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Alternative Approach to Evaluation of Absorption Correction Factor for Cylinder using Generalised Gaussian Quadrature Rule

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Abstract. This paper presents Numerical evaluation of Absorption correction factor for cylinder by using Generalised Gaussian quadrature rule. The new formula increases the accuracy in comparison with the original Gauss-Legendra quadrature rules and Simpson's method which were recently applied by Maslen(1999) and Takashi Ida(2010) et al. results obtained with the Generalised Gaussian quadrature method are compared with the existing formulae. It is shown that the Generalised Gaussian quadrature method has higher accuracy than the existing formulae.

Keywords: Finite element method, Generalised Gaussian quadrature rule, Numerical Integration.

AMS Mathematics Subject Classification (2010): 65R10

1. Introduction

The path traversed by a monochromatic beam of intensity I_0 through a homogeneous isotropic material of linear absorption coefficient μ. Then reduced intensity in the beam is given by

$$I = I_0 e^{-\mu T} \tag{1}$$

The path length T of the beam in the material (crystal) varies as the shape of the crystal. Therefore this equality can also be considered for the X-ray absorption for the crystalline solids whose absorption does not depend on the arrangement of the atoms in the unit cell. If the crystalline solid have a definite shape then different paths have different lengths T, then we have

$$L = \int_v I \, dv \tag{2}$$

Where v is the volume of the crystal the expression for the transmission coefficient is given by $A = \frac{1}{v}\int_v I_0 \, e^{-\mu T} \, dv$ (3)

This formula above Eq. (3) was formulated for the estimation of transmission factor in crystals of uniform cross-section as *A* depends on the thickness, the shape of the crystal

through which the beam has traversed and the Braggs angle θ, the angle of orientation with respect to incident and diffracted beams, A is termed as function of μ and θ i.e. A(μ, θ) where μ is linear absorption coefficient and the reciprocal of total over all absorption coefficient is called absorption correction factor A^*

In the past ***claasen*** solved the absorption coefficient *A* by geometrical construction for the cylindrical samples (tungsten) by graphical integration and later on as a result a table listing absorption correction factor A^* where tabulated in *International tables for X-ray crystallography(1959)* as a function of Braggs angle θ and μR, where R is the radius of the cylinder. which have a maximum error of one percent. This tabled numerical values can also be considered as absorption for single crystal circular cylinder samples provided the beam is perpendicular to the axis of the cylinder and later on Maslen (1999) tabled the numerical values of Absorption correction factor $A^*(\mu R, \theta)$ for cylinder in *International tables for crystallography Vol. C* (1975) by solving integral

$$A^*(\mu R,\theta) = \frac{4}{\pi}\int_0^{\frac{\pi}{2}}\int_0^{1} x\, exp(-\mu R\{[1-x^2sin^2(\theta-y)]^{1/2} + [1+x^2sin^2(\theta-y)]^{1/2}\})\ \cosh(2\mu R\, x\, sin\theta\, siny)\, dx\, dy \tag{4}$$

Proposed by Dwiggins (1975) using Simpsons numerical integration. Due to the existence of the singularity in the integrant at x = 1 and $\emptyset = \frac{\pi}{2} - \theta$ the formula was not favorable for the application of numerical integration. Thorkildsen and Larsen (1998a,b) proposed another formula

$$A(\mu R,\theta) = \frac{2}{\pi sin2\theta}\int_0^{2\theta}\int_0^{\pi-2\theta} exp\left[\frac{-2\mu R sinx\cos(y-\theta)}{cos\theta}\right]\sin(x+y)\sin(x-y+2\theta)\, dxdy \tag{5}$$

Takashi ida (2010) applied Gauss-Legendere quadrature formula to solve the above Eq. (5) over the range $0 \leq \mu R \leq 2.5$ and $0 \leq \theta \leq 90^0$ and achieved much more accuracy in the numerical values then Simpsons method applied to Diwiggins Eq. (4)

In this paper we have applied General Gaussian Quadrature rule to calculate $A^*(\mu R, \theta)$ the absorption correction factor using C.W. Dwiggins two-dimension integral formula Eq. (4), this method will improve the accuracy and efficiency of the finite element approach and make it more competitive with other Numerical methods like Gauss Legendre quadrature and Simpson's methods. It is easily recognized that in this approach the computational convenience, speed and accuracy are enhanced many fold.

