) E_n(f; B) \sim 2 \text{vol}(\Omega) E_n(f; B), \quad (8)$$

where $E_n(f; B) = \inf_{\phi \in \mathbb{P}_n} \max_{P \in B} |f(P) - \phi(P)|$. The decay rate of $E_n(f; B)$ as $n \rightarrow \infty$ depends on the regularity of f , by a multivariate version of Jackson

theorem; in particular, if $f \in C^{k+1}(B)$ then $E_n(f; B) = \mathcal{O}(n^{-k})$, cf. e.g. [15]. From this point of view, we mark a difference with respect to other methods like [1], that are by construction restricted to polynomials.

3 Implementation and numerical tests

The computational steps necessary for the construction of the quadrature formula (6), exact for \mathbb{P}_n^3 on an arbitrary polyhedron Ω , can be briefly summarized as follows:

- (i) determine a Cartesian bounding box for the polyhedron and compute the nodes $\{P_i\}$ and weights $\mathbf{u} = \{u_i\}$, $1 \leq i \leq \nu$, of a quadrature formula exact for \mathbb{P}_{2n}^3 for a given absolutely continuous measure $d\mu = \sigma(P)dP$ on the bounding box;
- (ii) compute an orthonormal basis $\{\phi_1, \dots, \phi_N\}$ of \mathbb{P}_n^3 with respect to $d\mu$, and the corresponding Lebesgue moments $\mathbf{m} = \{m_1, \dots, m_N\}$, $m_j = \int_{\Omega} \phi_j(P) dP$, by the divergence theorem via the (oriented) planar polygonal faces of the polyhedron

$$m_j = \int_{\partial\Omega} \phi_j(P) n_1(P) dS = \sum_{faces} \int_{face} \phi_j(P) n_1^{face} dS ,$$

where dS is the surface measure, $\phi_j(P) = \int \phi_j(P) dx$ is a primitive with respect for example to x , that is $\partial_x \phi_j(P) = \phi_j(P)$, and n_1 is the first component of the outward normal vector to the polyhedral surface, which is constant on each planar face;

- (iii) form the Vandermonde-like matrix $V = V_n(\{P_i\}) = [\phi_j(P_i)] \in \mathbb{R}^{\nu \times N}$ and compute the final weights as a scaling of a matrix-by-vector product as

$$\mathbf{w} = \text{diag}(\mathbf{u}) V \mathbf{m} ,$$

or in a Matlab-like notation $\mathbf{w} = \mathbf{u} . * V \mathbf{m}$.

Notice that (i) can be made completely independent of the polyhedron, by choosing a reference box such as $[-1, 1]^3$, via an affine change of variables (namely, a translation plus scaling of variables) which affects the integrals and the weights only by multiplicative constants. On the other hand, (iii) depends on the polyhedron only via the moment vector \mathbf{m} computed in (ii), because

- the Vandermonde-like matrix can be computed once and for all in the reference cube.

This aspect is particularly relevant in the application to polyhedral FEM, where quadrature has to be applied to a potentially very large number of different polyhedral elements.

Concerning (ii), assuming again with no loss of generality that $B = [-1, 1]^3$, the computation is substantially simplified by choosing a product type orthogonal basis, like e.g. the Chebyshev basis

$$\phi_j(P) = c_j T_\alpha(x) T_\beta(y) T_\gamma(z)$$

where $(\alpha, \beta, \gamma) \in \{0, 1, \dots, n\}^3$, $0 \leq \alpha + \beta + \gamma \leq n$, the c_j are normalization constants, and the index j corresponds to a suitable ordering of the triples, for example a lexicographical ordering. In particular, if j corresponds to a certain triple (α, β, γ) , then $c_j = a_\alpha a_\beta a_\gamma$, where $a_0 = 1/\sqrt{\pi}$ and $a_k = \sqrt{2/\pi}$ for $k > 0$. Indeed, a primitive in this case is analytically known,

$$\phi_j(P) = c_j \int_0^x T_\alpha(x) dx T_\beta(y) T_\gamma(z)$$

where $\int_0^x T_\alpha(x) dx = \frac{T_{\alpha+1}(x)}{2(\alpha+1)} - \frac{T_{\alpha-1}(x)}{2(\alpha-1)}$ for $\alpha \geq 2$, whereas trivially $\int_0^x T_0(x) dx = x$, $\int_0^x T_1(x) dx = x^2/2$; cf. e.g. [11]. The integrals on the planar faces in (ii) can be computed in several ways, for example by the formulas based on piecewise product Gauss-Legendre quadrature, developed in [19]. For a complete discussion on the computation of the polyhedral moments for the product Chebyshev basis, we refer the reader to [21, §2.1].

