PHYSOR 2004 -The Physics of Fuel Cycles and Advanced Nuclear Systems: Global Developments
Chicago, Illinois, April 25-29, 2004, on CD-ROM, American Nuclear Society, Lagrange Park, IL. (2004)

Two Dimensional Functional Expansion Tallies for Monte Carlo Simulations

David P. Griesheimer and William R. Martin*
Department of Nuclear Engineering & Radiological Sciences, University of Michigan, Ann Arbor, MI 48109

The functional expansion tally (FET) is a technique that allows higher order information about spatial flux distributions to be obtained from traditional Monte Carlo simulations, allowing a continuous representation of the scalar flux throughout a tally region. In this paper we present a new formulation for the 2D track length FET and its implementation in a modified version of MCNP4c. To verify our methodology we used the FET to create a Legendre polynomial approximation for the distribution of scalar flux in a 2-D PWR pin cell. The numerical results with FET were compared to a highly resolved mesh tally in a benchmark Monte Carlo simulation and confirm that the FET converges to the correct spatial flux distribution.

KEYWORDS: Monte Carlo Simulation, Track Length Tally, Functional Expansion, Orthogonal Functions, Legendre Polynomials

1. Introduction

Monte Carlo simulations for neutron transport calculations provide an excellent method for estimating integral quantities such as average scalar flux over large volumes. Unfortunately, the variance of these estimates increases dramatically as the tally volumes are reduced. This means that dividing a cell into histogram-style bins and using a mesh tally to estimate the spatial flux shape over the cell can require extremely large numbers of histories to reduce the uncertainty in each mesh to an acceptable level. Also, increasing the spatial resolution of a tally in this way can require adding additional surfaces to the geometry. Tracking particles through these extra surfaces can add a significant amount of run-time to the simulation.

One approach to this problem is the functional expansion tally (FET), a technique that allows Monte Carlo to tally not only the zeroth spatial moment of flux in each cell but also higher moments with respect to some set of basis functions. These moments can then be used to create a functional expansion of the spatial flux distribution within the cell. Previous work on the use of Monte Carlo tallies to estimate spatial flux expansion coefficients has yielded promising results in one dimensional test cases [1,2,3]. This work has indicated that the resulting functional expansions converge to the correct spatial flux distribution in the tally region as the number of expansion terms is increased. Presently this work has been generalized to spatial expansions of the flux in two dimensions.

2. Two Dimensional FET Estimator

2.1. Formulation of the 2D FET Track Length Estimator

We begin by considering a three dimensional region defined on the domain $x \in [x_0, x_1]$,

* Corresponding author, Tel. 734-764-5534, FAX 734-763-4540, E-mail: wrm@umich.edu

$y \in [y_0, y_1]$ and $z \in [z_0, z_1]$. The spatial flux over the x-y domain can be written as a functional expansion in some appropriate set of orthonormal basis functions,

$$\phi(x,y) = \sum_{i=0}^{I}\sum_{j=0}^{J} c_{ij}\,\psi_i(x)\psi_j(y). \tag{1}$$

The expansion coefficients c_{ij} in Eq. (1) can be evaluated using the orthogonality property of the basis set $\{\psi\}_0^\infty$ to yield

$$c_{ij} = \int_{x_0}^{x_1}\int_{y_0}^{y_1}\int_{z_0}^{z_1} \phi(x,y)\psi_i(x)\psi_j(y)\,dz\,dy\,dx. \tag{2}$$

The functional expansion technique uses an unbiased estimator for Eq. (2) to calculate the spatial expansion coefficients of the flux during a Monte Carlo simulation. The estimator,

$$\widehat{c_{ij}} = \frac{1}{N}\sum_{n=1}^{N}\sum_{k=1}^{K_n} G\left(x_{n,k}, x_{n,k+1}, y_{n,k}, y_{n,k+1}\right) \tag{3}$$

where,

$$G_{i,j}(x_k, x_{k+1}, y_k, y_{k+1}) = \begin{cases} \dfrac{w_{n,k}\,d_{n,k}}{\left(x_{n,k+1} - x_{n,k}\right)} \displaystyle\int_{x_{n,k}}^{x_{n,k+1}} \psi_i(x)\psi_j\left(\frac{\varphi_{n,k}}{\mu_{n,k}}\left(x - x_{n,k}\right) + y_{n,k}\right)dx & \text{For } \mu_{n,k} \geq \varphi_{n,k} \\ \dfrac{w_{n,k}\,d_{n,k}}{\left(y_{n,k+1} - y_{n,k}\right)} \displaystyle\int_{y_{n,k}}^{y_{n,k+1}} \psi_i\left(\frac{\mu_{n,k}}{\varphi_{n,k}}\left(y - y_{n,k}\right) + x_{n,k}\right)\psi_j(y)\,dy & \text{For } \mu_{n,k} \leq \varphi_{n,k} \\ w_{n,k}\,d_{n,k}\,\psi_i\left(x_{n,k}\right)\psi_j\left(y_{n,k}\right) & \text{For } \mu_{n,k} = \varphi_{n,k} = 0 \end{cases}$$

results from a modification to the traditional track length estimator [4] for scalar flux in a region.

