

# Positive Scattering Cross Sections Using Constrained Least Squares

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## Abstract

A method to create a positive Legendre expansion from truncated Legendre cross section libraries is presented. Cross section moments of order two and greater are modified by a constrained least squares algorithm, subject to the constraints that the zeroth and first moments are unchanged, and that the standard discrete ordinate scattering matrix is positive. A method using the maximum entropy representation of the cross section, which reduces the error in the modified moments is also presented. These methods are implemented in the PARTISN code, and numerical results from a transport calculation using highly anisotropic scattering cross sections with an exponential discontinuous spatial scheme are presented.

## 1 Introduction

The scattering cross section used in the discrete ordinates solution of the neutron transport equation is usually represented by a truncated Legendre expansion (Bell 1970). If there is a large degree of anisotropy, the expanded cross section may exhibit non-physical negative regions. When these negative regions are severe enough, negative discrete ordinates scattering sources may result. The Monte Carlo community has developed several methods which address the issue of negative Legendre scattering cross sections, and Brockmann provides a survey of some of these (Brockmann 1981). In this work we perform a least squares minimization upon the Legendre cross section moments in an effort to find a positive cross section representation which may be used directly in a discrete ordinate transport code.

One of the first instances that a least squares method has been applied to Legendre cross section function expansions is in the code CLEM (Slavik 1968), which used least squares minimization to adjust the Legendre moments in an attempt to gain a positive expansion. The angular domain is discretized on an equally spaced 101 point fixed mesh. Positivity is checked by testing the Legendre expansion of the approximate moments for negativity at each of the 101 mesh points. The authors of CLEM state that a disadvantage of their procedure is that the first moment of the cross section will be changed, affecting the transport calculation and the resulting flux. They have adapted CLEM to hold the first moment constant, but comment that it would often be impossible to find an approximate nonnegative truncated Legendre series.

Landesman and Morel (Landesman 1989) have proposed a constrained least squares method to adjust the Legendre moments of the one dimensional angular Fokker-Planck operator. To impose positivity on the truncated Legendre cross section expansion, the Legendre moments are modified subject to the constraints that the zeroth and first order moments remain unchanged, and that every element in the one-dimensional Galerkin (Morel 1989) scattering matrix using the least squares adjusted moments is positive. The modified Legendre expansion of the cross section is only required to be positive at the quadrature points. The first two constraints preserve the momentum transfer properties of the scattering

cross section. The result is  $N-1$  Legendre moments which are unique to its particular quadrature set.

In this paper we extend Landesman and Morel's method to multidimensional Galerkin quadrature, and show that unsatisfactory results are obtained. The method is then applied to standard multidimensional  $S_N$  quadrature, with much more positive results. The relative error of the modified moments is reduced by applying a method using the maximum entropy representation of the scattering cross section. Finally, results from a transport calculation using this method are presented.

## 2 Least Squares with Multidimensional Galerkin Quadrature

A Galerkin scattering matrix, as defined by Morel (Morel 1989), is constructed from three fundamental matrices. These three matrices are: a discrete-to-moment matrix, a diagonal cross section matrix, and a moment-to-discrete matrix. The discrete-to-moment matrix maps the discrete values of the angular flux to angular flux moments. The cross section matrix maps the angular flux moments to angular scattering source moments. Finally, the moment-to-discrete matrix maps the scattering source moments to discrete angular source values. This sequence is illustrated as follows:

$$\phi = \mathbf{D}\psi , \quad (1)$$

$$\xi = \Sigma\phi = \Sigma\mathbf{D}\psi , \quad (2)$$

$$S = \mathbf{M}\xi = \mathbf{M}\Sigma\mathbf{D}\psi . \quad (3)$$

Here  $S$  is the discrete scattering source and  $\psi$  is the discrete angular flux. The Galerkin approximation is defined such that the trial space elements obtained by interpolating the discrete scattering source have the same moments as those of equation (2). This requirement results in the relationship

