NPRE 555 Computational Project-3
Spring 2018

Discrete Ordinate Method Using Radau's Quadrature Set

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I. Abstract

In this report, the discrete ordinate method using the Radau's quadrature set is discussed and implemented. The report starts with deriving the necessary equations used to develop a code, to solve a one-dimension slab geometry, with vacuum boundary conditions, making use of Marshak's boundary conditions. Then, results obtained by using this method are compared with using Gauss-Legendre's quadrature set and also Chebyshev's quadrature set. A study of the spatial convergence and the order of accuracy of the Radau's method is demonstrate at the end.

The problem that we are dealing with in this report, is a two-region infinite bare slab of moderator which has total thickness $L = 6\ cm$. The first region has ($\Sigma t = 1\ Cm^{-1}$, $\Sigma a = 0.5\ Cm^{-1}$) and contains a uniformly distributed isotropic unit source $\left(1 \frac{n}{Cm-s}\right)$ for $(0 < x < 2\ Cm)$. The second region has no source, and has ($\Sigma t = 1.5\ cm^{-1}$, $\Sigma a = 1.2\ cm^{-1}$) for $(2\ Cm < x < 6\ Cm)$.

II. Discrete Ordinates Equations

The idea of discrete ordinate is to approximate the integration of the partial flux term using a certain numerical integration. As an approximate method that can capture the effect of the angle discretization in the space is that using certain set of quadrature that approximate the solution. In the following we derived the equations needed to develop a computer code to solve the discrete ordinate solution of a slab geometry using Marshak's boundary conditions.

$For\ one\ speed, one\ dimensional, steady\ state, the\ transport\ eqn\ is\ as\ follows:$

$$\mu \frac{d\psi}{dx} + \Sigma_t(x)\, \psi(x,\mu) = \frac{\Sigma_s(x)}{2} \int_{-1}^{1} d\mu' \psi(x,\mu') + \frac{S(x)}{2}$$

$S_n \rightarrow general\ eqn.$

$$\mu_i \frac{d\psi(x,\mu_i)}{dx} + \Sigma_t(x)\psi(x,\mu_i) = \frac{\Sigma_s(x)}{2} \sum_{i=1}^{N} \omega_i\, \psi(x,\mu_i) + \frac{S(x)}{2} \qquad i = 1,2,\ldots,N$$

$$\therefore\ \psi^m{}_{i\pm1,n}(x_{i\pm1},\mu_n) = A^{\pm}{}_{i,n}(x_i,\mu_n)\ \psi^m{}_{i\mp1,n}(x_{i\mp1},\mu_n) + B^{\pm}{}_{i,n}(x_i,\mu_n)\ Q^{m-1}{}_i\,(x_i)$$

$where,$

$i: 'even" \rightarrow i\ (from\ 2-l)\ :\ is\ the\ index\ of\ the\ central\ point,$

$i+1: index\ of\ the\ right\ edge\ of\ each\ mesh,$

$i_1: index\ of\ the\ left\ edge\ of\ each\ mesh.$

$\underline{Marshak's\ Boundary\ conditions}$:

1) $\psi^{m}{}_{1,n}(x_1,\mu_n) = 0\ (for\ \mu_n > 0)$

2) $\psi^{m}{}_{l+1,n}(x_{l+1},\mu_n) = 0\ (for\ \mu_n < 0)$

$\underline{By\ using\ the\ Diamond\ difference\ approach}$:

$$\therefore\ \alpha_n = 0\ , \qquad A^{\pm}{}_{i,n} = \frac{2\mu_n \mp \sum_{ti}(x_i)\Delta_i}{2\mu_n \pm \sum_{ti}(x_i)\Delta_i} \quad , \qquad B^{\pm}{}_{i,n} = \frac{\pm 2\Delta_i}{2\mu_n \pm \sum_{ti}(x_i)\Delta_i}$$

$$Q_i{}^{m-1}(x_i) = \frac{1}{2}\Big(\Sigma_{is}(x_i)\ Q_i{}^{m-1}(x_i) + S_i(x_i)\Big)$$

$$\varphi_i{}^{m-1}(x_i) = \sum_{n}^{N} \omega_n\ \psi_{i.n}{}^{m-1}\ (x_i,\mu_n)$$

$\underline{For\ Diamond\ difference}$:

$$(\alpha_n = 0\ ) \rightarrow\ \ \psi^{m-1}{}_{i,n}(x_i,\mu_n) = \tfrac{1}{2}\ \Big(\psi^{m-1}{}_{i+1,n}(x_{i+1},\mu_n) +\ \psi^{m-1}{}_{i-1,n}(x_{i-1},\mu_n)\Big)$$

$\underline{Source\ Convergence\ criterion}$:

$$Maximum\ difference\ for\ all\ x_i\ :\ \left(\tfrac{|\varphi_i{}^{m}(x_i) - \varphi_i{}^{m-1}(x_i)\,|}{\varphi_i{}^{m-1}(x_i)}\right) < \varepsilon_{\varphi}$$

$\underline{I. Forward\ sweeping}$:

