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Gauss Legendre – Gauss Jacobi Quadrature Rules over a Tetrahedral Region

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Abstract

This paper presents a Gaussian quadrature method for the evaluation of the triple integral $I = \iiint_T f(x, y, z)\,dxdydz$, where $f(x, y, z)$ is an analytic function in x, y, z and T refers to the standard tetrahedral region: $\{(x, y, z) \mid 0 \le x, y, z \le 1, x + y + z \le 1\}$ in three space (x, y, z). Mathematical transformation from (x, y, z) space to (u, v, w) space maps the standard tetrahedron T in (x, y, z) space to a standard 1-cube: $\{(u, v, w) / 0 \le u, v, w \le 1\}$ in (u, v, w) space. Then we use the product of Gauss-Legendre and Gauss-Jacobi weight coefficients and abscissas to arrive at an efficient quadrature rule over the standard tetrahedral region *T*. We have then demonstrated the application of the derived quadrature rules by considering the evaluation of some typical triple integrals over the region *T*.

Keywords: Finite element method, Gauss Legendre – Gauss Jacobi quadrature rules, Tetrahedral region, Standard 1-cube, Orthogonal polynomials

1. Introduction

In recent years, we have been witnessing finite element method (FEM) gaining importance due to the most obvious reason that it can provide solutions to many complicated problems that would be intractable by other numerical techniques [1,2]. In FEM it may be possible to perform some of the integration analytically, particularly if constant or linear elements are used to discretise the surface or boundary curve of the given region. However, with higher order elements or for more complex distorted elements the integrals become too complicated for analytical integration and the numerical integration is essential, among various integration schemes, Gauss Legendre quadrature which can evaluate exactly the $(2n\text{-}1)^{\text{th}}$ order polynomial with n-Gaussian points is most commonly used in view of the accuracy and efficiency of calculations [3]. The triangular and tetrahedral elements are very widely used in finite element analysis. The versatility of these elements can be further enhanced by improved numerical integration schemes. Mathematically, the problem can be defined as the evaluation of the following integrals

$$II = \int_0^1 \int_0^{1-L_1} F(L_1, L_2, L_3)\ dL_2 dL_1 \tag{1}$$

where L_1, L_2, L_3 are the well known area co-ordinates and

$$III = \int_0^1 \int_0^{1-L_1} \int_0^{1-L_1-L_2} G(L_1, L_2, L_3, L_4)\ dL_3 dL_2 dL_1 \tag{2}$$

where L_1, L_2, L_3, L_4 are the well known volume co-ordinates.