$$\mathbf{M} = \mathbf{D}^{-1} . \quad (4)$$

To construct the matrix  $\mathbf{M}$  for three-dimensional Galerkin quadrature, a subset of spherical harmonics for the trial and weighting space is used. Morel has found the following subset of spherical harmonics, when used in conjunction with the triangular Legendre-Tchebychev (Lathrop 1965) quadrature, produce an invertible  $\mathbf{M}$  matrix of the form

$$\mathbf{M}_{m,(l,k)} = \frac{2l+1}{4\pi} \left[ (2 - \delta_{k,0}) \frac{(l-|k|)!}{(l+|k|)!} \right]^{\frac{1}{2}} Y_{l,k}(\hat{\Omega}_m) . \quad (5)$$

The limits on  $l$  and  $k$  in equation (5) are;

$$\begin{aligned} l &= 0, N-1, \quad k = -l, l, \\ \text{and } l &= N, \quad k < 0, \\ \text{and } l &= N, \quad k > 0 \text{ odd,} \\ \text{and } l &= N+1, \quad k < 0 \text{ even.} \end{aligned}$$

Here the row index  $m$  is the  $m^{\text{th}}$  quadrature direction, the column index  $(l,k)$  is related to each combination of  $l$  and  $k$ , and  $N$  is the quadrature or  $S_N$  order. This results in being able to use  $N+1$  Legendre cross sections moments with three-dimensional Galerkin quadrature.

A Fortran code was written to create the three-dimensional Galerkin quadrature matrices, and then attempt a least squares adjustment of the Legendre scattering cross section moments subject to the constraints that the zeroth and first order moments remain unchanged, and that every element in the multidimensional Galerkin scattering matrix,  $\mathbf{M}\mathbf{\Sigma}\mathbf{D}$ , is positive. The functional minimized is

$$\Delta\sigma_l = \sum_{l=0}^L (\sigma_l^* - \sigma_l)^2, \quad (6)$$

where  $\sigma_l^*$  is the least squares modified moment of order  $l$ . The constrained least squares algorithm used is the LSEI (Hanson 1978) routine from the SLATEC (Vanevender 1982) subroutine library. SLATEC is publically available on the world wide web and was also used by Landesman and Morel. We refer to this method as the Least Squares Galerkin Quadrature, or LSGQ.

This method is analyzed with two sets of  $P_4$  cross sections. The Legendre expansion for test case one is strictly positive. Test case two is a downscatter cross section for hydrogen, from energy group 18 to 22, from the Los Alamos 30 group  $P_4$  MENDF5 (Little 1986) cross section library. Table 1 lists the scattering cross section moments for test case one, and the resulting moments from the LSGQ method for  $S_N$  orders  $S_8$ ,  $S_{10}$ , and  $S_{12}$ . The code calculated nine Legendre moments for  $S_8$ , eleven for  $S_{10}$ , and thirteen for  $S_{12}$ , which is the maximum number of moments contained within the diagonal matrix  $\mathbf{\Sigma}$  in the three-dimensional Galerkin quadrature formulation. The relative error of the least squares modified moments compared to the original Legendre moments of orders two through four are also reported.

It is noted from Table 1 that none of the cross section moments are changed for quadrature orders eight and 10. This is expected since the cross section expansion in this case is positive everywhere. However,

Table 1: LSGQ modified Legendre moments of test case one for varying  $S_N$  orders

