NUMERICAL INTEGRATION OVER ARBITRARY TETRAHEDRAL ELEMENT BY TRANSFORMING INTO STANDARD 1-CUBE

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ABSTRACT

In this paper, we are using two different transformations to transform the arbitrary linear tetrahedron element to a standard 1-Cube element and obtain the numerical integration formulas over arbitrary linear tetrahedron element implementing generalized Gaussian quadrature rules, with minimum computational time and cost. We also obtain the integral value of some functions with singularity over arbitrary linear tetrahedron region, without discretizing the tetrahedral region into P^3 tetrahedral regions. It may be noted the computed results are converging faster than the numerical results in referred articles and are exact for up to 15 decimal values with minimum computational time. In a tetrahedral sub-atomic geometry, a focal particle is situated at the middle with four substituents that are situated at the sides of a tetrahedron. The bond edges are $\cos-1(-\frac{1}{3}) = 109.4712206...^{\circ} \approx 109.5^{\circ}$ when each of the four substituents are the same, as in methane (CH4) and in addition its heavier analogs. The impeccably symmetrical tetrahedron has a place with point amass Td, yet most tetrahedral particles have brought down symmetry. Tetrahedral atoms can be chiral. Mathematically the problem is to evaluate the volume integral over a arbitrary tetrahedron transforming the triple integral over arbitrary linear tetrahedron into the integrals over a standard 1-cube using two different parametric transformations.

Keywords- generalized Gaussian quadrature; linear tetrahedral elements; classical Gauss quadrature; finite element methods

INTRODUCTION

Numerical methods date back to Archimedes who tried to calculate the area of a circle, which happened even before the field of integral calculus was formed. Finite element method (FEM), is an ideal numerical method for a wide range of engineering, biomedical, etc., problems due to its rich mathematical formulation and the ability to model complex geometries using unstructured meshes and employing elements that can be individually tagged makes the method unique. It stems from properly-posed functional minimization principles. Numerical integration is an essential tool to evaluate integrals over iso-parametric tetrahedral elements, as in Fig.1.

In a tetrahedral sub-atomic geometry, a focal particle is situated at the middle with four substitutents that are situated at the sides of a tetrahedron. The bond edges are $\cos-1(-\frac{1}{3}) = 109.4712206...^{\circ} \approx 109.5^{\circ}$ when each of the four substituents are the same, as in methane (CH4) and in addition its heavier analogs. The impeccably symmetrical tetrahedron has a place with point amass Td, yet most tetrahedral particles have brought down symmetry. Tetrahedral atoms can be chiral.



Fig.1 Tetrahedron with four vertices

Innumerable formulae have been developed for quadrature like Newton cotes formulae and the classical Gauss quadrature formulae, because of the simplicity of the problem and its practical value. The traditional Gaussian quadrature rules are greatly productive when the capacities to be coordinated are very much approximated by polynomials; however, in the event that the integrands are unique in relation to polynomials they don't perform well. Standard practice has been to use Gauss integration by Stroud [1996], Cattani [1990] and Rathod [1996, 1998]. Since such principles utilize a minimal number of test focuses to accomplish a coveted level of exactness. This economy is imperative for productive firmness lattice estimations. The generalization, of the traditional Gauss quadrature rules, called as generalized-Gaussian quadrature (GGQ) are introduced by Karlin and Studden (1966) and numerical scheme for the construction of GGQ was presented by Ma et. al., (1996). Also generalized Gaussian quadrature method over (0, 1) introduced by Ma et al., in [1996] has been verified to give more precise results than the traditional Gauss Legendre quadrature rules over (-1, 1) as in [2005, 2007] and also it is applicable for functions with end point singularities. Rathod et al., {20005] proposed Gauss-Legendre quadrature rule for the numerical integration of an arbitrary function over the standard tetrahedron by transforming the standard tetrahedron into a standard 2-cube. As Rathod et al.,

[2007] has used a product rule based on zeros and weight coefficients of the Gauss Legendre - Gauss Jacobi quadrature rules, using one of the parametric transformations to transform a standard tetrahedron into a standard 1-cube, as in Fig.2. Also, Rathod et al., in 2011 has proposed another parametric transformation to transform a standard tetrahedron into a standard 1-cube and have applied the product rule for numerical integration which has a higher precision.



