NPRE 555 Computer Project 3 Report

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1 T_N Approximation

In CP 2, the neutron transport equation was solved by P_N approximation, which was shown to be a powerful method to get satisfactory results of slab reactor with isotropic scattering and source. However, it convergences slowly with anisotropic scattering [1].To improve this, T_N approximation which uses Chebyshev polynomials to replace Legendre polynomials is proposed. Most of previous studies focused on solving criticality problem using T_N approximation. It is also shown that T_N can be applied to eigenvalue spectrum and diffusion length calculation for bare and reflected slab or spheres [2]. In addition, T_N approximation can be used for slab with strongly anisotropic scattering [3] as well. However, for weak absorber, the result accuracy using T_N method is not comparable to that using P_N approximation [1].

The basic idea of solving neutron transport problems using T_N approximation method is expanding differential flux, cross section and neutron sources using Chebyshev polynomials [1]. Then, the transport equation can be simplified and solved by applying orthogonality and recurrence relation of Chebyshev polynomials. In this report, instead of criticality problem where T_N approximation is widely used, the scalar neutron flux distribution in a 1-D slab reactor with isotropic scattering and isotropic source will be solved using T_N approximation.

2 Problem Description

2.1 Basic problem

The problem solve in CP 2 using P_N method is chosen as the basic problem. The flux distribution in a 1-D slab reactor with isotropic scattering and isotropic source will be solved using one-speed neutron transport equation. The entire domain is uniformly divided into $M-1$ cells and the material properties are summarized in Table. 1.

Table 1: Material properties of reactor

Σ_t	$0.17\ cm^{-1}$
Σ_s	$0.10\ cm^{-1}$
Q	$10\ cm^{-3}s^{-1}$

The basic problem will be solved using T_1 approximation and the results will be compared with those evaluated using P_1 and P_3 approximation methods.

2.2 Challenging problems

2.2.1 Spatial convergence

Spatial convergence will be conducted for T_1 approximation and the result will be used in hight order accuracy approximation. Initially, the entire domain is divided into 10 grid nodes and a initial guess of scalar flux ϕ_0 distribution is obtained. Then, the mesh size will increase with increment of 1 and the relative error ε will be compared to convergence criteria ε_0. If $\varepsilon \leq \varepsilon_0$, the mesh is considered converged. ε of mesh size $M+1$, ε_{M+1}, is defined as:

$$\varepsilon_{M+1} = \frac{|\mathrm{avg}\,[\phi_0(\mathrm{M}+1)] - \mathrm{avg}\,[\phi_0(\mathrm{M})]|}{\mathrm{avg}\,[\phi_0(\mathrm{M})]}$$

2.2.2 Order of accuracy convergence

A general solution of T_N approximation for 1-D slab reactor will be obtained. As is similar to P_N, only odd ordered T_N approximations are considered. Then, the order of accuracy, N, will increase gradually with increment of 2. The relative error ε will be compared to the threshold ε_0, if $\varepsilon \leq \varepsilon_0$, the result is considered converged. And ε of T_{N+2} approximation (ε_{N+2}) is defined as:

$$\varepsilon_{N+2} \equiv \frac{\max|\phi_0(T_{N+2}) - \phi_0(T_N)|}{\phi_0(T_N)}$$

3 Theory

The one-dimensional neutron transport equation, for isotropic scattering and source, is:

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

Expand $\psi(x,\mu)$ and $Q(x,\mu)$ using Chebyshev polynomials of first kind:

$$\psi(x,\mu) = \frac{\phi_0(x)}{\pi\sqrt{1-\mu^2}} T_0(\mu) + \frac{2}{\pi\sqrt{1-\mu^2}} \sum_{n=1}^{N} \phi_n(x) T_n(\mu)$$

$$Q(x,\mu) = \frac{Q_0(x)}{\pi\sqrt{1-\mu^2}} T_0(\mu) + \frac{2}{\pi\sqrt{1-\mu^2}} \sum_{n=1}^{N} Q_n(x) T_n(\mu)$$