$For\ \mu_n > 0\ , \mu_1 = 0.57735\ \ , \omega_1 = 1$

$$\psi^{m}{}_{i+1,n}(x_{i+1},\mu_n) = A^{+}{}_{i,n}(x_i,\mu_n)\ \ \psi^{m}{}_{i-1,n}(x_{i-1},\mu_n) +\ B^{+}{}_{i,n}(x_i,\mu_n)\ Q^{m-1}{}_{i}(x_i)$$

$\underline{II. Backward\ sweeping}$:

$For\ \mu_n < 0\ ,\ \ \ \mu_2 = 0.57735\ \ , \omega_2 = 1$

$$\psi^{m}{}_{i-1,n}(x_{i-1},\mu_n) = A^{-}{}_{i,n}(x_i,\mu_n)\ \ \psi^{m}{}_{i+1,n}(x_{i+1},\mu_n) +\ B^{-}{}_{i,n}(x_i,\mu_n)\ Q^{m-1}{}_{i}(x_i)$$

In Table-1, the first 4 orders of Radau's quadrature sets are inserted, [1] While Table-2 and Table-3, are the sets for Chebyshev quadrature and Gauss quadrature respectively.

Table-1 Radau's Quadrature Set

N	$\pm\mu_n$	ω_n
2	1	1
4	0.4472136	0.833333
	1	0.16666667
6	0.0813570	0.5548584
	0.7650553	0.3784750
	1	0.0666667
8	0.2092992	0.4124591
	0.5917002	0.3411227
	0.8717401	0.2107042
	1	0.0357143

Table-2 Chebyshev's Quadrature Set

N	$\pm\mu_n$	ω_n
2	0.77459	0.43033
4	0.50029	0.23937
	0.89223	0.23937
6	0.44298	0.15991
	0.71215	0.15991
	0.92930	0.15991

Table-3 Gauss' Quadrature Set

$\pm\mu_n$	ω_n
0.57735	1.00
0.33998	0.65214
0.86113	0.34785
0.23861	0.46791
0.66120	0.36076
0.93246	0.17132

III. The Algorithm and Results

In this part, we will discuss how the developed codes work, and then we will introduce the results of each code. In this project three main codes were developed. One for implementing the discrete ordinate solution using the Radau's quadrature set, for a prespecified number of space meshes, and 4 quadrature. Then, it compares its results with the results obtained from implementing the discrete ordinate using Gauss-Legendre's quadrature set and Chebyshev's quadrature set. The second code is to apply a space convergence study, and the last one is to increase the order of accuracy of the method and demonstrate accuracy convergence of the method.

The main algorithm of the code developed is to calculate $\varphi_i{}^m(x_i)$ and $Q_i{}^m(x_i)$ to find $\psi^m{}_{i,n}(x_i, \mu_n)$ at each point using an iterative scheme. The iterations should stop when the value of $\varphi_i{}^m(x_i)$ became stable for successive iterations. So that, the difference between them satisfied a certain convergence criterion ε_φ as expressed in the previous section. A sweeping to the right, in order to find $\psi^m{}_{i+1,n}(x_{i+1}, \mu_n)$ for positive quadrature and a sweeping to the left to find $\psi^m{}_{i-1,n}(x_{i-1}, \mu_n)$ for negative quadrature at each point is used while iterating. A careful consideration should be given to the change of region as the material properties are different between the two regions. During all of this we keep the boundary conditions of zero incoming current at the vacuum boundaries.