Fig.2 Tetrahedron transformed into 2-Cube

Rathod et al., [2005, 2011] have evaluated the numerical integration of arbitrary functions applying Gauss Legendre quadrature rules, over the p^3 tetrahedral regions using one of the parametric transformations to transform a standard tetrahedron into a standard 1-cube by discretization of standard tetrahedral region V_i into p^3 tetrahedral regions each of which has volume equal to <u>1</u> units.

 $\overline{6p^3}$

In reference, Mamatha and Venkatesh [2015], have evaluated the numerical integration of arbitrary integrands by decomposing standard tetrahedral region T(0,1) into four hexahedral element regions H(-1,1) using Gauss quadrature rules. With minimum number of divisions of the tetrahedral region they have shown the convergence of integral values to exact solutions, and also the number of computations and errors are reduced drastically.

In this paper we try to obtain the numerical integration formulas over arbitrary linear tetrahedron by using two different transformations to transform the integral over a linear tetrahedron to a standard 1-cube element, implementing generalized Gaussian quadrature rules and also obtain the integral values of some arbitrary functions without discretization of arbitrary linear tetrahedron region into many tetrahedral regions. Integral values obtained using these quadrature nodes and weights for different integrands are tabulated in this paper and it is established that these quadrature rules give better accuracy for the integrands, including with end point singularities, with minimum computational time and cost.

The problem can be defined mathematically as evaluation of the integral defined in (1):

$$I = \int_{0}^{1} \int_{0}^{1-x} \int_{0}^{1-x-y} f(x, y, z) dz dy dx$$
(1)

by transforming the triple integral over linear tetrahedron into the integrals over a standard 1-cube.

I. Volume Integration Over an Arbitrary Tetrahedron by Transforming Into a Standard 1-Cube

In the reference article by Rathod [2005], the author has applied Gauss-Legendre quadrature rule for numerical integration over the standard tetrahedron by transforming the standard tetrahedron into a standard 2-cube. And in [2007] they have applied the same method by discretizing the tetrahedral region into p^3 tetrahedral regions. In another article of Rathod [2007, 2011], he has applied the Gauss Legendre- Gauss Jacobi quadrature product rules to evaluate integrals over arbitrary tetrahedral regions by an affine-transformation to transform an arbitrary tetrahedron in (X,Y,Z) space into an orthogonal tetrahedron (x, y, z) and then transforming the tetrahedral region into a standard 1-Cube $(0 \le \xi_1, \xi_2, \xi_3 \le 1)$. In this paper, we use generalized Gaussian quadrature rules to evaluate integrals over arbitrary tetrahedral regions by transforming the orthogonal tetrahedron into a standard 1-cube

 $(0 \le \xi_1, \xi_2, \xi_3 \le 1)$ by using two parametric representations as in (5) and (8) and show that the numerical evaluation of integrands converges faster with minimum computational time and cost.

A. Volume Co-ordinates for an Arbitrary Linear Tetrahedron

For transforming the tetrahedral region into a standard 1-Cube, the limits of integration have to be mapped to $(0 \le \xi_1, \xi_2, \xi_3 \le 1)$ in (ξ_1, ξ_2, ξ_3) space. This is achieved by transforming the (x, y, z) to the natural coordinates

$$(\xi_1, \xi_2, \xi_3)$$
 using the equation

$$x = N_{1}x_{1} + N_{2}x_{2} + N_{3}x_{3} + N_{4}x_{4}$$

$$y = N_{1}y_{1} + N_{2}y_{2} + N_{3}y_{3} + N_{4}y_{4}$$

$$z = N_{1}z_{1} + N_{2}z_{2} + N_{3}z_{3} + N_{4}z_{4}$$

$$N = N_{1} + N_{2} + N_{3} + N_{4}$$
(2)

The ratio of the volumes of tetrahedron based on an internal point C, as in Fig.3, in the total volume element is identified as the physical nature of the coordinates.

$$N_1 = \frac{volume \ of \ C_{234}}{volume \ of \ C_{1234}}, \quad N_2 = \frac{volume \ of \ C_{134}}{volume \ of \ C_{1234}},$$

$$N_4 = \frac{volume \, of \, C_{123}}{volume \, of \, C_{1234}}$$

The (x, y, z) coordinates transformed to natural coordinates (ξ_1, ξ_2, ξ_3) using the (2),

$$x = N_i x_i ; y = N_i y_i ; z = N_i z_i ;$$
 (3)