T_n are orthogonal with the weight $\frac{1}{\sqrt{1-x^2}}$ over the interval $[-1,1]$. Therefore, we have:

$$\int_{-1}^{1} \frac{T_n(x)T_m(x)}{\sqrt{1-x^2}}dx = \begin{cases} 0 & n \neq m \\ \pi & n = m = 0 \\ \frac{\pi}{2} & n = m \neq 0 \end{cases}$$

The recurrence relation of the Chebyshev polynomials of the first kind is:

$$2\mu T_n(\mu) = T_{n+1}(\mu) + T_{n-1}(\mu)$$

Using the orthogonality of T_n and recurrence relation, the neutron transport equation can be written as:

$$\frac{d\phi_1(x)}{dx} + \Sigma_t \phi_0(x) = \Sigma_s \phi_0(x) + Q_0(x)$$

$$\frac{d\phi_2(x)}{dx} + \frac{d\phi_0(x)}{dx} + 2\Sigma_t \phi_1(x) = 2Q_1(x)$$

$$\frac{d\phi_{n+1}(x)}{dx} + \frac{d\phi_{n-1}(x)}{dx} + 2\Sigma_t \phi_n(x) = \frac{[1+(-1)^n]}{1-n^2}\Sigma_s \phi_0(x) + 2Q_n(x), \quad n \geq 2$$

3.1 General equations

For T_{2N+1} approximation, $d\phi_{2N+2}/dx = 0$. Therefore, for $n \neq 0$ and $n \neq 2N+1$,

$$\frac{d\phi_{n+1}(x)}{dx} + \frac{d\phi_{n-1}(x)}{dx} + 2\Sigma_t \phi_n(x) = \frac{[1+(-1)^n]}{1-n^2}\Sigma_s \phi_0(x) + 2Q_n(x), \quad n \geq 2$$

where:

$$\phi_n(x) = \int_{-1}^{1} \psi(x,\mu)T_n(\mu)d\mu$$

$$Q_n(x) = \int_{-1}^{1} Q(x,\mu)T_n(\mu)d\mu$$

If we introduce new set of variables F_n for T_{2N+1} approximation ($N \geq 1$) and define:

$$F_N = \phi_{2N}$$

$$F_n = \phi_{2n} + \phi_{2n+2}$$

The odd ordered T_n equation gives:

$$\begin{aligned}\phi_{2n+1}(x) &= \frac{1}{2\Sigma_t}\left[2Q_{2n+1}(x) - \frac{d\phi_{2n+2}(x)}{dx} - \frac{d\phi_{2n}(x)}{dx}\right] \\ &= \frac{1}{2\Sigma_t}\left[2Q_{2n+1}(x) - \frac{dF_n(x)}{dx}\right]\end{aligned}$$

Plug $\phi_{2n+1}(x)$ and $\phi_{2n-1}(x)$ into $2n_{th}$ ordered T_n equation:

$$\frac{d}{dx}\left\{\frac{1}{2\Sigma_t}\left[2Q_{2n+1}(x) - \frac{dF_n(x)}{dx}\right]\right\} + \frac{d}{dx}\left\{\frac{1}{2\Sigma_t}\left[2Q_{2n-1}(x) - \frac{dF_{n-1}(x)}{dx}\right]\right\} + 2\Sigma_t\phi_{2n}(x) = \frac{2\Sigma_s}{1-4n^2}\phi_0(x) + 2Q_{2n}(x)$$

And

$$\phi_{2n} = F_n - F_{n+1} + F_{n+2}\cdots = \sum_{m=0}^{N-n}(-1)^m F_{n+m}$$

For isotropic source and scattering:

$$Q_{2n+1} = Q_{2n-1} = 0$$

$$\boxed{-\frac{d^2F_n(x)}{dx^2} - \frac{d^2F_{n-1}(x)}{dx^2} + 4\Sigma_t^2\sum_{m=0}^{N-n}(-1)^m F_{n+m}(x) = \frac{4\Sigma_s\Sigma_t}{1-4n^2}\sum_{m=0}^{N}(-1)^m F_m + 4\Sigma_t Q_{2n}(x)} \tag{1}$$