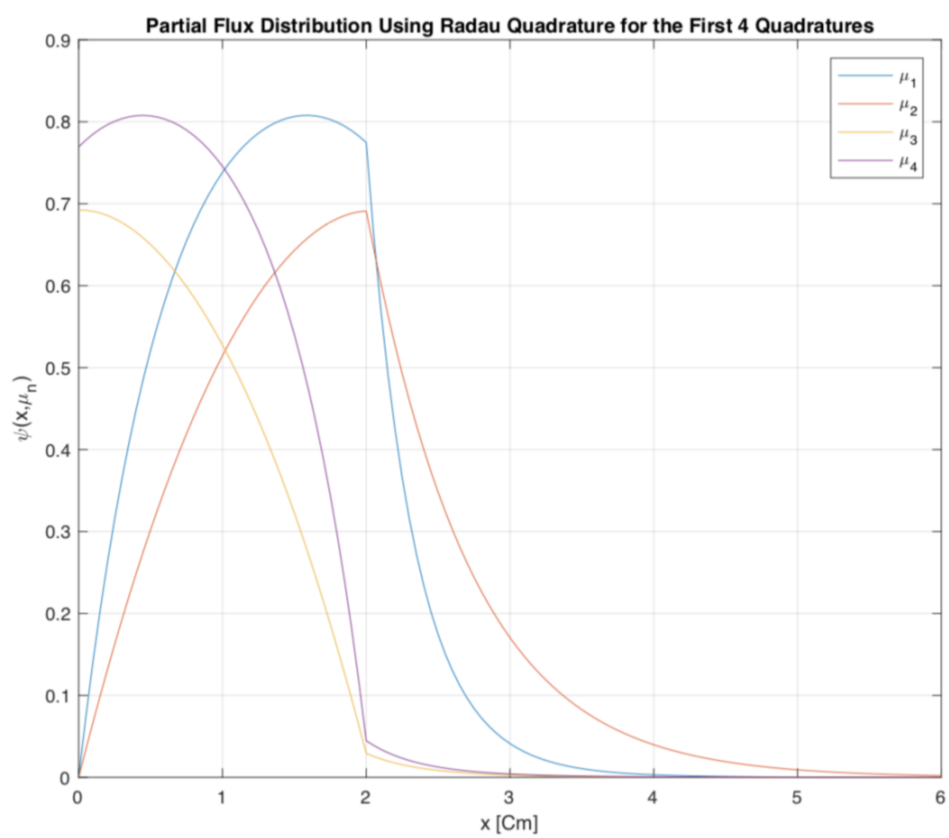

Figure 1 Partial Fluxes Using Radau Quadrature

In Figure-1, The partial fluxes corresponding to the 4th order Radau's set is shown. In Figure-2, the rightward and leftward angular fluxes distributions for this order is introduced, and in Figure-3, the scalar flux distribution is introduced.