Finally, the cost of (iii) is substantially that of a matrix-by-vector product. Even though it is not the dominant one, with the choice of the total-degree product Chebyshev basis and of the tensorial Gauss-Chebyshev rule, this cost could be even lowered since it essentially corresponds to a discrete cosine transform of the moment vector, that can be accelerated by the FFT.

The numerical tests below have been performed using Matlab R2024A on an Intel Core Ultra 5 125H processor, with frequency 3.60 GHz and 16 GB of RAM. A preliminary non-optimized version of the Matlab code, named *cheapQ*, is available at [18]. In our implementation, to compute a *cheap* formula with degree of exactness n on Ω , in accordance to Theorem 2.1 we used as set of nodes those of a tensorial Gauss-Chebyshev rule on $[-1, 1]^3$ with degree of exactness $2n$, namely $(n+1)^3$ nodes, scaled to the bounding box.

In Figure 2 we show the relative integration errors for the random polynomials $g_k(x, y, z) = (a_k x + b_k y + c_k z + d_k)^n$ on the three polyhedral domains of Figure 1, where a_k, b_k, c_k, d_k are uniform random coefficients in $[-1, 1]$. The domains have been obtained starting from suitable point clouds by the Matlab built-in command **alphashape**, which also provides the boundary facets. For each even n in the range between 4 and 20, we have made 200 tests and computed the average logarithmic relative error $\sum_{k=1}^{200} \log(E(g_k))/200$, displayed by a black circle. The relative errors $E(g_k)$ have been computed using as reference integral the value produced by a tessellation-based formula with exactness degree n , taken from [21]. We have chosen even degree of exactness n , since in a possible application to FEM these correspond to polynomial elements of degree $n/2$. The numerical experiments show that as expected, such average errors are not far from machine precision.

Next in Table 1 we list the average cputimes in seconds of the *CheapQ* algorithm. We notice that, as expected, the results for Ω_2 are higher in view of the larger number of facets of the domain. On the other hand, with the two polyhedral elements with 20 facets, we see a good performance, with times ranging from the order of 10^{-3} seconds per element for the lowest degrees to 10^{-2} seconds for degree 20. These times are up to one order of magnitude lower than those of the tetrahedra-free Tchakaloff-like formulas with positive weights and interior nodes, that we have recently constructed in [21] by moment-matching with NonNegative Least Squares. Finally in Table 2 we report the stability ratios $\sum_{j=1}^n |w_j|/\text{vol}(\Omega_i)$. We can see that these quantities do not exceed 2 and tend to decrease towards 1 as n increases, as suggested by Theorem 1.

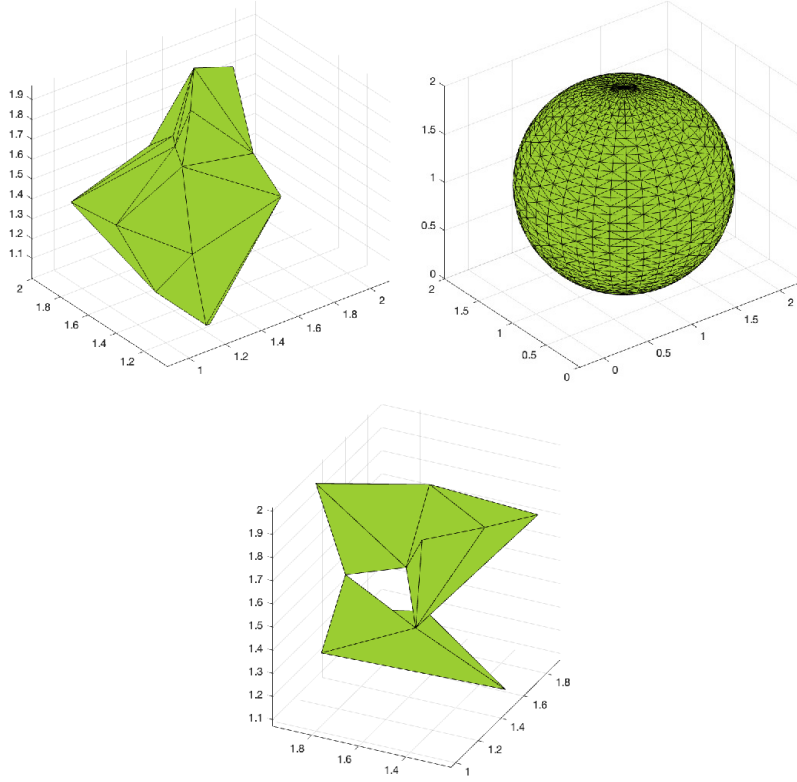


Figure 1: Examples of polyhedral domains. Left: Ω_1 (nonconvex, 20 facets); Center: Ω_2 (convex, 760 facets); Right: Ω_3 (multiply connected, 20 facets).