 $N_1 + N_2 + N_3 + N_4 = 1$, where (x_i, y_i, z_i) are the coordinates of vertex of the tetrahedron



Fig. 3. Volume Co-ordinates

B. Affine Transformation for an Arbitrary Linear Tetrahedron

The transformation between the (x, y, z) to the natural coordinates (ξ_1, ξ_2, ξ_3) in (3) is rewritten by substituting $N_1 = \xi_1, N_2 = \xi_2, N_3 = \xi_3$, as

$$x = \xi_{1} x_{14} + \xi_{2} x_{24} + \xi_{3} x_{34} + x_{4}$$

$$y = \xi_{1} y_{14} + \xi_{2} y_{24} + \xi_{3} y_{34} + y_{4}$$

$$y = \xi_{1} z_{14} + \xi_{2} z_{24} + \xi_{3} z_{34} + z_{4}$$
with
$$(4)$$

$$x_{ij} = x_i - x_j$$
; $y_{ij} = y_i - y_j$; $z_{ij} = z_i - z_j$

By the parametric representation in (4), we have for the volume element (1), represented as

$$I = \iiint_{T} f(x, y, z) dx dy dz$$

$$= \iiint_{V} f(x(\xi_{1}, \xi_{2}, \xi_{3})y(\xi_{1}, \xi_{2}, \xi_{3})z(\xi_{1}, \xi_{2}, \xi_{3}))|J|d\xi_{1}d\xi_{2}d\xi_{3}d\xi_{4}d\xi_{4}d\xi_{5$$

$$|J| = \begin{vmatrix} x_1 - x_4 & x_2 - x_4 & x_3 - x_4 \\ y_1 - y_4 & y_2 - y_4 & y_3 - y_4 \\ z_1 - z_4 & z_2 - z_4 & z_3 - z_4 \end{vmatrix},$$

= 6 (volume of tetrahedron)

is the unit orthogonal tetrahedron spanned by the vertices < (0, 0, 0), (1, 0, 0), (0, 1, 0), (0, 0, 1) > .

II. Transformation of Integrals Over an arbitrary Tetrahedron into Integrals Over a Standard 1-Cube

In this section, we transform the triple integral of the form in (1) into the integrals over the standard 1-Cube $(0 \le \xi_1, \xi_2, \xi_3 \le 1)$ by using two parametric transformations.

Transformation-I: Consider the integral in (1), let us write the parametric representation as in (5) x = lmn, y = lm(1-n), z = l(1-m); (5) where $0 \le l, m, n \le 1$, such that it completely

describes the region $0 \le l, m, n \le 1$, such that it completely

 $x + y + z = 1, x \ge 0, y \ge 0, z \ge 0.$

Then the differential volume and the determinant of the Jacobian are

 $dxdydz = |J| dl dm dn = l^2 m dl dm dn$ and

$$|J| = \frac{\partial(x, y, z)}{\partial(l, m, n)} = \begin{vmatrix} \frac{\partial x}{\partial l} & \frac{\partial x}{\partial m} & \frac{\partial x}{\partial n} \\ \frac{\partial y}{\partial l} & \frac{\partial y}{\partial m} & \frac{\partial y}{\partial n} \\ \frac{\partial z}{\partial l} & \frac{\partial z}{\partial m} & \frac{\partial z}{\partial n} \end{vmatrix} = -l^2 m \quad (6)$$

Thus, the volume integral in (1) is transformed over a standard 1-cube by using the

$$I = \int_{0}^{1} \int_{0}^{1} \int_{0}^{1} f(lmn, lm(1-n), l(1-m)) l^{2}m \, dl \, dm \, dn \quad (7)$$