2. Generalised Gaussian quadrature

Let us consider the integral of the form

$$\int_a^b q(x)\, \emptyset(x)dx = \sum_{k=1}^{n} W_k^{(n)}\, \emptyset(x_k^n) \tag{6}$$

with $x_k^n \in [a,b]$ and $W_k^{(n)} \in R$ for all $k = 1,2,3,---,n$. The points x_k^n and coefficients $W_k^{(n)}$ are referred to as sampling points and weights coefficients.

The quadrature formula given in Eq.(6) is said to be Generalized Gaussian quadrature rule with respect to the functions $\{\emptyset_k\}_{k=1}^{2n}$, if it integrals exactly all the 2N functions. The Generalized Gaussian quadrature rule with respect to the system of function defined as $\{1, \ln x, x, x \ln x\, , x^2, x^2 \ln x, x^3, x^3 \ln x\, , - - -, x^{n-1}, x^{n-1} \ln x\}$ on [0, 1] for N = 5,10,15, 20, 40 are given in Table 1 (J. Ma. et al., 1996). we shall be using these sampling points and its weights in the product of polynomial and logarithmic function in this paper

3. Numerical method

The integral of the Eq. (4) can be transformed to square region $\{(\xi, \eta) / 0 \leq \xi \leq 1, 0 \leq \eta \leq 1\}$, the mathematical transformation is

$x = \xi$ and $y = \frac{\pi}{2}\eta$ (7)

We have

$A^*(\mu R, \theta) = \frac{4}{\pi}\int_0^1 \int_0^1 f\big(x(\xi\, ,\eta), y(\xi\, ,\eta)\big)\, J d\xi d\eta$ (8)

Where $J\,(\xi\, ,\eta)$ is the Jacobians of the transformation

$$J(\xi\, ,\eta) = \begin{vmatrix} \frac{\partial x}{\partial \xi} & \frac{\partial y}{\partial \xi} \\ \frac{\partial x}{\partial \eta} & \frac{\partial y}{\partial \eta} \end{vmatrix} = \frac{\pi}{2}$$

From Eq. (8) , we can write as

$$A^*(\mu R, \theta) = \frac{4}{\pi}\int_0^1 \int_0^1 f\left(\xi, \frac{\pi}{2}\eta\right) \frac{\pi}{2}\, d\xi\, d\eta$$

$$= \frac{4}{\pi}\sum_{i=1}^{m}\sum_{j=1}^{n} \frac{\pi}{2}\, w_i w_j\, f\big(x(\xi_i\, ,\eta_j)\, , y(\xi_i\, ,\eta_j)\big)$$ (9)

where $\xi_{i\,,}\, \eta_j$ are sampling points and w_i, w_j are corresponding weights. We can rewrite Eq. (9) as

$A^*(\mu R, \theta) = \frac{4}{\pi}\sum_k^{N=m\times n} W_k f(x_k, y_k)$ (10)

where $W_k = \frac{\pi}{2}\, w_i\, w_j$ (10a)

$x_k = \xi\,,$ (10b)

$y_k = \frac{\pi}{2}\eta\,,$ (10c)

if $k = 1,2,3, \ldots\,,\ i, j = 1,2,3, \ldots$

we present the following algorithm to calculate sampling points and weights as

***Step* 1**. $k \to 1$

***Step* 2**. $i = 1, m$

***Step* 3**. $j = 1, n$

$W_k = \frac{\pi}{2}\, w_i\, w_j\,,\ x_k = \xi_i\,,\ y_k = \frac{\pi}{2}\eta_j$

$k = k + 1$

***Step* 4**. *compute step* 3

***Step* 5**. *compute step* 2

to computed the sampling points and corresponding weights based on the above algorithm for order N = 5, 10, 15, 20 and are listed in table 1