The basic problem of integrating an arbitrary function of two variables over the surface of the triangle, were first given by Hammer, Marlowe and Stroud [4], and Hammer and Stroud [5,6]. Cowper [7] provided a table of Gaussian quadrature formulae with symmetrically placed integration points. Lyness and Jespersen [8] made an elaborate study of symmetric quadrature rules by formulating the problem in polar co-ordinates. Lannoy [9] discussed the symmetric 4-point integration formula, which is presented in [7]. Laurie [10] derived a 7-point integration rule and discussed the numerical error in integrating some functions. Laursen and Gellert [11] gave a table of symmetric integration formulae up to a precision of degree ten. Dunavant [12] presented some extensions to the integration formulae given by Lyness and Jespersen [8] and also gave tables of integration formulae with precisions of degree from eleven to twenty. Sylvester [13] derived some numerical integration formulae for triangles as product of one-dimensional Newton Cotes rules of closed type as well as open type. The precision of these integration formulae is limited to a degree ten atmost for various reasons. Lether [14] and Hillion [15] derived the formulae for triangles as product of one-dimensional Gauss Legendre and Gauss Jacobi quadrature rules. The precision of these formulae is again up to degree seven. This is because the zeros and weight coefficients of Gauss Jacobi orthogonal polynomials with weight functions x, x^2, x^3 were available for polynomials of degree up to six only. Even today the zeros and weights for the integral $\int_0^1 x^r f(x)\, dx$, r = 0,1,2 are not available beyond a formula of order-eight as documented in Abramowicz and Stegun [16]. Reddy [17] and Reddy and Shippy [18] derived the 3-point, 4-point, 6-point and 7-point rules of precision 3, 4, 6 and 7 respectively which gave improved accuracy. Since the precision of all the formulae derived by the authors [4-18] is limited to a precision of degree ten and it is not likely that the techniques can be extended much further to give a greater accuracy which may be demanded in future, Lague and Baldur [19] proposed the product formulae based only on the sampling points and weight coefficients of Gauss Legendre quadrature rules. By the proposed method of [19] this restriction is removed and one can now obtain numerical integration rules of very high degree of precision as the derivation now rely on standard Gauss Legendre quadarature rules. However, the Lague and Baldur [19] have not worked out explicit weight coefficients and sampling points for application to integrals over a triangular surface. Rathod et al [20, 21, 22] provided this information in a systematic manner in their recent work. For tetrahedral regions, four volume coordinates L_1, L_2, L_3, L_4 are involved and we have to compute numerically the integral III stated in Eq. (2). Numerical integration formulae for III with a degree of precision d=1,2,3 are listed in Zienkiewicz [1] and these are based on reference [4]. Rathod et al [23] proposed product formulae based on Gauss Legendre quadrature rule for the numerical integration of an arbitrary function over the standard tetrahedron. In this paper, we propose the product rule based on Gauss Legendre - Gauss Jacobi quadrature rules which has a higher precision than our earlier work [23], and are based on zeros and weight coefficients of the Gauss Legendre Gauss - Jacobi quadrature rules $\int_0^1 x^r f(x)\, dx$, r = 0,1,2.

2. Gauss quadrature formulas

Given any n distinct points $-1 \le x_1 < x_2 < \dots\dots\dots < x_{n-1} < x_n \le 1$ (3)

and weight function $w(x)$ which is positive and integrable on the interval [-1,1], we can find constants $A_1, A_2, \dots\dots\dots, A_n$ so that the formula

$$\int_{-1}^{1} f(x)w(x)\, dx = \sum_{k=1}^{n} A_K f(x_k) + E(f) \tag{4}$$

is exact (that is $E(f)$)=0) whenever $f(x)$ is a polynomial of degree $\le(n-1)$. But it was Gauss [24] who proved that for a certain special choice of $x_1, x_2, ..., x_n$, we can find $A_1, A_2, ..., A_n$ so that the formula (4) has degree of exactness equal to $(2n-1)$, (i.e., $E(f)$)=0 if f is a polynomial of degree $\le(2n-1)$). Let $w(x)=(1-x)^{\alpha}(1+x)^{\beta}, (\alpha,\beta>-1)$ be the weight functions. These weight functions are known as Jacobi weights and the corresponding orthogonal polynomials are known as Jacobi polynomials $P_n^{(\alpha,\beta)}(x)$. Let $x_1, x_2, ..., x_n$ be the zeros of the n^{th} degree Jacobi Polynomials $P_n^{(\alpha,\beta)}(x)$. It is well known (see [25, p349]) that the corresponding Gaussian quadrature formula is given by

$$(f\in\pi_{2n-1})=\int_{-1}^{1} w(x)f(x)dx=\sum_{k=1}^{n} f(x_k)A_K^{(\alpha,\beta)}+E_{2n-1}(f) \tag{5}$$

where
$$A_k^{(\alpha,\beta)}=\frac{2^{\alpha+\beta+1}\Gamma(\alpha+n+1)\Gamma(\beta+n+1)}{\Gamma(n+1)\Gamma(\alpha+\beta+n+1)(1-x_k^2)[P_n^{(\alpha,\beta)\prime}(x)]^2} \tag{6}$$

$$(1-x)^{\alpha}(1+x)^{\beta}P_n^{(\alpha,\beta)}(x)=\frac{(-1)^n}{2^n n!}\frac{d^n}{dx^n}[(1-x)^{n+\alpha}(1+x)^{n+\beta}] \tag{7}$$