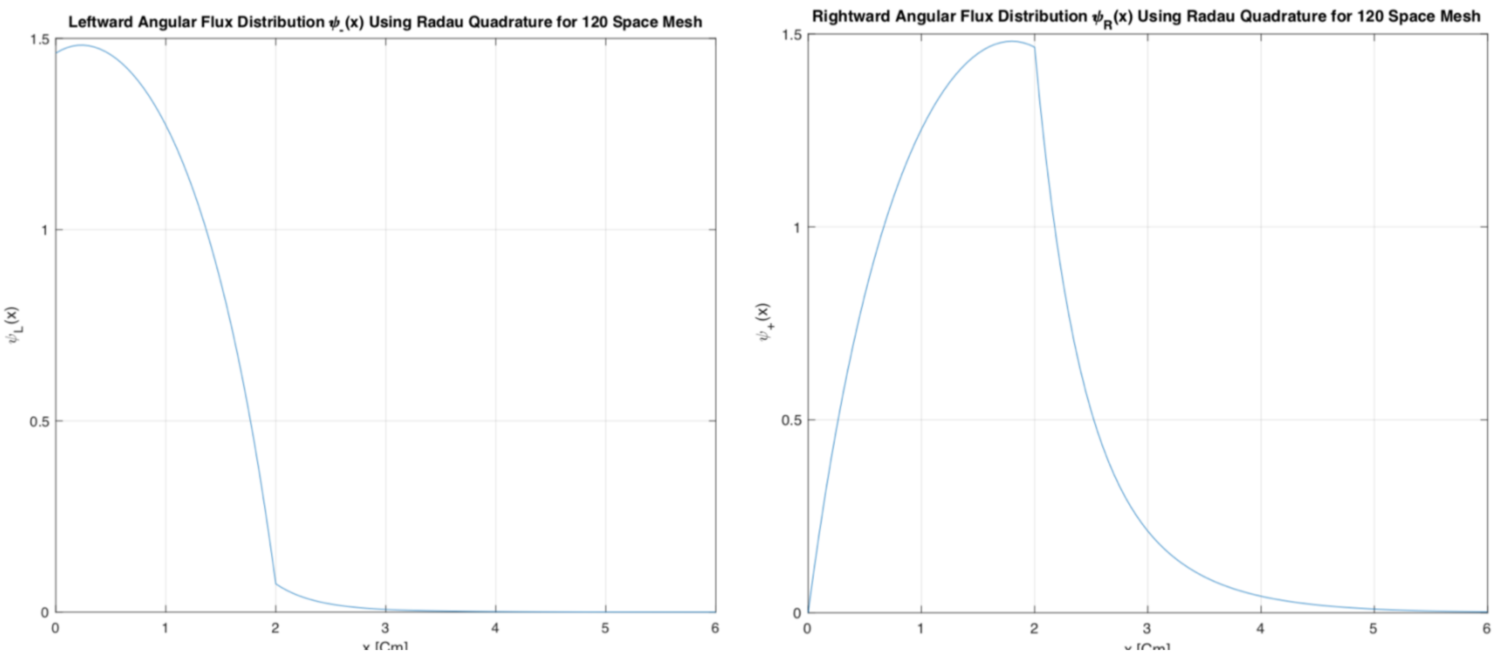

Figure 2 The Rightward and Leftward Angular Fluxes

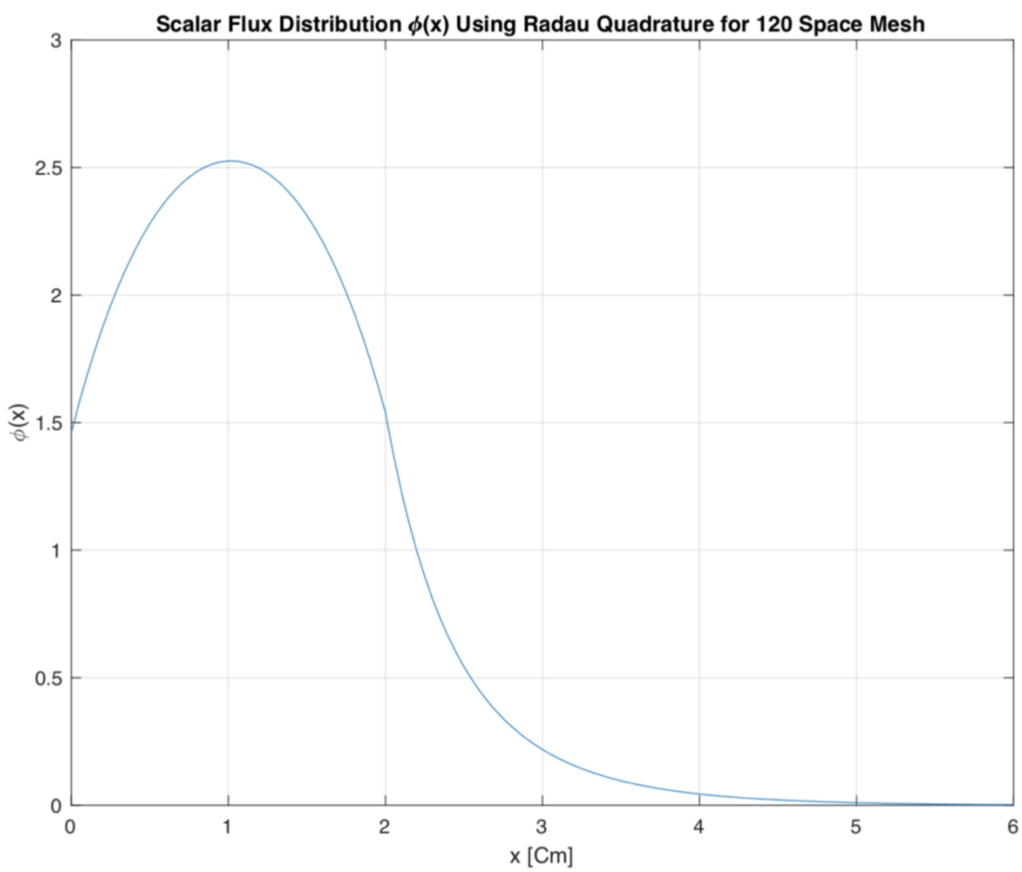

Figure 3 Scalar Flux Distribution

A comparison between the leftward angular fluxes, rightward angular fluxes, and scalar fluxes distributions, are estimated using Gauss-Legendre's quadrature vs Radau's quadrature can be found in Figure-4, and Figure-5, respectively.