Moment Order	Original	$S_8 - P_9$		$S_{10} - P_{11}$		$S_{12} - P_{13}$	
		Least Squares	Rel. Error	Least Squares	Rel. Error	Least Squares	Rel. Error
0	1.0	1.0	0.0	1.0	0.0	1.0	0.0
1	0.5	0.5	0.0	0.5	0.0	0.5	0.0
2	0.2	0.2	0.0	0.2	0.0	0.1976	0.012
3	0.005	0.005	0.0	0.005	0.0	7.381E-3	0.563
4	0.001	0.001	0.0	0.001	0.0	1.265E-3	0.265

for the  $S_{12}$  quadrature, the least squares algorithm adjusted the second through fourth order moments as much as 50 percent. The least squares algorithm modifies the Legendre moments only if an element of the multidimensional Galerkin scattering matrix is negative, which is a constraint that has been placed on the system. This indicates that the three-dimensional Galerkin scattering matrix is not positive, even though the Legendre expansion of the scattering cross section is positive everywhere. Further tests indicate that when even higher ordered Galerkin scattering matrices are used, the resulting LSGQ modified moment expansion differs more from the original positive cross section.

Table 2 lists the LSGQ modified moments and their relative error with varying  $S_N$  orders for the second test cross section. Again, the relative errors for moments of order two through four tend to increase

Table 2: LSGQ modified Legendre moments of test case two for varying  $S_N$  orders

Moment Order	Original	$S_8 - P_9$		$S_{10} - P_{11}$		$S_{12} - P_{13}$	
		Least Squares	Rel. Error	Least Squares	Rel. Error	Least Squares	Rel. Error
0	0.37248	0.37248	0.0	0.37248	0.0	0.37248	0.0
1	0.05706	0.05706	0.0	0.05706	0.0	0.05706	0.0
2	-0.17203	-9.619E-2	0.441	-8.866E-2	0.485	-8.653E-2	0.497
3	-0.08190	-5.003e-2	0.389	-5.499E-2	0.329	-3.930E-2	0.520
4	0.10697	1.851E-2	0.827	2.013E-2	0.812	9.530E-3	0.911

when a higher ordered Galerkin scattering matrix is used in the least squares calculation. The errors in the LSGQ modified moments are large enough to bring the method into question.

To summarize, we have demonstrated some peculiar behavior of the LSGQ method. When the original Legendre cross section expansion is inherently positive, the LSGQ method modifies the original moments as higher ordered Galerkin quadrature scattering matrices are used, which indicates that the elements of the higher ordered Galerkin scattering matrices are not positive. A possible cause may be ill-conditioning introduced in the matrix inversion process. The condition number of the Galerkin moment to discrete matrix,  $\mathbf{M}$ , increases as the quadrature order is increased. This may result in the numerical inversion of  $\mathbf{M}$  having increased roundoff error and possibly introduce small negative components in the Galerkin scattering matrix. In addition to the possible ill-conditioning, we note that while the Galerkin representation of the flux is positive at the quadrature points, the interpolate of the angular flux may contain negative regions. Multiplication of the interpolate by a scattering cross section may excite these non-positive regions. Thus the positivity of the scattering source may also be a function of the stability of the angular flux interpolant. Further research in this area is required.

The relative errors of the LSGQ modified moments increase as the Galerkin quadrature is increased. A higher quadrature order allows the least squares algorithm to use more Legendre moments in its search for a positive Galerkin scattering matrix. It is reasonable, and desirable, that the errors should decrease as more Legendre moments are used to represent a scattering cross section, but this is not the case with the LSGQ method.

The second test case also resulted in modified cross section moments that had rather large relative errors. Such error in the cross section moments may affect the results of a transport calculation, especially if the angular flux moments of order two or greater are relatively large in magnitude. For this reason, the multidimensional LSGQ method is not recommended as a viable method for the generation of a positive scattering source. This is contrary to the one-dimensional method (Landesman, 1989), which works well. The reason for the failure of the multidimensional method is not understood.