Transformation-II: Consider the integral in (1), let us write the parametric representation as

$$x = l, y = m(1-l), z = n(1-l)(1-m);$$
 (8)
where

 $1-x-y-z = (1-l)(1-m)(1-n), 0 \le l, m, n \le 1$ such that it completely describes the region

$$x + y + z = 1, x \ge 0, y \ge 0, z \ge 0.$$

Then the differential volume and the determinant of the Jacobian are

$$dxdydz = |J| dl dmdn = (1-l)^{2}(1-m) dl dmdn \quad \text{and}$$

$$\begin{split} \xi_{3} \\ J| &= \frac{\partial(x, y, z)}{\partial(l, m, n)} = \begin{vmatrix} \frac{\partial x}{\partial l} & \frac{\partial x}{\partial m} & \frac{\partial x}{\partial n} \\ \frac{\partial y}{\partial l} & \frac{\partial y}{\partial m} & \frac{\partial y}{\partial n} \\ \frac{\partial z}{\partial l} & \frac{\partial z}{\partial m} & \frac{\partial z}{\partial n} \end{vmatrix} = (1 - l)^{2} (1 - m) \quad (9) \end{split}$$

Hence the volume integral in (1) is transformed over a standard 1-cube by using the transformation-2, as in (8), is given by (10).

$$I = \int_{0}^{1} \int_{0}^{1} \int_{0}^{1} \left[f(l, m(1-l), n(1-l)(1-m)(1-l)^{2}(1-m) \right] dl dm dn.$$
(10)

III. Numerical integration:

One can now apply generalized Gauss quadrature rule to evaluate integrals in 7 and 10

$$I = \int_{0}^{1} \int_{0}^{1} \int_{0}^{1} f(lmn, lm(1-n), l(1-m)) l^{2}m \, dl \, dm \, dn$$
$$I = \sum_{m=1}^{N} a_{m} g(x_{m}, y_{m}, z_{m})$$
(11)

$$I = \int_{0}^{1} \int_{0}^{1} \int_{0}^{1} f(l, m(1-l), n(1-l)(1-m)(1-l)^{2}(1-m)dldmdn$$
$$I = \sum_{m=1}^{N} k_{m}h(x_{m}, y_{m}, z_{m})$$
(12)

where

$$\begin{split} h(x_m, y_m, z_m) &= f(l, m(1-l), n(1-l)(1-m)(1-l)^2(1-m); \\ g(x_m, y_m, z_m) &= f(lmn, lm(1-n), l(1-m)); \text{ are} \\ \text{abscissas} \qquad \text{and} \qquad k_m &= (1-l)^2(1-m) w_i w_j w_k; \end{split}$$

 $c_m = l^2 m w_i w_j w_k$, are weight coefficients of generalized Gauss quadrature rule and N is the number of sampling points.

Integral values in (11) and (12), obtained using these generalized Gaussian quadrature rules nodes and weights for different integrands based on availability of analytical solutions are tabulated and the effectiveness of the parametric transformation of the proposed method is tested.

Numerical Examples: We consider some typical integrands whose integral values are known on standard tetrahedral domain and with the exact value of the integrals [2005, 2007].

$$I_{1} = \iiint_{T} \frac{1}{\sqrt{(1 - x - y)^{2} + z^{2}}} dx dy dz$$
(13)

$$I_{2} = \iiint_{T} (x + y + z)^{\frac{1}{2}} dx dy dz$$
(14)

$$I_{3} = \iiint_{T} (x + y + z)^{-\frac{1}{2}} dx dy dz$$
(15)

$$I_{4} = \iiint_{T} \sin(x + y^{2} + z^{4}) dx dy dz$$
(16)

$$I_{5} = \iiint_{T} \frac{1}{(1+x+y+z)^{4}} dx dy dz$$
(17)

$$I_6 = \iiint_T x^3 \sin(y\pi) \sin(z\pi) dx dy dz$$
(18)

We evaluate the numerical solution to the integrals in (11) and (12) considering the arbitrary integrands in (13, 18), by applying generalized Gaussian quadrature (GGQM) integration method whose results are given in Appendix (Table–I). It is observed that the computed results (GGQM) are converging faster than the Gauss-Legendre quadrature (GLQM) numerical method in 2005, 2007 and as compared to the Gauss-Legendre and Gauss-Jacobi quadrature (GLJQM) numerical method in 2007 and 2011 without discretization of tetrahedral regions we are able to obtain the numerical results exact up to 15 decimal places. As in (18), we have computed the numerical solution to the integral with the singularity function, which is not computed in the referred articles.