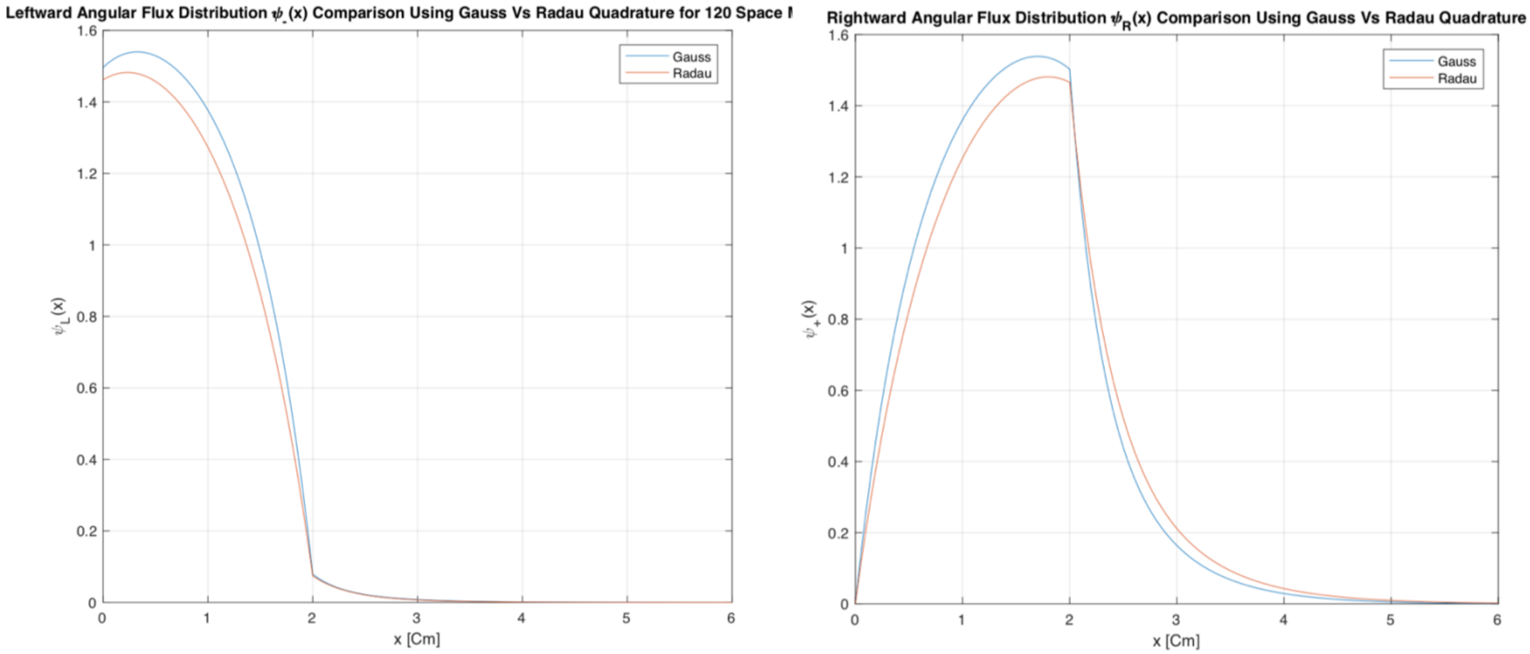

Figure 4 Comparison for the leftward and rightward angular fluxes for G-L Vs Radau

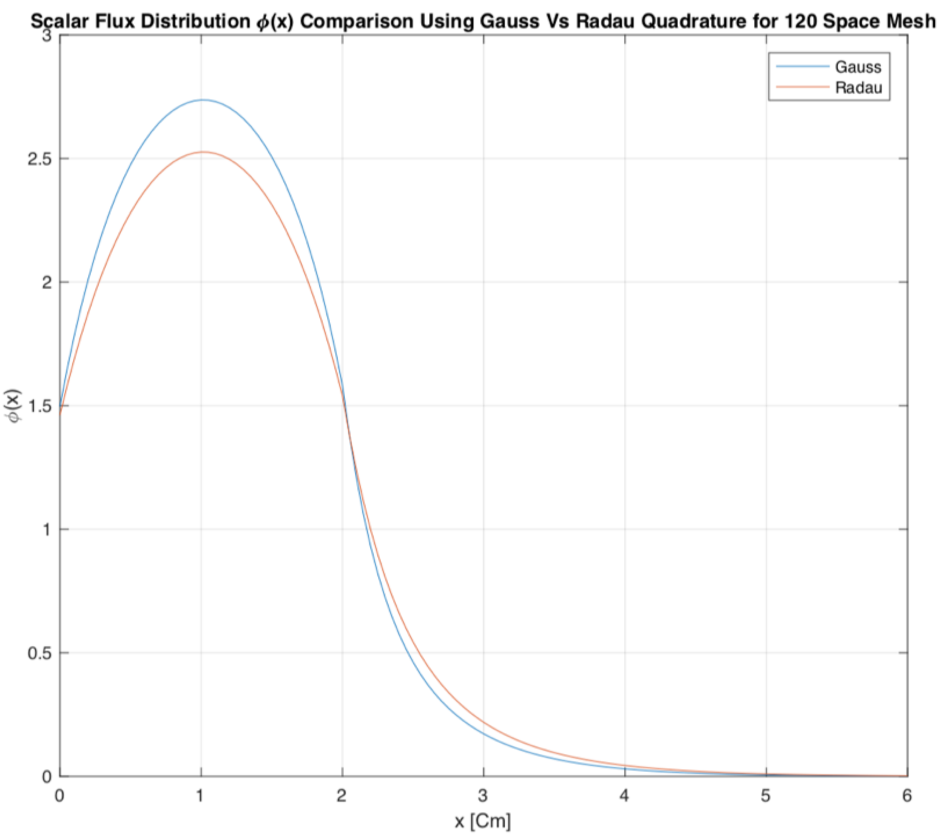

Figure 5 Comparison for the scalar fluxes for G-L Vs Radau

A comparison between the leftward angular fluxes, rightward angular fluxes, and scalar fluxes distributions, estimated using Gauss-Legendre's quadrature vs Radau's quadrature vs Chebyshev's quadrature can be found in Figure-6 and Figure-7, respectively.