### 3 Least Squares Modified Cross Section Moments with Standard $S_N$ Quadrature

Each element of the standard  $S_N$  scattering matrix,

$$\mathbf{S}_{mm'} = \sum_{l=0}^L \sigma_l P_l(\hat{\Omega}_{m'} \cdot \hat{\Omega}_m) w_{m'} , \quad (7)$$

is guaranteed to be positive if the quadrature weights are positive and the Legendre expansion of the cross section function has a positive value at each combination of  $(\hat{\Omega}_{m'}, \hat{\Omega}_m)$ . To find a positive truncated Legendre expansion of the scattering cross section, we propose a variation of LSGQ method. The following functional is minimized,

$$\Delta\sigma_l = \left[ \frac{(\sigma_l - \sigma_l^*)(\sigma_0 - |\sigma_l|)}{\sigma_0} \right]^2 \quad (8)$$

subject to the constraints that the zeroth and first Legendre cross section moments remain unchanged, and that each element in the standard  $S_N$  scattering matrix is positive, or

$$\sum_{l=0}^L \sigma_l^* P_l(\hat{\Omega}_{m'} \cdot \hat{\Omega}_m) w_{m'} \geq 0. \quad (9)$$

The third constraint, equation (9) ensures a positive representation of the scattering cross section at all points where the Legendre cross section function will be evaluated. This functional differs from the one minimized in the LSGQ method by the addition of the weight,

$$\frac{(\sigma_0 - |\sigma_l|)}{\sigma_0}. \quad (10)$$

The purpose of this weight is to allow more freedom to adjust moments that are small in magnitude. If a cross section moment is small compared to the zeroth moment, it is less likely to make a large contribution to the cross section expansion, and therefore have little effect on the results of a transport calculation. We refer to this method as least squares with  $S_N$  quadrature, or LSSN.

A Fortran code has been written to calculate the LSSN modified cross section moments. This code takes the original cross section moments as input, and then outputs the least squares solution to the order requested by the user. If the least squares solver cannot satisfy the constraints with the requested output Legendre order, it aborts the procedure, and indicates that a higher Legendre order is required for a positive solution. The final order of the LSSN modified Legendre expansion which is required for positivity is dependent on the average cosine of the scattering angle. The required order is only a function of  $\bar{\mu}$  since only the zeroth and first cross section moments are fixed, while the upper moments can be modified in the least squares sense.

Test cases one and two were again used to analyze this method. For these calculations, the code performed the LSSN method on the  $P_4$  Legendre cross section moments, and returned Legendre moments of order one less than the user requested quadrature order, i.e., a 13<sup>th</sup> order expansion was returned when an  $S_{14}$  quadrature was used.

The Legendre expansion of test case one is strictly positive, and the LSSN method returned cross section moments which matched the original moments exactly, regardless of the  $S_N$  order requested. This behavior is expected since the original Legendre expansion does not need to be modified for the cross section to be nonnegative. This is unlike the LSGQ method, which began to modify the moments as the

$S_N$  and Legendre order was increased.

Table 3 lists the original moments for test case two, the calculated moments using the LSSN method, and the relative error of the moments of order two through four for quadratures of  $S_6$  through  $S_{10}$ . These data begin with  $S_6$  since the LSSN method calculated a positive cross section expansion with only a  $P_5$  expansion. The relative error of the cross section moments is much lower than the relative error from the LSGQ method. Also, the relative error decreases as the output Legendre order is increased, which is a desirable feature.

Table 3: LSSN modified moment comparison for test case two

		$S_6 - P_5$		$S_8 - P_7$		$S_{10} - P_9$	
Order	Original	LSSN	Rel Error	LSSN	Rel Error	LSSN	Rel Error
0	0.3727	0.3727	0.0	0.3727	0.0	0.3727	0.0
1	0.05707	0.05707	0.0	0.05707	0.0	0.05707	0.0
2	-0.1728	-0.1190	.3081	-0.1355	0.2124	-0.1451	0.1564
3	-0.08191	-0.04113	0.4978	-0.05614	0.3145	-0.06480	0.2088
4	0.1069	0.04167	0.6105	0.05593	0.4771	0.06166	0.4235

To summarize, the LSSN method produces modified Legendre moments that are better behaved than the LSGQ method. The relative error of the modified moments for each test case is less than those of the LSGQ method, and they decrease with increasing Legendre order. Each test case also produces a set of Legendre moments which appear to approach the original moments as the requested Legendre order increased.