In this paper, we need integrals over (0,1), and hence we shall refer to the Gauss-Jacobi rules derived in Villadsen and Michelson [26], though it is possible for us to derive these from the formulas quoted in Eqs. (5)-(7). The formulas can be very systematically generated from [26] as given in the following:

$$\int_{0}^{1}(1-x)^{\alpha}x^{\beta}f(x)dx=\sum_{i=1}^{n} w_i^{(\alpha,\beta)}f(x_i)+E_{2n-1}(f) \tag{8}$$

where x_i's are the zeros of $P_N^{(\alpha,\beta)}(x)$ over (0,1) and

$$P_N^{(\alpha,\beta)}(x)=\frac{(-1)^N\Gamma(\beta+1)}{\Gamma(N+\beta+1)}(1-x)^{-\alpha}x^{-\beta}\frac{d^N}{dx^N}[(1-x)^{N+\alpha}x^{N+\beta}]$$
$$=\sum_{i=0}^{N}(-1)^{N-i}\gamma_{N,i}^{(\alpha,\beta)}x^i \tag{9}$$

$$\gamma_{N,i}^{(\alpha,\beta)}=\frac{(N-i+1)}{i}\frac{(N+\alpha+\beta+i)}{(\beta+i)}\gamma_{N,i-1}^{(\alpha,\beta)},\quad i=1,2,.......,N \text{ and } \gamma_{N,0}^{(\alpha,\beta)}=1 \tag{10}$$

and the weight coefficients $w_i^{(\alpha,\beta)}$ are given by

$$w_i^{(\alpha,\beta)}=\frac{(2N+\alpha+\beta+1)}{x_i(1-x_i)}\frac{C_N^{(\alpha,\beta)}}{[P_N^{(1)\,(\alpha,\beta)}(x_i)]^2}$$

$$P_N^{(\alpha,\beta)}(x)=\frac{P_N^{(\alpha,\beta)}(x)}{\gamma_{N,N}^{(\alpha,\beta)}},\qquad \gamma_{N,N}^{(\alpha,\beta)}=\frac{\Gamma(2N+\alpha+\beta+1)}{\Gamma(N+\alpha+\beta+1)\Gamma(N+\beta+1)}$$

$$C_N^{(\alpha,\beta)} = \frac{\Gamma(N+\alpha+\beta+1)\Gamma(N+\beta+1)\Gamma(N+1)\Gamma(N+\alpha+1)}{\{\Gamma(2N+\alpha+\beta+1)\}^2 \ (2N+\alpha+\beta+1)} \tag{11}$$

We shall now present the special case of formulas of Eq. (8) for $\alpha = 0$. This gives us the following Gauss-Jacobi quadrature rule $(\alpha = 0, \beta = 0,$ refers to the Gauss-Legendre quadrature rule over (0,1)).

$$\int_0^1 x^\beta f(x)dx = \sum_{i=1}^{n} w_i^{(0,\beta)} f(x_i) + E_{2n-1}(f) \tag{12}$$

where x_i's are the zeros of $P_N^{(0,\beta)}(x)$ over (0,1) and

$$P_N^{(0,\beta)}(x) = \frac{(-1)^N \beta!}{(N+\beta)!} \sum_{k=0}^{N} (-1)^k C_k^N \frac{(N+\beta+k)!}{(\beta+k)!} x^k = \sum_{k=0}^{N} (-1)^{N-k} \gamma_k^N x^k \tag{13}$$

$$\gamma_k^N = \frac{(N-k+1)}{k} \frac{(N+\beta+k)}{(\beta+k)} \gamma_{k-1}^N, \quad k = 1, 2, ..., N \text{ and } \gamma_0^N = 1 \tag{14}$$

and the weight coefficients $w_i^{(0,\beta)}$ are given by

$$w_i^{(0,\beta)} = \frac{(2N+\beta+1)}{x_i(1-x_i)} \frac{C_N^{(0,\beta)}}{[P_N^{(1)\,(0,\beta)}(x_i)]^2} \tag{15}$$

where $$C_N^{(0,\beta)} = \frac{\left[\dfrac{N!\,(N+\beta)!}{(2N+\beta)!}\right]^2}{(2N+\beta+1)} \tag{16}$$

If necessary, one can find the abscissas and weight coefficients for higher order rules by the procedure outlined in Eqs. (12)-(16) and computer programs already available in [26].