Then, we can reduce the number of variables from $2N+2$ to $N+1$. Discretizing Eq 1:

$$\boxed{-\frac{F_n^{i-1} - 2F_n^i + F_n^{i+1}}{\Delta x^2} - \frac{F_{n-1}^{i-1} - 2F_{n-1}^i + F_{n-1}^{i+1}}{\Delta x^2} + 4\Sigma_t^2\sum_{m=0}^{N-n}(-1)^m F_{n+m}^i - \frac{4\Sigma_s\Sigma_t}{1-4n^2}\sum_{m=0}^{N}(-1)^m F_m^i = 4\Sigma_t Q_{2n}^i} \tag{2}$$

3.2 Special cases

If $n = 0$,

$$\boxed{-\frac{d^2F_0(x)}{dx^2} + 2\Sigma_t^2\sum_{m=0}^{N}(-1)^m F_m(x) = 2\Sigma_s\Sigma_t\sum_{m=0}^{N}(-1)^m F_m + 2\Sigma_t Q_0(x)}$$

3.3 Solution

Therefore, $F_n(x)$ of T_{2N+1} approximation with M grid nodes can be obtained by solving the following linear algebra system:

$$\mathbf{AF} = \mathbf{Q}$$

where $\mathbf{A}$ is the coefficient matrix with size $(N+1)M \times (N+1)M$, $\mathbf{F} = [f_0, f_1, \dots f_{(N+1)M-1}]^T$ is the vector of neutron fluxes and $\mathbf{Q} = [Q_0, Q_1, \dots Q_{(N+1)M-1}]$. And

$$f_{nM+i} = F_n^i$$

$$Q_{nM+i} = 4\Sigma_t Q_{2n}^i$$

3.4 Marshak Boundary Condition

The Marshak boundary conditions are given as:

$$\int_0^1 \psi(0,\mu)T_k(\mu)d\mu = 0, \quad k = 1,3,5,\dots,N.$$

$$\int_{-1}^0 \psi(a,\mu)T_k(\mu)d\mu = 0, \quad k = 1,3,5,\dots,N.$$

This type of B.C. yields:

$$H_k\phi_0(0) + \sum_{n=1}^{2N+1} H_{n,k}\phi_n(0) = 0 \tag{3}$$

$$I_k\phi_0(a) + \sum_{n=1}^{2N+1} I_{n,k}\phi_n(a) = 0 \tag{4}$$

where:

$$H_k = \int_0^1 \frac{T_k(\mu)}{\sqrt{1-\mu^2}}d\mu = \begin{cases} \pi/2 & k = 0 \\ \frac{\sin(k\pi/2)}{k} & k \geq 1 \end{cases}$$

$$H_{n,k} = \int_0^1 \frac{2T_k(\mu)T_n(\mu)}{\sqrt{1-\mu^2}}d\mu = \begin{cases} \pi/2 & n = k \neq 0 \\ \frac{\sin((n+k)\pi/2)}{(n+k)} + \frac{\sin((n-k)\pi/2)}{(n-k)} & n \neq k \end{cases}$$

$$I_k = \int_{-1}^0 \frac{T_k(\mu)}{\sqrt{1-\mu^2}}d\mu = \begin{cases} \pi/2 & k = 0 \\ -\frac{sin(k\pi/2)}{k} & k \geq 1 \end{cases}$$

$$I_{n,k} = \int_{-1}^0 \frac{2T_k(\mu)T_n(\mu)}{\sqrt{1-\mu^2}}d\mu = \begin{cases} \pi/2 & n = k \neq 0 \\ -\frac{\sin[(n+k)\pi/2]}{(n+k)} - \frac{\sin[(n-k)\pi/2]}{(n-k)} & n \neq k \end{cases}$$

It is noticed that k only takes odd number, so for odd n, $I_{n,k} = 0$, if $n \neq k$. Only even ordered ϕ_n are left in Eq. 3 and 4.