#### 4 The Role of Maximum Entropy with the LSSN Method

In an effort to reduce the relative error of the LSSN modified cross section moments even further, we have implemented an algorithm which uses the method of maximum entropy (Moskelev 1993) (Baker 1995). The LSSN method described in the previous section uses the given cross section moments (up to order  $L$ ) as input, which is often of order less than required for a positive cross section representation. The higher cross section moments, of order  $L+1$  and greater, which are required for positivity, are initially set to zero, resulting in a truncated expansion which may be far from convergent. This truncated series is considered as an initial guess for the LSSN algorithm. It is postulated that if the least squares solver had a more convergent, and hence a more positive series from which to work, less of a change to the original Legendre moments of order two or greater would be required.

To find more moments, the exponential representation of the scattering cross section found from the maximum entropy technique is used. By projecting the exponential representation over Legendre polynomials of order greater than that given in the cross section library, as shown here,

$$\sigma_l = \int_{-1}^1 d\mu P_l(\mu) \exp\left(\sum_{l'=0}^L \lambda_{l'} P_{l'}(\mu)\right), \quad L+1 \leq l < N, \quad (11)$$

estimated Legendre moments of order  $L+1$  and greater can be calculated. Thus, if an  $N-1$  order expansion is requested using the LSSN method with an  $S_N$  quadrature of order  $N$ , it can use these

additional moments as an initial guess for moments of order L+1 to N-1. This method is denoted as LSSN/ME, where the ME is an abbreviation for maximum entropy. If the exponential representation is not available, then one can revert to using the LSSN method.

This proposal was analyzed using the LSSN Fortran program presented previously. The program used N-1 input moments as the initial expansion, where the L+1 to N-1 upper moments were calculated from the cross section's exponential representation. If the cross section expansion is strictly positive, as is the case for test case one, then no least squares modification is required. For test data we use the group one self scattering cross section for carbon from the Los Alamos 30 group MENDF library. Table 4 lists the original moments, the resulting LSSN/ME modified moments, and the relative error for moments of order two through four. The results presented here are for a ninth order Legendre expansion with an  $S_{10}$  quadrature. The relative error of the second order moment is slightly greater than the case when the LSSN algorithm is used. However, the relative error of the third and fourth order moments have improved.

Table 4: LSSN/ME modified moments comparison for carbon cross section

Order	Original	$P_9 - S_{10}$ from $P_9$ (LSSN/ME)		$P_9 - S_{10}$ from $P_4$ (LSSN)	
		LSSN/ME	Rel Error	LSSN	Rel Error
0	0.070211	0.070211	0.0	0.070211	0.0
1	0.063745	0.063745	0.0	0.063745	0.0
2	0.052652	0.052868	0.004102	0.052476	0.003342
3	0.039704	0.040034	0.008312	0.03896	0.01874
4	0.027427	0.02765	0.008244	0.02582	0.05839

Further comparison of the LSSN and LSSN/ME least squares methods using cross sections from the Los Alamos MENDF5  $P_4$  cross section library have been made. These data indicate that the LSSN/ME method resulted in approximately the same, or a significantly lower, relative error of the modified moments. It is therefore recommended that the LSSN/ME method be used over the LSSN method when the approximated moments from maximum entropy are available.

## 5 Results from a Sample Transport Problem

The LSSN/ME method was implemented in the parallel discrete ordinate transport code PARTISN (Alcouffe 1998). In this section, the results for an example problem consisting of a cube of natural carbon are presented. The atom density of the carbon is 0.1314 barns/cm<sup>2</sup>. The cube is 55 cm on a side, with a spatial mesh of 22x22x22 in the x, y, and z directions respectively. The cross sections used are from the Los Alamos MENDF 30 group  $P_4$  cross section set. Only the first two groups of the cross section set were used for this example problem. The scattering cross sections at these energies are forward peaked and their  $P_4$  Legendre expansions exhibit negative regions in the interval from  $-1 \leq \mu_0 \leq +1$ . The mean free path for neutrons in the first energy group is on the order of 5 cm, thus the carbon cube is approximately 11 mean free paths in the x, y, and z directions.