3. Formulation of integrals over a tetrahedron

The finite element method for three-dimensional problems with tetrahedron element requires the numerical integration of expressions containing product of shape functions and their global derivatives over a standard tetrahedron T with coordinates (0,0,0),(1,0,0),(0,1,0) and (0,0,1) in the natural coordinate space (*x,y,z*) say. The numerical integration of an arbitrary function f, over the tetrahedron T is given by

$$I = \iiint_T f(x,y,z)dxdydz = \int_0^1 dx \int_0^{1-x} dy \int_0^{1-x-y} f(x,y,z)dz$$

$$= \int_0^1 dy \int_0^{1-y} dx \int_0^{1-x-y} f(x,y,z)dz \qquad (17)$$

It is now required to find the value of the integral by a quadrature formula:

$$I = \sum_{m=1}^{N} c_m f(x_m, y_m, z_m) \qquad (18)$$

where c_m are the weights associated with the sampling points (x_m, y_m, z_m) and N is the number of pivotal points related to the required precision.

The integral I of Eq. (17) can be transformed into an integral over the cube: $\{(u,v,w) \mid 0 \le u,v,w \le 1\}$ by the substitution

$$x = uvw\,,\ y = uv(1-w),\ z = u(1-v) \qquad (19)$$

Then the determinant of the Jacobian and the differential volume are

$$\frac{\partial(x,y,z)}{\partial(u,v,w)} = \begin{vmatrix} \frac{\partial x}{\partial u} & \frac{\partial x}{\partial v} & \frac{\partial x}{\partial w} \\ \frac{\partial y}{\partial u} & \frac{\partial y}{\partial v} & \frac{\partial y}{\partial w} \\ \frac{\partial z}{\partial u} & \frac{\partial z}{\partial v} & \frac{\partial z}{\partial w} \end{vmatrix} = -u^2 v \ \text{and}$$

$$dxdydz = \left| \frac{\partial(x,y,z)}{\partial(u,v,w)} \right| dudvdw = u^2 v \ dudvdw \qquad (20)$$

Then on using Eqs. (19) and (20) in Eq. (17), we have

$$I = \int_0^1 \left(\int_0^{1-x} \left(\int_0^{1-x-y} f(x,y,z)dz \right) dy \right) dx$$

$$= \int_0^1 \int_0^1 \int_0^1 f(uvw,\ uv(1-w),\ u(1-v))u^2 v dudvdw \qquad (21)$$

Eq. (21) represents an integral over the standard 1-cube: $\{(u,v,w) \mid 0 \le u,v,w \le 1\}$. We shall now use the Gauss Legendre – Gauss Jacobi quadrature rules described in the previous section 2 and developed in Eqs. (12)-(16) to approximate the triple integral of Eq. (21) above. We thus have:

$$I \approx \sum_{i=1}^{\alpha} \sum_{j=1}^{\beta} \sum_{k=1}^{\gamma} \lambda_i^{(\alpha)} \mu_j^{(\beta)} \nu_k^{(\gamma)} \times f\left[u_i^{(\alpha)} v_j^{(\beta)} w_k^{(\gamma)}, u_i^{(\alpha)} v_j^{(\beta)} (1 - w_k^{(\gamma)}), u_i^{(\alpha)} (1 - v_j^{(\beta)}) \right]$$

$$= \sum_{m=1}^{N=(\alpha\times\beta\times\gamma)} c_m f(x_m, y_m, z_m) \qquad (22)$$

where, it is obvious that

$$c_m = \lambda_i^{(\alpha)} \mu_j^{(\beta)} \nu_k^{(\gamma)}, \quad x_m = u_i^{(\alpha)} v_j^{(\beta)} w_k^{(\gamma)}, \quad y_m = u_i^{(\alpha)} v_j^{(\beta)} (1 - w_k^{(\gamma)}), \ \ z_m = u_i^{(\alpha)} (1 - v_j^{(\beta)})$$

in which the pairs $(\lambda_i^{(\alpha)}, u_i^{(\alpha)}), (\mu_j^{(\beta)}, v_j^{(\beta)})$ and $(\nu_k^{(\gamma)}, w_k^{(\gamma)})$ refer to the abscissas and weight coefficients of Gauss-Legendre and Gauss-Jacobi quadrature rules over (0,1) of order α, β and γ respectively for the integral $\int_0^1 x^r f(x)\,dx$, r = 0,1,2. In the present analysis we shall assume $\alpha = \beta = \gamma$.