CONCLUSIONS

In this research article, we have evaluated the volume integral of an integrand over arbitrary tetrahedral region by first transforming into standard tetrahedron and later by using two different transformations we transform standard tetrahedron in (x, y, z) space into a standard 1-Cube in (l, m, n)space. We have used generalized Gaussian quadrature method for the evaluation of the triple integral, as in (1). It may be noted that almost all the numerical results which we have obtained is exact for more than ten decimal values, converging faster than the numerical results by Rathod [2011]. Also, without discretization of tetrahedral regions we are obtaining the exact integral values as compared to the numerical results in Rathod [2005, 2007] by reducing the number of computations. We observed that the numerical results obtained with Transformation-2 for the integrands are more accurate with analytical solutions compared to the results obtained with Transformation-1.

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1

Appendix Table

$I_1 = \iiint_T \frac{1}{\sqrt{(1-x-y)^2 + z^2}} dx dy dz = 0.440686793 \mathfrak{D}9772$							
			Tra	nsformation-1			
GLOM by Rathod[2005]							
IV	GGQM	11	GLJQM[11]	P ³ =6 ³	$P^{3}=7^{3}$	$P^{3}=8^{3}$	
5	0.401433409154618	7	0.431524943273086	0.438056467746589	0.438461566166572	0.438525199025403	
10	0.429349205239327	8	0.432737244267085	0.438494153586623	0.438837020656758	0.438853915428304	
15	0.435393554019928	9	0.434234187958587	0.438800139004454	0.439099456872214	0.439083654085687	
20	0.437634725073964	10	0.433942502667705	0.439022470568174	0.439290122690003	0.439250549614584	
Transformation-2							
A.		A.	GLJQM by Rathod and GLQM by Rathod[20		LQM by Rathod[2007]]	
1	GGQM	11	Shafiqul[2007]	$P^{3}=6^{3}$	$P^{3}=7^{3}$	$P^{3}=8^{3}$	
5	0.440685900461525	7	0.434255520664723	0.440032854640855	0.440156655061396	0.440009086267002	
10	0.440686793510637	8	0.435031208274682	0.440028320026023	0.440152657197482	0.440005515259131	
15	0.440686793509740	9	0.436135693229094	0.440025722427437	0.440150367069788	0.440003469650297	
20	0.440686793509771	10		0.440024154598790	0.440148984820863	0.440002234985244	

$I_2 = \iiint_T (x+y+z)^{\frac{1}{2}} dx dy dz = 0.142857142\7143							
			Tran	sformation-1			
			GLJOM BY		GLQM by Rathod[2005]	
N	GGQM	N	RATHOD[2011]	P ³ =6 ³	$P^{3}=7^{3}$	P ³ =8 ³	
5	0.142857129401889	7	0.143260558916461	0.142857145351164	0.142857144311217	0.142857143768345	
10	0.142857142856268	8	0.142857190262350	0.142857143904410	0.142857143467725	0.142857143239767	
15	0.142857142857140	9	0.142857169357884	0.142857143341263	0.142857143139396	0.14285743034018	
20	0.142857142857143	10	0.142488864056452	0.142857143098771	0.142857142998018	0.142857142945423	
Transformation-2							
37		N	GLJQM by Rathod and	(GLQM by Rathod[2007]	
IN	GGQM	IN	Shafiqul[2007]	P ³ =6 ³	$P^{3}=7^{3}$	$P^{3}=8^{3}$	
5	0.142857116529782	7	0.142857173245610	0.142857143720264	0.142857143360363	0.142857143172488	
10	0.142857142852559	8	0.142857152996523	0.142857143208842	0.142857143062192	0.142857142985637	
15	0.142857142857117	9	0.142857152535564	0.142857143016253	0.142857142949907	0.142857142915274	
20	0 142857142857143	10		0 142857142935285	0 142857142902701	0 142857142885692	