The problem was run with a Legendre-Tchebychev  $S_{16}$  quadrature. The fixed angular surface source was placed at the center four mesh cells on the  $z = 0$  face. Only one angular direction was given a non-zero

value, resulting in a beam along one quadrature direction. The direction cosines for this direction are  $\mu = -0.1026789$ ,  $\eta = -0.1026789$ , and  $\xi = 0.9894009$ , which correspond to the direction which is closest to normal on the front face. The fixed source was only specified in group one. Since results of this problem using the linear discontinuous spatial scheme resulted in negative scalar fluxes, the exponential discontinuous (Wareing 1997) scheme was chosen for the spatial discretization.

Also included are the results from a Monte Carlo calculation using the code MCNP<sup>TM</sup> (Briesmeister, 1997). The cross sections used in the MCNP calculation are also from the Los Alamos MENDF 30 group cross section library, which have been processed with the maximum entropy technique and divided into 30 equiprobable angular bins, using Baker's XREP module (Baker 1996). The MCNP calculation used 20 million histories, and tallies were performed on an 11x11x11 spatial meshing.

Figures 1 and 2 present the resulting scalar fluxes for groups one and two respectively. The  $S_N$  scalar flux was volume averaged over the appropriate spatial cells to recover a cell averaged quantity equivalent to the coarser meshing of the Monte Carlo calculation. The scalar flux in these figures is for the spatial cells bordering the  $z = 55$  cm face, fixed in the center along the  $x$  direction, and varied along the  $y$  direction. The  $S_N$  solutions using the LSSN/ME scattering source method shows good agreement with Monte Carlo solution. The errorbars on the MCNP scalar fluxes indicated in the figures is for one standard deviation.

## 6 Conclusions

In this paper, we have extended the least squares method proposed by Landesman and Morel to multidimensional Galerkin quadrature. This was shown to produce unsatisfactory results, and further study is needed into the origin of this failure. We have therefore developed a variation to this method which modifies the Legendre cross section moments in a least squares sense such that the zeroth and first moments remain unchanged, and that standard discrete ordinate scattering matrix is positive. To reduce the relative error of the modified moments, a method using the maximum entropy representation of the cross section has been devised. Moments of order  $L+1$  and greater are estimated by projecting the exponential representation of the cross section over the appropriate Legendre polynomials. These extra moments are then used as input to the constrained least squares algorithm. Results from an anisotropic carbon cross sections demonstrated a reduction in the relative error of the modified moments. Finally, the carbon example problem demonstrated that the LSSN/ME method produced results that were consistent with a multigroup Monte Carlo calculation on a difficult, highly anisotropic problem with exponential discontinuous spatial differencing.

## Acknowledgments

This work was performed under the auspices of the United States Department of Energy.