4. Some numerical results

We consider some typical integrals with known exact values

Example1 Let us consider the following multiple integrals which are generalised to three-dimensions from Reddy and Shippy [18].

$$I_1 = \int_0^1 \int_0^{1-x} \int_0^{1-x-y} \sqrt{(x+y+z)}\,dzdydx = 0.142857142857143$$

$$I_2 = \int_0^1 \int_0^{1-x} \int_0^{1-x-y} \frac{dzdydx}{\sqrt{(x+y+z)}} = 0.200000000000000$$

$$I_3 = \int_0^1 \int_0^{1-x} \int_0^{1-x-y} \left[(1-x-y)^2 + z^2\right]^{\frac{-1}{2}} dzdydx = 0.440686793509772$$

Example 2 We now consider the following multiple integrals from Stroud [6].

$$I_4 = \int_0^1 \int_0^{1-x} \int_0^{1-x-y} Sin(x+2y+4z)\,dzdydx = 0.131902326890181$$

$$I_5 = \int_0^1 \int_0^{1-x} \int_0^{1-x-y} (1+x+y+z)^{-4}\,dzdydx = 0.020833333333333$$

We have tabulated the numerical values for I_1, I_2 and I_3 of example-1 and I_4 and I_5 of example-2, in Tables 1 and 2 respectively.

5. Conclusions

In this paper we have derived Gaussian quadrature method for the evaluation of the triple integral $\iiint_T f(x,y,z)\,dxdydz$, where $f(x, y, z)$ is an analytic function in and T

refers to the standard tetrahedral region: $\{(x,y,z) \mid 0 \le x,y,z \le 1, x+y+z \le 1\}$ in three space (x, y, z). Mathematical transformation from (x, y, z) space to (u,v,w) space maps the standard tetrahedron T in (x, y, z) space to a standard 1-cube: $\{(u,v,w) / 0 \le u,v,w \le 1\}$ in (u,v,w) space. Then we use the product of Gauss-Legendre and Gauss-Jacobi weight coefficients and abscissas to arrive at an efficient quadrature rule over the standard tetrahedral region *T*. We have then demonstrated the application of the derived quadrature rules by considering the evaluation of some typical triple integrals over the region *T*.

Table 1 Numerical results of triple integrals in example-1

n^3	I_1	I_2	I_3
2^3	0.142942021837018	0.198763628315142	0.373050560741083
3^3	0.142569950931711	0.199205880631040	0.401003305350442
4^3	0.142859942312556	0.199879880172048	0.415402464798632
5^3	0.142857974957635	0.199948586087860	0.422997550101168
6^3	0.142857440261375	0.199975068156754	0.427626629757130
7^3	0.143260558916461	0.200674960303585	0.431524943273086
8^3	0.142857190262350	0.199992401298026	0.432737244267085
9^3	0.142857169357884	0.199995417776173	0.434234187958587
10^3	0.142488864056452	0.199607363698843	0.433942502667705

Table 2 Numerical results of triple integrals in example- 2

n^3	I_4	I_5
2^3	0.131086148130859	0.020575578288408
3^3	0.131573257676406	0.020767180573211
4^3	0.131902220378017	0.020832433738594
5^3	0.131902327536958	0.020833289256266
6^3	0.131902326829507	0.020833331321815
7^3	0.132384495652103	0.020916599226093
8^3	0.131902317683351	0.020833329020945
9^3	0.131902326175840	0.020833332878624
10^3	0.131643059515503	0.020806898469793

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