2.2. Derivation of the 2D FET Track Length Estimator

The derivation of the estimator for Eq. (2) is a generalization of the proof presented by Spanier [1] in 1999. The proof begins by partitioning the expansion domain into P and Q equally spaced partitions in the x- and y-directions, respectively. Equation (2) can then be written as the sum of the integrals taken over each partition,

$$c_{ij} = \sum_{p=1}^{P}\sum_{q=1}^{Q}\int_{x_p}^{x_{p+1}}\int_{y_q}^{y_{q+1}}\int_{z_0}^{z_1} \phi(x,y)\psi_i(x)\psi_j(y)\,dz\,dy\,dx. \tag{4}$$

If the x and y partitions (Δx_p and Δy_p) are sufficiently small then it is reasonable to express ψ_n over an interval by its Taylor expansion about the midpoint of the interval,

$$\psi_i(x) = \psi_i(x_{p+1/2}) + O(\Delta x_p) \;\; \forall \;\; x \in [x_p, x_{p+1}]. \tag{5}$$

Using this relationship allows Eq. (4) to be rewritten as

$$c_{ij} = \sum_{p=1}^{P}\sum_{q=1}^{Q}\left(\psi_i(x_{p+1/2}) + O(\Delta x_p)\right)\left(\psi_j(y_{q+1/2}) + O(\Delta y_q)\right)\int_{x_p}^{x_{p+1}}\int_{y_q}^{y_{q+1}}\int_{z_0}^{z_1}\phi(x,y)\,dz\,dy\,dx\,. \tag{6}$$

The third factor in Eq. (6) is the integrated scalar flux over the (p,q) partition, a quantity that can also be interpreted as the amount of track length generated by all particles passing through the partition,

$$\int_{x_p}^{x_{p+1}}\int_{y_q}^{y_{q+1}}\int_{z_0}^{z_1}\phi(x,y)\,dz\,dy\,dx = D_{pq}, \tag{7}$$

where D_{pq} is the total track length generated in the (p,q) partition. An unbiased estimator for D_{pq} can be written as

$$\widehat{D_{pq}} = \frac{1}{N}\sum_{n=1}^{N}\sum_{k=1}^{K_n} t_{n,k,p,q}\, w_{n,k}\,, \tag{8}$$

where N is the total number of particles started, K_n is the total number of events (collision, surface crossing, etc.) where the n^{th} particle can change direction, $w_{n,k}$ is the weight of the particle, and $t_{n,k,p,q}$ is the path length traveled in the partition $\Delta x_p \Delta y_q$ by particle n as it travels from event k to $k+1$. Substituting Eq. (8) into Eq. (6) and manipulating gives an estimator for the expansion coefficient c_{ij},

$$\widehat{c_{ij}} = \frac{1}{N}\sum_{n=1}^{N}\sum_{k=1}^{K_n} w_{n,k}\sum_{p=1}^{P}\sum_{q=1}^{Q}\left(\psi_i(x_{p+1/2}) + O(\Delta x_p)\right)\left(\psi_j(y_{q+1/2}) + O(\Delta y_q)\right) t_{n,k,p,q}\,. \tag{9}$$

This estimator was developed for an arbitrary mesh defined over the expansion domain. Taking the limit of Eq. (9) as the partition goes to zero, $\Delta x_p \to 0$ and $\Delta y_q \to 0$, gives

$$\widehat{c_{ij}} = \frac{1}{N}\sum_{n=1}^{N}\sum_{k=1}^{K_n} w_{n,k}\int_{t_{n,k}}\psi_i(x)\psi_j(y)\,dt, \tag{10}$$

where the second factor in the summation is a path integral taken over $t_{n,k}$, the path traveled by particle n as it moves between events k and $k+1$. The path integral in Eq. (10) can be written in Cartesian coordinates, yielding