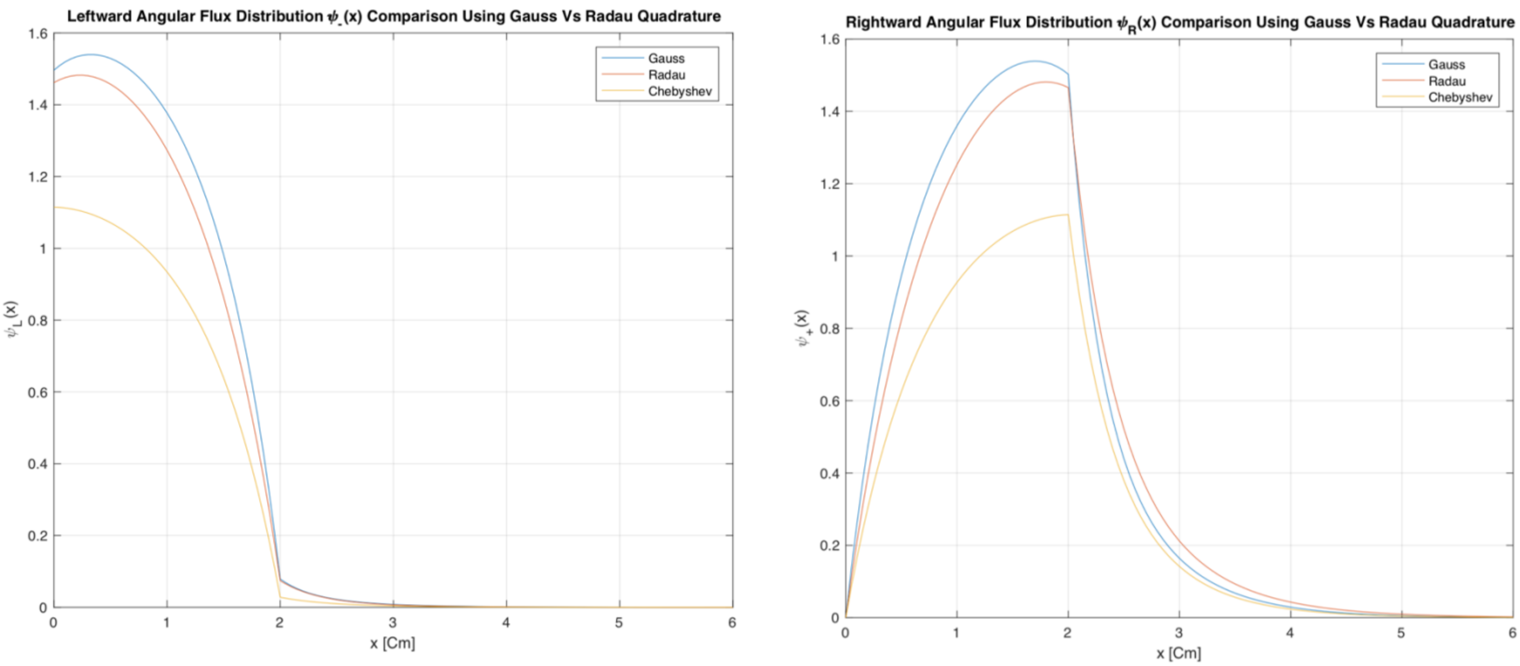

Figure 6 Comparison for the leftward and rightward angular fluxes for G-L Vs Radau Vs Chebyshev

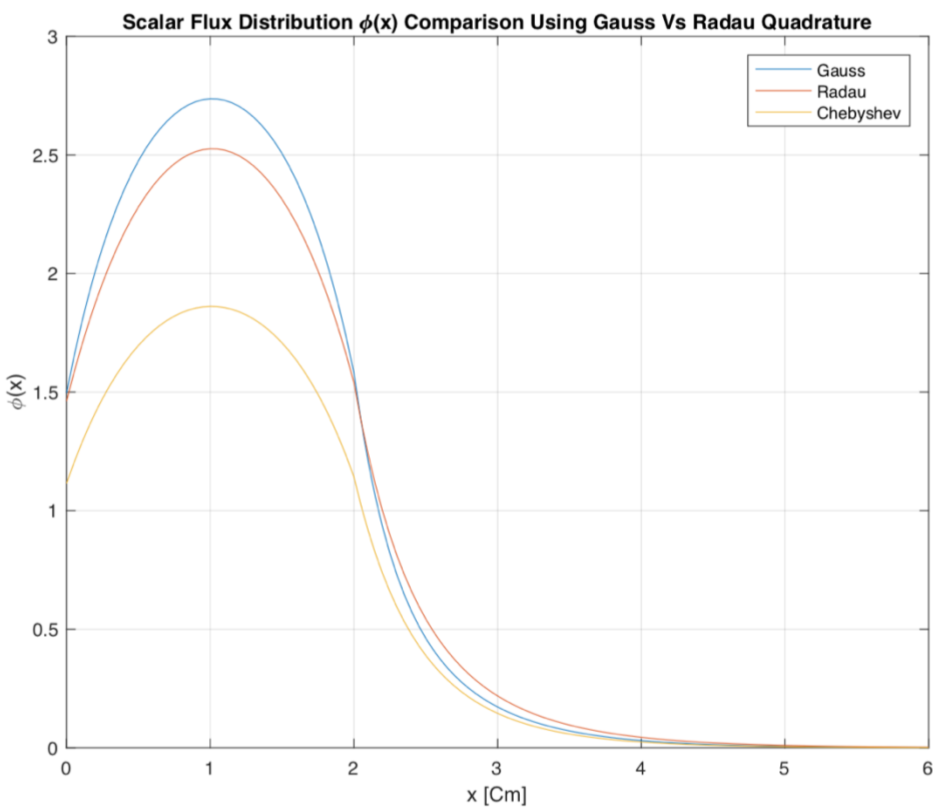

Figure 7 Comparison for the scalar fluxes for G-L Vs Radau Vs Chebyshev

IV. Spatial Convergence using Radau's Quadrature

A study of the spatial convergence, is done by changing the number of space meshes in a systematic way and calculate the difference in the scalar flux between the different iterations till it match a certain convergence criterion, exactly as done before, is carried out. This procedure is somewhat challenging because in order to avoid being bothered by the plain that separate the two regions, we have to consider the number of meshes that covers the slab to be only multiples of 3. The error estimated vs the number of spatial meshes is introduced in Figure-8.