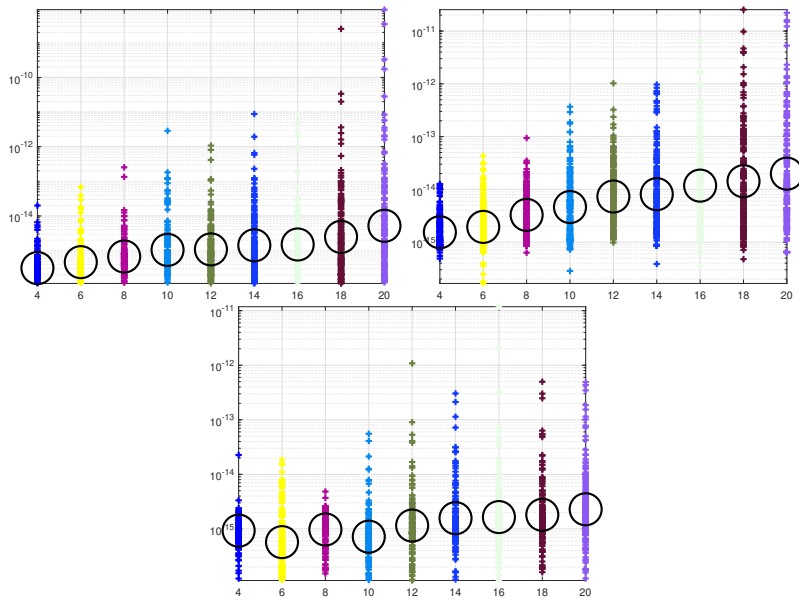


Figure 2: Relative errors $E(g_k)$ of the tetrahedra-free rule over 200 polynomial integrands of the form $g_k = (a_k x + b_k y + c_k z + d_k)^n$ on the three polyhedra of Figure 1, where a_k, b_k, c_k, d_k are uniform random coefficients in $[-1, 1]$ and $n = 4, 6, 8, \dots, 20$; the circles correspond to the average logarithmic error $\sum_{k=1}^{200} \log(E(g_k))/200$.

deg n	4	6	8	10	12	14	16	18	20
Ω_1	1.2-e03	1.4-e03	1.7-e-03	2.3-e03	3.4e-03	5.1e-03	7.7e-03	1.9e-02	3.4e-02
Ω_2	3.0e-02	3.4e-02	4.3e-02	5.9e-02	8.2e-02	1.2e-01	1.8e-01	4.4e-01	9.7e-01
Ω_3	8.1e-04	9.0e-04	1.1e-03	1.7e-03	2.3e-03	3.5e-03	5.4e-03	1.3e-02	2.6e-02

Table 1: Average cputimes (in seconds) of *CheapQ* on the domains of Fig. 1, varying the algebraic degree of exactness.

deg n	4	6	8	10	12	14	16	18	20
Ω_1	1.55	1.40	1.30	1.25	1.23	1.21	1.19	1.17	1.17
Ω_2	1.30	1.14	1.21	1.12	1.13	1.12	1.10	1.10	1.09
Ω_3	1.63	1.81	1.89	1.86	1.82	1.79	1.74	1.67	1.63

Table 2: Ratios $\sum_{j=1}^{\nu} |w_j| / \text{vol}(\Omega_i)$ for *CheapQ* on the domains of Fig. 1, varying the algebraic degree of exactness.

4 Conclusions

We have implemented a quadrature formula without sub-tessellation, which is exact for polynomials up to a given degree on polyhedral elements. The formula is based on hyperinterpolation in a bounding box and Chebyshev moment computation via the divergence theorem. The computational bulk is given by computation of the Chebyshev moments, since the final weights are obtained via a matrix-by-vector product where the matrix is element-independent, and can be computed once and for all. No conditioning issues arise, since no matrix factorization or inversion is needed. Moreover, the resulting quadrature formula is theoretically stable even in the presence of some negative weights. We are confident that the present method could become an additional tool, with some improved features with respect to [10] and other techniques adopted in the literature, for the efficient and stable computation of stiffness and mass matrices within polyhedral Finite Elements. Cheap but still accurate assembly of such matrices, due to the increasing adoption of polytopal FEM simulations, could have a non negligible fall-out on large scale numerical modelling.

Acknowledgements.

Work partially supported by the DOR funds of the University of Padova and by the INdAM-GNCS 2024 Project “Kernel and polynomial methods for approximation and integration: theory and application software”. This research has been accomplished within the Community of Practice “Green Computing” of the Arqus European University Alliance, the RITA “Research Italian network on Approximation”, the SIMAI Activity Group ANA&A, and the UMI Group TAA “Approximation Theory and Applications”.

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