$$\widehat{c_{ij}} = \frac{1}{N}\sum_{n=1}^{N}\sum_{k=1}^{K_n} w_{n,k}\int_0^{d_{n,k}}\psi_i(x(t))\psi_j(y(t))\sqrt{\left(\frac{dx}{dt}\right)^2 + \left(\frac{dy}{dt}\right)^2}\,dt, \tag{11}$$

where $d_{n,k}$ is the total distance traveled by particle n between events k and $k+1$. Since a particle can only change direction at an event k, the particle path between events k and $k+1$ is a straight line between the points $(x_{n,k}, y_{n,k})=(x(0), y(0))$ and $(x_{n,k+1}, y_{n,k+1})=(x(d_{n,k}), y(d_{n,k}))$. As the particle follows this path it has direction $\Omega_{n,k}=(\Omega_x, \Omega_y, \Omega_z)_{n,k}$ and directional cosines given by

$$\mu_{n,k}=Cos\left(\Omega_{x,n,k}\right) \qquad \varphi_{n,k}=Cos\left(\Omega_{y,n,k}\right). \tag{12}$$

Because the path is linear it is possible to parameterize either $y=f(x)$ or $x=f(y)$,

$$y=\frac{\varphi_{n,k}}{\mu_{n,k}}\left(x-x_{n,k}\right)+y_{n,k} \qquad dy=\frac{\varphi_{n,k}}{\mu_{n,k}}dx, \tag{13}$$

or,

$$x=\frac{\mu_{n,k}}{\varphi_{n,k}}\left(y-y_{n,k}\right)+x_{n,k} \qquad dx=\frac{\mu_{n,k}}{\varphi_{n,k}}dy. \tag{14}$$

Using the $y=f(x)$ parameterization Eq. (11) can be rewritten as

$$\widehat{c_{ij}}=\frac{1}{N}\sum_{n=1}^{N}\sum_{k=1}^{K_n}w_{n,k}\int_0^{d_{n,k}}\psi_i\left(x(t)\right)\psi_j\left(\frac{\varphi_{n,k}}{\mu_{n,k}}\left(x(t)-x_{n,k}\right)+y_{n,k}\right)\sqrt{1+\left(\frac{\varphi_{n,k}}{\mu_{n,k}}\right)^2}\,\frac{dx}{dt}dt. \tag{15}$$

Equation (15) now depends only on x and, following a change of variable, can be expressed

$$\widehat{c_{ij}}=\frac{1}{N}\sum_{n=1}^{N}\sum_{k=1}^{K_n}w_{n,k}\sqrt{1+\left(\frac{\varphi_{n,k}}{\mu_{n,k}}\right)^2}\int_{x_{n,k}}^{x_{n,k+1}}\psi_i\left(x\right)\psi_j\left(\frac{\varphi_{n,k}}{\mu_{n,k}}\left(x-x_{n,k}\right)+y_{n,k}\right)dx. \tag{16}$$

Following algebraic simplification Eq. (16) gives the final form of the estimator,

$$\widehat{c_{ij}}=\frac{1}{N}\sum_{n=1}^{N}\sum_{k=1}^{K_n}\frac{w_{n,k}\,d_{n,k}}{\left(x_{n,k+1}-x_{n,k}\right)}\int_{x_{n,k}}^{x_{n,k+1}}\psi_i\left(x\right)\psi_j\left(\frac{\varphi_{n,k}}{\mu_{n,k}}\left(x-x_{n,k}\right)+y_{n,k}\right)dx. \tag{17}$$

Returning to Eq. (11), if the $x=f(y)$ parameterization is used the final result becomes,

$$\widehat{c_{ij}}=\frac{1}{N}\sum_{n=1}^{N}\sum_{k=1}^{K_n}\frac{w_{n,k}\,d_{n,k}}{\left(y_{n,k+1}-y_{n,k}\right)}\int_{y_{n,k}}^{y_{n,k+1}}\psi_i\left(\frac{\mu_{n,k}}{\varphi_{n,k}}\left(y-y_{n,k}\right)+x_{n,k}\right)\psi_j\left(y\right)dy. \tag{18}$$

Equations (17) and (18) yield the same numerical result for particle paths that have nonzero values for $\mu_{n,k}$ and $\varphi_{n,k}$. Particles traveling parallel to either the x-axis ($\varphi_{n,k}=0$) or the y-axis ($\mu_{n,k}=0$) must use the form of the estimator that prevents division by zero. For the case where a particle is traveling parallel to the z-axis ($\mu_{n,k}=\varphi_{n,k}=0$) a new form of the estimator must be derived to prevent division by zero.