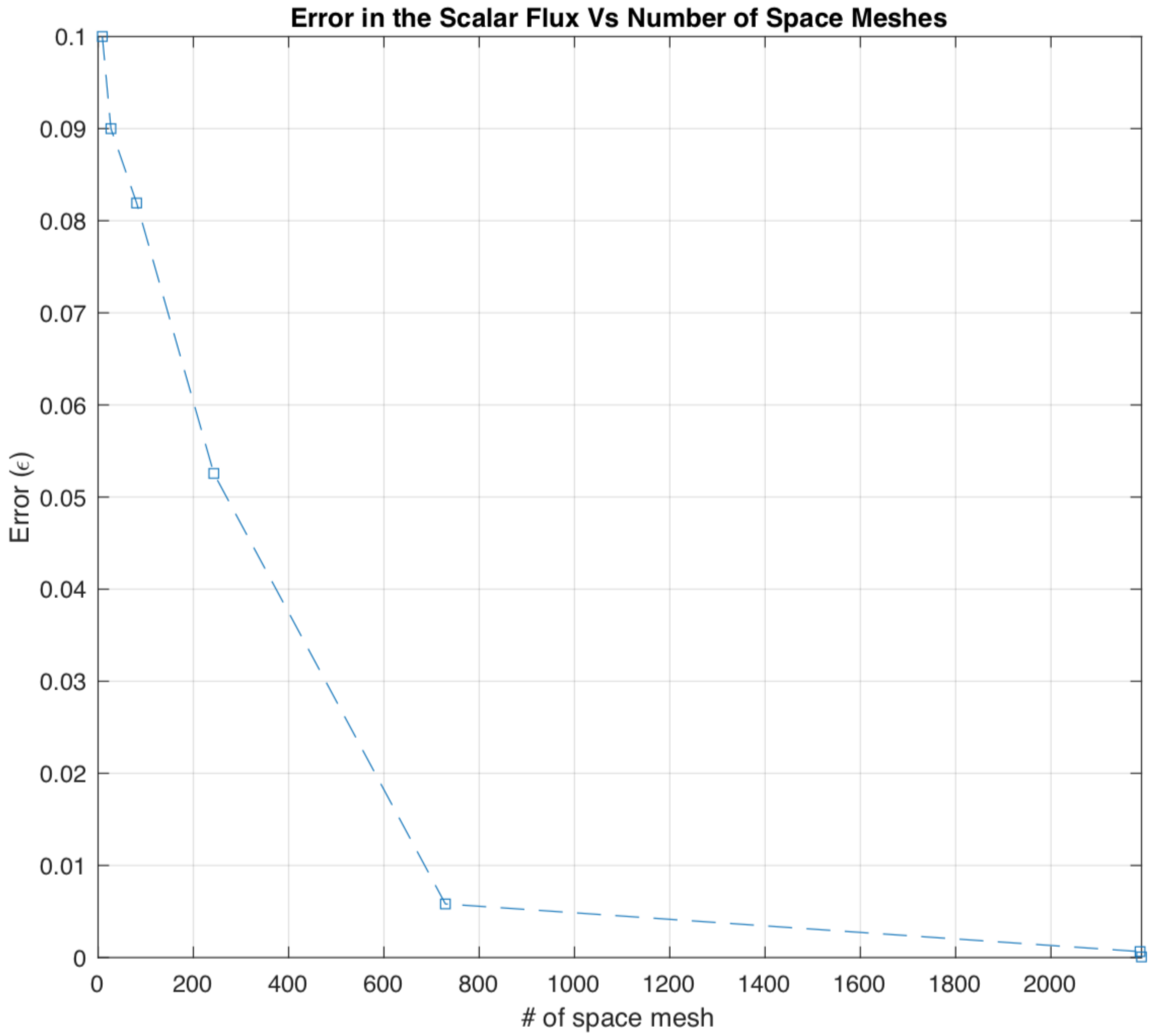

Figure 8 Spatial Convergence using Rabau's Quadrature

V. Accuracy Convergence using Radau's Quadrature

If we fixed the number of space meshes to be sufficiently a big number, we can study the accuracy convergence of using the Radau's quadrature with increasing the considered order of used quadrature by calculating the flux change between these iterations. The values obtained is inserted in Figure-9 for 81 meshes.