If $k = 2m+1$ and $n = 2a$,

$$H_{2m+1} = \int_0^1 \frac{T_{2m+1}(\mu)}{\sqrt{1-\mu^2}} d\mu = \frac{(-1)^m}{2m+1}$$

$$H_{2a,2m+1} = \int_0^1 \frac{2T_{2m+1}(\mu)T_{2a}(\mu)}{\sqrt{1-\mu^2}} d\mu = \frac{(-1)^{a+m}}{2a+2m+1} + \frac{(-1)^{a-m+1}}{2a-2m-1}$$

$$I_{2m+1} = \int_{-1}^0 \frac{T_{2m+1}(\mu)}{\sqrt{1-\mu^2}} d\mu = \frac{(-1)^{m+1}}{2m+1}$$

$$I_{2a,2m+1} = \int_{-1}^0 \frac{2T_{2m+1}(\mu)T_{2a}(\mu)}{\sqrt{1-\mu^2}} d\mu = \frac{(-1)^{a+m+1}}{2a+2m+1} + \frac{(-1)^{a-m}}{2a-2m-1}$$

For odd$^{\text{th}}$ ordered ϕ_{2n+1} at left boundary:

$$\begin{aligned}\phi_{2n+1}(0) &= -\frac{1}{H_{2n+1,2n+1}} \left\{ H_{2n+1} \sum_{m=0}^{N} (-1)^m F_m(0) + \sum_{a=1}^{N} H_{2a,2n+1} \sum_{m=0}^{N-a} (-1)^m F_{a+m}(0) \right\} \\ &= \frac{1}{2\Sigma_t} \left[2\cancelto{0}{\phi_{2n+1}} - \frac{dF_n(0)}{dx} \right] = -\frac{1}{2\Sigma_t} \frac{dF_n(0)}{dx}\end{aligned}$$

Using ghost nodes at left boundary,

$$\frac{1}{2\Sigma_t} \frac{F_n^1 - F_n^{-1}}{\Delta x} = \frac{1}{H_{2n+1,2n+1}} \left\{ H_{2n+1} \sum_{m=0}^{N} (-1)^m F_m^1 + \sum_{a=1}^{N} H_{2a,2n+1} \sum_{m=0}^{N-a} (-1)^m F_{a+m}^1 \right\}$$

$$\boxed{\Longrightarrow F_n^{-1} = F_n^1 - \frac{2\Sigma_t \Delta x}{H_{2n+1,2n+1}} \left\{ H_{2n+1} \sum_{m=0}^{N} (-1)^m F_m^0 + \sum_{a=1}^{N} H_{2a,2n+1} \sum_{m=0}^{N-a} (-1)^m F_{a+m}^0 \right\}}$$

where F_n^{-1} denotes the ghost point outside the entire domain. Similarly, at right boundary:

$$\begin{aligned}\phi_{2n+1}(a) &= -\frac{1}{I_{2n+1,2n+1}} \left\{ I_{2n+1} \sum_{m=0}^{N} (-1)^m F_m(a) + \sum_{a=1}^{N} I_{2a,2n+1} \sum_{m=0}^{N-a} (-1)^m F_{a+m}(a) \right\} \\ &= \frac{1}{2\Sigma_t} \left[2\cancelto{0}{\phi_{2n+1}} - \frac{dF_n(a)}{dx} \right] = -\frac{1}{2\Sigma_t} \frac{dF_n(a)}{dx}\end{aligned}$$

$$\boxed{\Longrightarrow F_n^M = F_n^{M-2} + \frac{2\Sigma_t \Delta x}{I_{2n+1,2n+1}} \left\{ I_{2n+1} \sum_{m=0}^{N} (-1)^m F_m^{M-1} + \sum_{a=1}^{N} I_{2a,2n+1} \sum_{m=0}^{N-a} (-1)^m F_{a+m}^{M-1} \right\}}$$

3.5 T_1 approximation

For T_1 approximation, only F_0 exists:

$$-\frac{d^2 F_0(x)}{dx^2} + 2\Sigma_t^2 F_0(x) = 2\Sigma_s \Sigma_t F_0(x) + 2\Sigma_t Q_0(x)$$

$$-\frac{F_0^{i-1}-2F_0^i+F_0^{i+1}}{\Delta x^2}+2\Sigma_t^2F_0^i-2\Sigma_s\Sigma_tF_0^i=2\Sigma_tQ_0(x)$$