k	x_k	y_k	W_k
1	0.005652228	0.008878499	0.000695822
2	0.073430372	0.008878499	0.004321186
3	0.284957404	0.008878499	0.009577693
4	0.619482264	0.008878499	0.011578448
5	0.915758083	0.008878499	0.006887316
6	0.005652228	0.115344158	0.004321186
7	0.073430372	0.115344158	0.026835388
8	0.284957404	0.115344158	0.059479296
9	0.619482264	0.115344158	0.071904369
10	0.915758083	0.115344158	0.042771545
11	0.005652228	0.447610044	0.009577693
12	0.073430372	0.447610044	0.059479296
13	0.284957404	0.447610044	0.131832889
14	0.619482264	0.447610044	0.159372441
15	0.915758083	0.447610044	0.094800992
16	0.005652228	0.973080465	0.011578448
17	0.073430372	0.973080465	0.071904369
18	0.284957404	0.973080465	0.159372441
19	0.619482264	0.973080465	0.192664936
20	0.915758083	0.973080465	0.114604677
21	0.005652228	1.438469433	0.006887316
22	0.073430372	1.438469433	0.042771545
23	0.284957404	1.438469433	0.094800992
24	0.619482264	1.438469433	0.114604677
25	0.915758083	1.438469433	0.068171366

Table 1: Generalised Gaussian quadrature rule of order N = 5

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μR	Exact	Dwiggins et. al	Maslen et al	Order	Computed value
0.1	1.18432	1.1843	1.1843	N=5 N=10 N=15 N=20	1.1845194836 1.1843662195 1.1843273883 1.1843273942
0.5	2.29961	2.2996	2.2996	N=5 N=10 N=15 N=20	2.2990541915 2.2996721602 2.2996132835 2.2996132774
1.0	5.09098	5.0907	5.0907	N=5 N=10 N=15 N=20	5.0905632101 5.0906423155 5.0909877128 5.0909870547
1.5	10.74774	10.7461	10.746	N=5 N=10 N=15 N=20	10.717315508 10.747033755 10.747740901 10.747740988
2.1	24.42587	24.4137	24.41	N=5 N=10 N=15 N=20	24.413544120 24.429115796 24.425806331 24.425878213
2.5	40.09687	40.0598	40.06	N=5 N=10 N=15 N=20	40.093367137 40.096510969 40.096531445 40.096874421

Table 2: Values of A^* for cylinder at $\theta = 0$

θ^0	Exact	Dwiggins et. al	Maslen et al	Order	Computed Value
0	5.09098	5.0907	5.9356	N=5 N=10 N=15 N=20	5.0917550823 5.0903521761 5.0909809533 5.0909807315
15	4.93242	4.9323	4.9323	N=5 N=10 N=15 N=20	4.9321135091 4.9324844063 4.9324648967 4.9324254079
30	4.54397	4.5439	4.5439	N=5 N=10 N=15 N=20	4.5437653242 4.5439456271 4.5439773164 4.5439760213
45	4.10228	4.1022	4.1022	N=5 N=10 N=15 N=20	4.1029754431 4.1022555764 4.1022887210 4.1022886500
60	3.72865	3.7286	3.7286	N=5 N=10 N=15 N=20	3.7281742193 3.7280321167 3.7286509350 3.7286506541
75	3.47912	3.4790	3.4790	N=5 N=10 N=15 N=20	3.4796452313 3.4791453709 3.4791220902 3.4791220993
90	3.38875	3.3886	3.3886	N=5 N=10 N=15 N=20	3.3876409521 3.3884200166 3.3887576218 3.3887547425

Table 3: Values of A^* for cylinder at $\mu R = 1$

4. Conclusion

Numerical integration approach for evaluating Absorption correction factor A^* using Generalized Gaussian quadrature rule is presented in detail, the results obtained are in excellent agreement with exact value, the good results shows that further developments of the present procedure for finding A^*

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