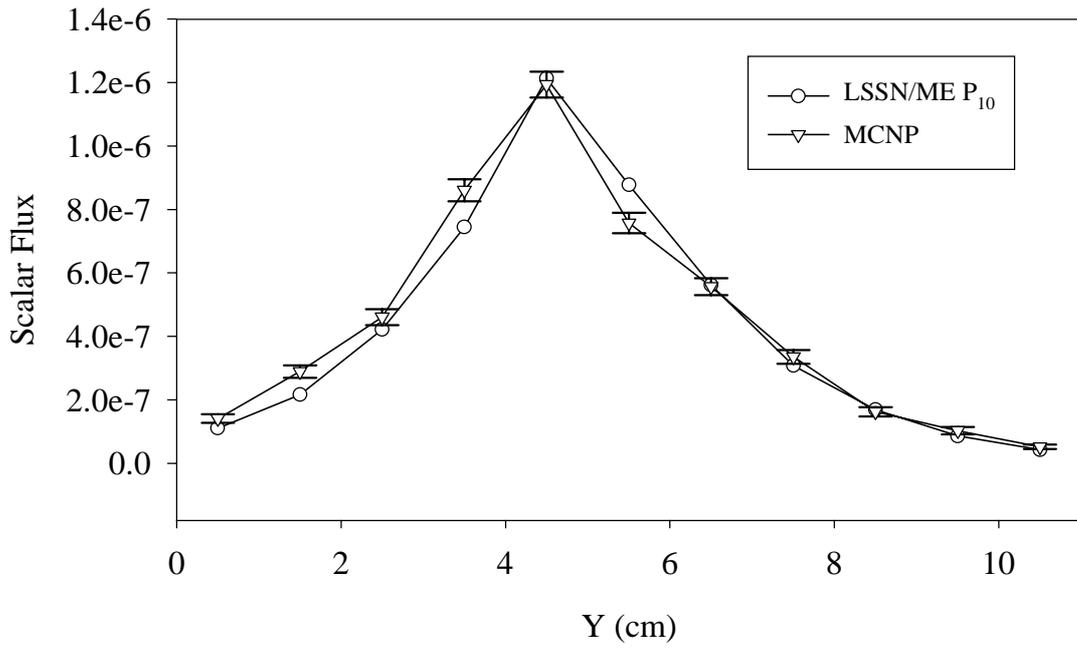


Figure 1: Group 1 scalar flux from fine mesh sample carbon problem

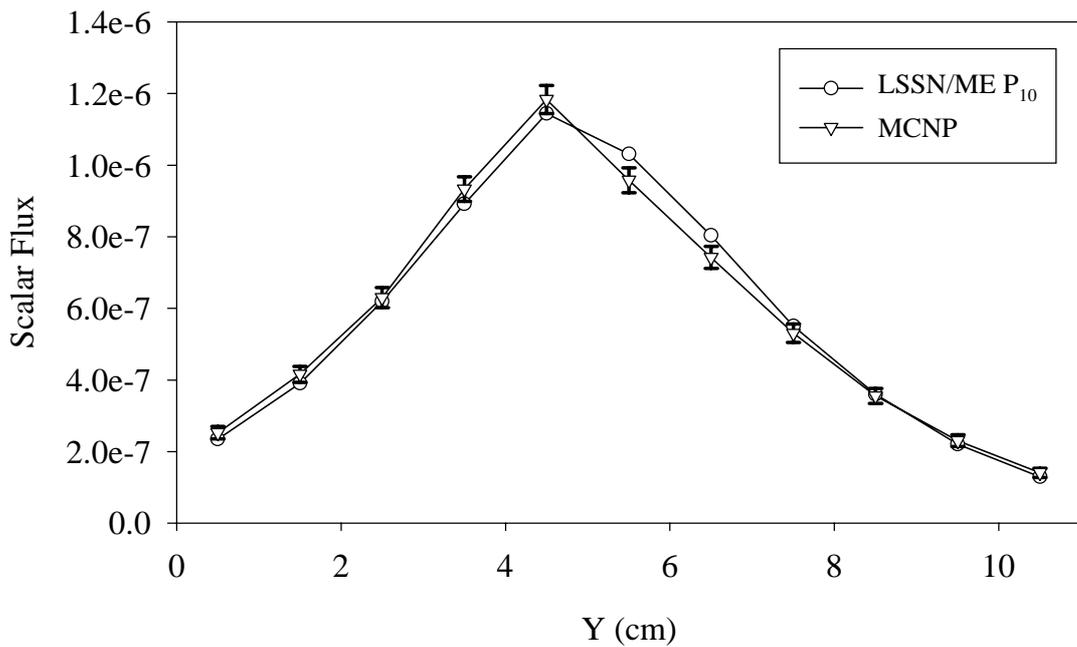


Figure 2: Group 2 scalar flux from fine mesh sample carbon problem

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