The Marshak boundary conditions give:

$$\phi_0(0)+\frac{\pi}{2}\phi_1(0)=F_0(0)-\frac{\pi}{4\Sigma_t}\frac{dF_0(0)}{dx}=0$$

$$-\phi_0(a)+\frac{\pi}{2}\phi_1(a)=-F_0(a)-\frac{\pi}{4\Sigma_t}\frac{dF_0(a)}{dx}=0$$

$$F_0^0-\frac{\pi}{4\Sigma_t}\frac{F_0^1-F_0^{-1}}{\Delta x}=0\Longrightarrow F_0^{-1}=F_0^1-\frac{4\Delta x\Sigma_t}{\pi}F_0^0$$

$$-F_0^{M-1}-\frac{\pi}{4\Sigma_t}\frac{F_0^M-F_0^{M-2}}{\Delta x}=0\Longrightarrow F_0^M=F_0^{M-2}-\frac{4\Delta x\Sigma_t}{\pi}F_0^{M-1}$$

Then, for $1\leq n\leq M-2$:

$$A[n,n]=\frac{2}{\Delta x^2}+2\Sigma_t^2-2\Sigma_s\Sigma_f$$

$$A[n,n-1]=A[n,n+1]=-\frac{1}{\Delta x^2}$$

At boundaries:

$$A[0,0]=A[M-1,M-1]=\frac{2}{\Delta x^2}+2\Sigma_t^2-2\Sigma_s\Sigma_f+\frac{4\Sigma_t}{\pi\Delta x}$$

$$A[0,1]=A[M-1,M-2]=-\frac{2}{\Delta x^2}$$

The source terms are given as:

$$Q[n]=2\Sigma_tQ_0=2\Sigma_tQ$$

4 Results & Discussion

4.1 Basic problem

The basic problem is solving using T_1 approximation and the result of scalar flux is shown and compared with results of P_1 and P_3 approximations in Fig. 1. In general, scalar fluxes obtained using T_1, P_1 and P_3 approximations follow the same pattern. In the middle of slab, the flux is almost constant. In this region, T_N and P_N agree perfectly with each other. Near boundaries, T_1 approximation behaviors similarly as P_3 approximation. However, in the shoulder region, the fluxes evaluated using T_1 and P_1 approximations are almost identical.