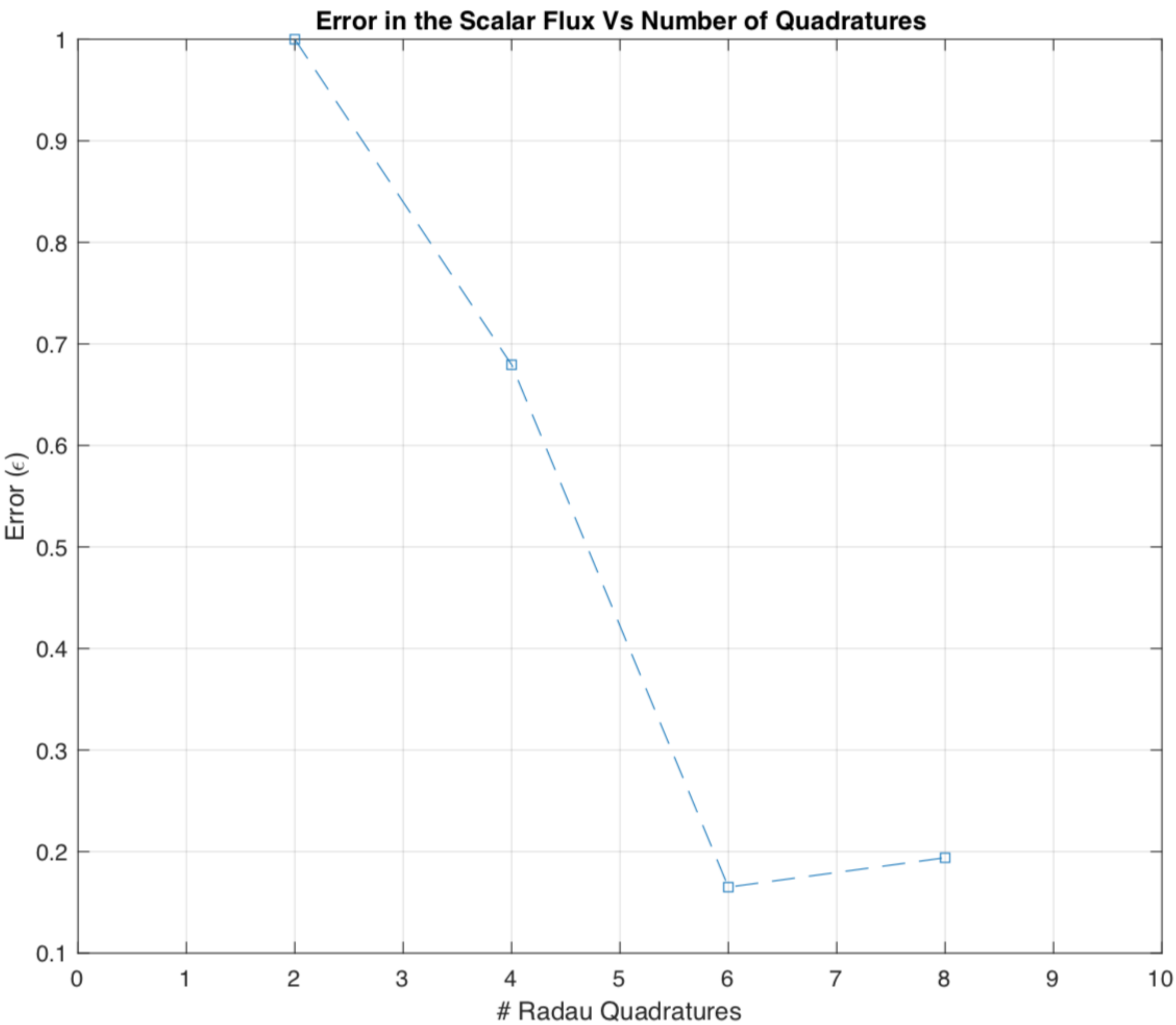

Figure 9 Accuracy Convergence using Rabau's Quadrature (the x-axis indicate the number of used quadrature which is the order of approximation)

As seen from the previous figure, increasing the order of approximation decreases the error and increases the accuracy, only till it reaches the 8^{th} order, which shouldn't be the case! And unfortunately, I couldn't get an access to the values of higher orders in the references that I had access to. I tried the code on the G-L approach and this problem didn't appear, which may mean that this method may have a problem with the accuracy for some orders, however it may also be due to a mistake in my code.

VI. Conclusion

The Rabau's quadrature set for solving the transport equation for a slab system, can be implemented easily for Cartesian systems, which provides a quick spatially converging solution. However, at the same time, its results are not as fast converging as the Gauss-Legendre's method. In addition, this method may diverge for certain higher orders, which doesn't make it reliable for many calculations. Maybe that's why this approach is rarely used for the neutronics calculations, and may be is used more for heat transfer calculations, where there is no source and destruction terms like in neutronics. It is worth mentioning that for the three used quadrature sets the Gauss-Legendre's set is far more better than the rest two, and the Rabau's method is better than the Chebyshev's method, as estimated for 4 order quadrature for each set.

VII. References

[1] S. Chandrasekhar, Radiative Transport, Dover Publication, Chapter II,1960.

[2] W. A. Fiveland, Discrete Ordinate Methods for Radiative Heat Transfer in Isotropically and Anisotropically Scattering Media, ASME-JHT, Vol. 109, 1987.

[3] W. A. Fiveland, Discrete-Ordinates Solutions of the Radiative Transport Equation for Rectangular Enclosures, ASME-JHT, Vol. 106, 1984.

[4] Beyer, W. H. CRC Standard Mathematical Tables, 28th ed. Boca Raton, FL: CRC Press, p. 466, 1987.