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$I_{3} = \iiint_{T} (x + y + z)^{-\frac{1}{2}} dx dy dz = 0.20000000000000000000000000000000000$							
			Tra	nsformation-1			
N	N GLQM BY GLQM by Rathod[2005]]	
			RATHOD[2011]	P ³ =6 ³	$P^{3}=7^{3}$	$P^{3}=8^{3}$	
5	0.199999899961675	7	0.200674960303585	0.199999243473790	0.199999485415138	0.199999631466358	
10	0.199999999859248	8	0.199992401298026	0.199999591454682	0.199999722109779	0.199999800981524	
15	0.1999999999997098	9	0.199995417776173	0.199999764024885	0.199999839491058	0.199999885047250	
20	0.1999999999999820	10	0.199607363698843	0.199999856139718	0.199999902147048	0.199999929920004	
	Transformation-2						
N	GGQM	N	GLJQM by Rathod	(GLQM by Rathod[2007]	
			and Shafiqul[2007]	P ³ =6 ³	$P^{3}=7^{3}$	P ³ =8 ³	
5	0.200000275082718	7	0.199995955453215	0.199999924909213	0.199999948923666	0.199999963420324	
10	0.20000002496569	8	0.199996036650226	0.199999960197440	0.199999972926523	0.199999980610609	
15	0.2000000068057	9	0.199997676631442	0.199999977310639	0.199999984566824	0.199999988947120	
20	0.20000000004693	10		0.199999986302052	0.199999990682733	0.199999993327192	

$I_4 = \iiint_T \sin(x + y^2 + z^4) dx dy dz = 0.131902326 \circledast 0181$						
			Tra	ansformation-1		
N	GGQM N GLJQM BY GLQM by Rathod[2005]]	
			RATHOD[2011]	P ³ =6 ³	$P^{3}=7^{3}$	$P^{3}=8^{3}$
5	0.131888262041085	7	0.132384495652103	0.131902326890182	0.131902326890182	0.131902326890182
10	0.131902326893353	8	0.131902317683351	0.131902326890181	0.131902326890181	0.131902326890181
15	0.131902326890182	9	0.131902326175840	0.131902326890181	0.131902326890182	0.131902326890181
20	0.131902326890182	10	0.131643059515503	0.131902326890182	0.131902326890182	0.131902326890182
Transformation-2						
N	GGQM	GGOM N GLJOM by Rathod GLOM by Rathod[2007]]	
			and Shafiqul[2007]	P ³ =6 ³	$P^{3}=7^{3}$	$P^{3}=8^{3}$
5	0.131901021445645	7	0.131902324856213	0.131902326890182	0.131902326890182	0.131902326890182
10	0.131902326890124	8	0.131902314247159	0.131902326890181	0.131902326890181	0.131902326890181
15	0.131902326890182	9	0.131902325772292	0.131902326890181	0.131902326890181	0.131902326890181
20	0.131902326890182	10		0.131902326890182	0.131902326890182	0.131902326890182

$I_{5} = \iiint_{T} \frac{1}{(1+x+y+z)^{4}} dx dy dz = 0.02083333333333333333333333333333333333$						
			Tra	nsformation-1		
N	GGQM N GLJQM BY GLQM by Rathod[2005]					
			RATHOD[2011]	P ³ =6 ³	$P^{3}=7^{3}$	$P^{3}=8^{3}$
5	0.020834525016257	7	0.020916599226093	0.0208333333333328	0.02083333333333333	0.02083333333333333
10	0.020833333335968	8	0.020833329020945	0.02083333333333333	0.02083333333333333	0.02083333333333333
15	0.02083333333333333	9	0020833332878624	0.02083333333333333	0.02083333333333333	0.02083333333333333
20	0.02083333333333333	10	0.020806898469793	0.02083333333333333	0.02083333333333333	0.02083333333333333
	Transformation-2					
N GGQM N GLJQM by Rathod			GLQM by Rathod[2007]			
			and Shafiqul[2007]	P ³ =6 ³	$P^{3}=7^{3}$	$P^{3}=8^{3}$
5	0.020833253744181	7	0.020833332245126	0.0208333333333170	0.02083333333333331	0.02083333333333333
10	0.020833333333470	8	0.020833332255096	0.02083333333333333	0.02083333333333333	0.02083333333333333
15	0.02083333333333333	9	0.020833333237911	0.02083333333333333	0.02083333333333333	0.02083333333333333
20	0.02083333333333333	10		0.02083333333333333	0.02083333333333333	0.02083333333333333

$I_6 = \iiint_T x^3 \sin(y\pi) \sin(z\pi) dx dy dz = 0.0011802 \text{\texttt{5}42112911}$					
Ν	GGQM	GGQM			
	Transformation-1	Transformation-2			
5	0.001174767313633	0.001172338527940			
10	0.001180215414563	0.001180215405319			
15	0.001180215421129	0.001180215421129			
20	0.001180215421129	0.001180215421129			