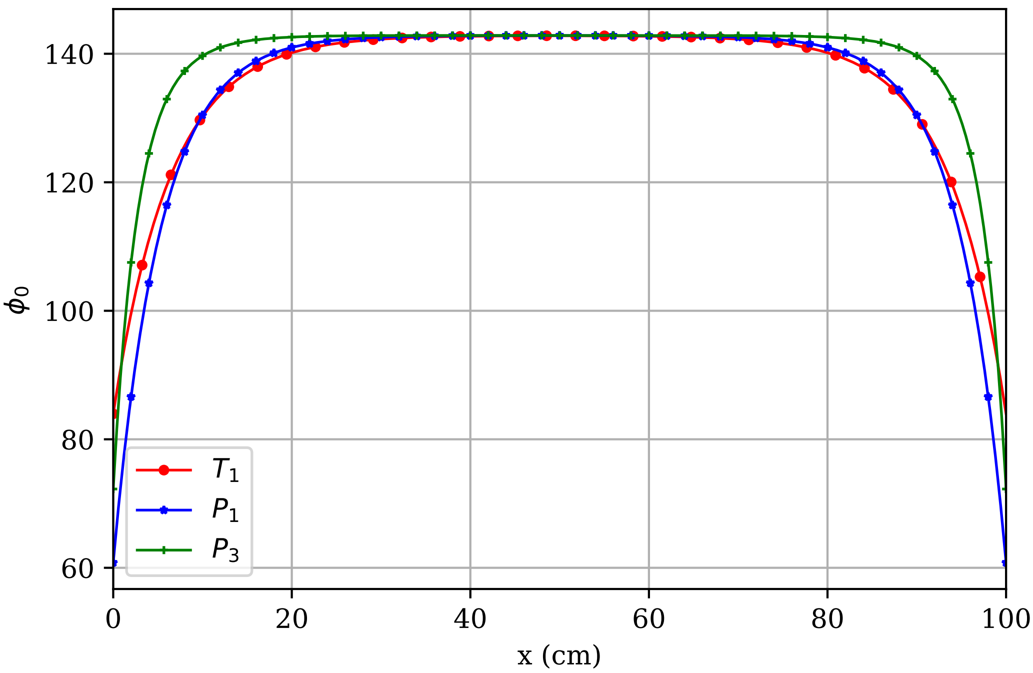

Figure 1: Comparison of T_N and P_N methods

4.2 Challenging problems

4.2.1 Spatial convergence

The change of relative error ε with mesh size increasing is summarized in Fig. 2. The threshold ε_0 is set to be 1×10^{-6} and the refined mesh size is 619. It is shown that ε monotonically decreases as mesh becomes more refined. And it decreases more slowly as mesh size increases.

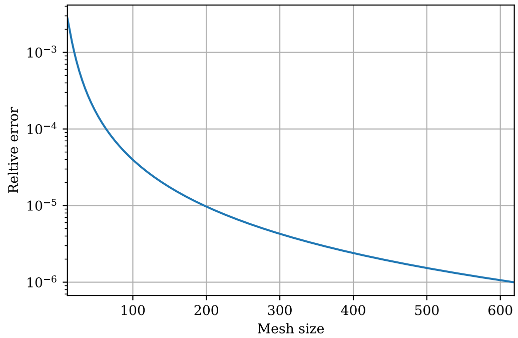

Figure 2: Spatial convergence

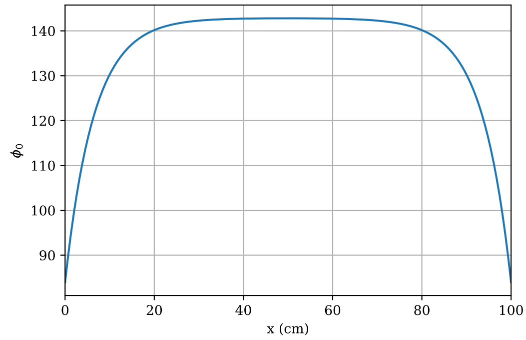

Figure 3: Converged scalar flux with T_1 approximation

4.2.2 Order of accuracy convergence

After conducting spatial convergence, influence of order of accuracy on the results are studied by changing the order of T_N approximation incrementally. The convergence criteria $\varepsilon_0 = 1 \times 10^{-3}$. The results of order of accuracy convergence are summarized in Fig. 4. The converged scalar flux is plotted in Fig. 5 and compared with lower order of accuracy in Fig. 6. Based on Fig. 6, in general, ε decreases as order of accuracy increases. However, error does not change monotonically. On the contrary, it decreases jaggedly as higher ordered approximation is made.

In summary, T_{23} approximation is sufficient to provide satisfactory solutions of neutron transport equation. Based on Fig. 6, the finally converged result is located between results from P_1 and P_3 approximations. It is closer to P_3 approximation than P_1 approximation. It can be noticed that solutions of T_{11} and T_{23} are almost identical. However, the computational power needed continuous to increases as the order of accuracy becomes higher. Therefore, further increases of order of accuracy do not benefit much.

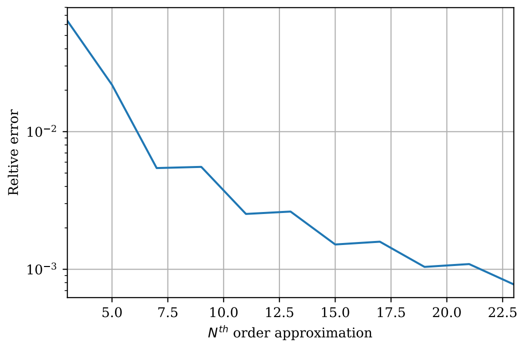

Figure 4: Order of accuracy convergence

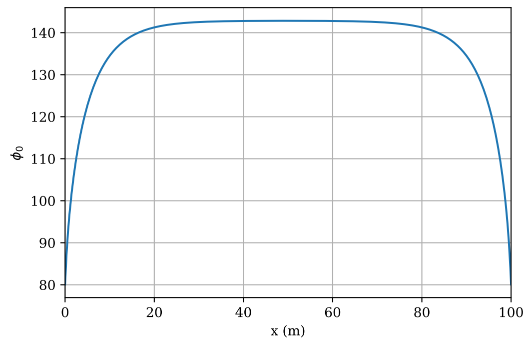

Figure 5: Converged scalar flux

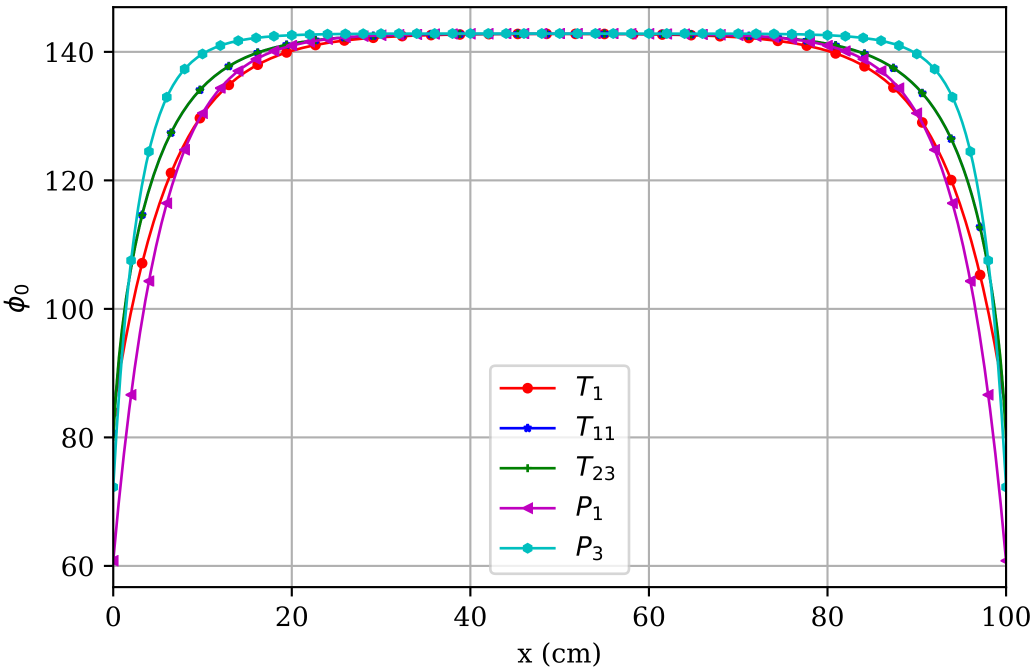

Figure 6: Comparison of T_N and P_N methods after convergence studies

5 Conclusion

In conclusion, T_N approximation method can be a powerful tool to solve one-speed neutron transport equation in 1-D slab. It can be roughly concluded that results of T_N approximation agree with those of P_N approximation. However, required computational power and computer memory increase dramatically as the order of accuracy increase, even for the simplest 1-D problem. Therefore, the algorithm and code should be improved to apply to complex geometries and multi-group problems.

References

[1] Fikret Anli, Faruk Yaşa, Süleyman Güngör, and Hakan Öztürk. Tn approximation to neutron transport equation and application to critical slab problem. *Journal of Quantitative Spectroscopy and Radiative Transfer*, 101(1):129–134, 2006.

[2] EGE Ökkeş, Hakan Öztürk, and Ahmet Bülbül. Diffusion approximation to neutron transport equation with first kind of chebyshev polynomials. *SDÜ Fen Edebiyat Fakültesi Fen Dergisi*, 10(2), 2015.

[3] Ayhan Yilmazer. Solution of one-speed neutron transport equation for strongly anisotropic scattering by tn approximation: Slab criticality problem. *Annals of Nuclear Energy*, 34(9):743–751, 2007.