Starting with Eq. (17), the fundamental theorem of calculus can be used to evaluate the definite integral in terms of the antiderivatives of the integrand, denoted $F(x)$,

$$\widehat{c_{ij}} = \frac{1}{N}\sum_{n=1}^{N}\sum_{k=1}^{K_n} w_{n,k}\, d_{n,k} \frac{F\left(x_{n,k+1}\right) - F\left(x_{n,k}\right)}{\left(x_{n,k+1} - x_{n,k}\right)}. \tag{19}$$

Taking the limit as $\varphi_{n,k} \to 0$ yields,

$$\lim_{x_{n,k} \to x_{n,k+1}} \widehat{c_{ij}} = \frac{1}{N}\sum_{n=1}^{N}\sum_{k=1}^{K_n} w_{n,k}\, d_{n,k}\, F'\left(x_{n,k}\right). \tag{20}$$

Evaluating $F'(x_{n,k})$ gives the original integrand evaluated at $x_{n,k}$ for a final result,

$$\widehat{c_{ij}} = \frac{1}{N}\sum_{n=1}^{N}\sum_{k=1}^{K_n} w_{n,k}\, d_{n,k}\, \psi_i\left(x_{n,k}\right)\psi_j\left(y_{n,k}\right) \text{ when } \mu_{n,k} = \varphi_{n,k} = 0. \tag{21}$$

Taken together Eq. (17), (18) and (21) give the final estimator for c_{ij}, shown in Eq. (3).

3. Monte Carlo Implementation and Numerical Results

3.1. MCNP Implementation

In order to verify the 2D FET estimator, Eq. (3) was implemented in a modified version of MCNP4c [5] with the set of Legendre polynomials chosen as the expansion basis set. Because the Legendre polynomials are defined only on the domain $[-1,1]$ the code must first scale the spatial expansion domain to fit the Legendre domain. The scalar flux distribution over the scaled 2-D region can then be expanded in terms of Legendre polynomials,

$$\phi(\tilde{x}, \tilde{y}) = \sum_{i=0}^{I}\sum_{j=0}^{J} \frac{(2i+1)(2j+1)}{4} c_{ij}\, \psi_i(\tilde{x})\, \psi_j(\tilde{y}), \tag{22}$$

where $\tilde{x}$ and $\tilde{y}$ are the scaled spatial variables. Once the expansion domain has been appropriately scaled, expansion coefficients can be estimated by using Eq. (3) during the random walk simulation. The Monte Carlo code evaluates the function $G_{i,j}(x_k, x_{k+1}, y_k, y_{k+1})$ after every particle transport operation and stores the cumulative sum over all histories. After the simulation has finished this sum is normalized by the number of starting particles to give the final estimate. Unfortunately, the function G_{ij} contains an integral that is not easy to evaluate analytically for an arbitrary path. To overcome this difficulty we have chosen to evaluate the integral numerically using Gauss-Legendre quadrature. The use of Gauss-Legendre quadrature and the Legendre polynomial recursion relationships allows for a fast and flexible evaluation algorithm that can be used to generate arbitrary order expansion coefficients. For testing purposes a 10^{th} order Gauss-Legendre quadrature was implemented, which allows up to a 9×9 (10 terms in both the x- and y-directions) order spatial expansion over the region.

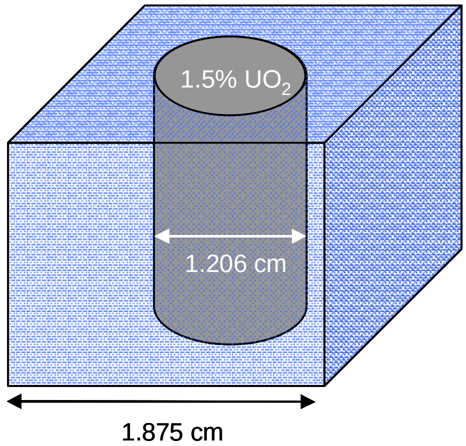

Figure 1. Simulated PWR fuel pin model used for benchmark testing of the Legendre functional expansion tally (FET) implemented in MCNP4c.

3.2. PWR Pin Cell Results

The code was tested on an infinite lattice of simulated PWR fuel pins. Each fuel pin cell (Figure 1) is a 1.5% enriched 0.603 cm radius UO_2 pellet surrounded by light water. The pin cells were modeled as infinitely long and arranged in a square lattice with a pitch of 1.875 cm. The modified version of MCNP4c was used to estimate the first 10×10 Legendre moments of the thermal flux distribution over the x-y plane of the fuel pin cell for varying numbers of total source particles. These moments were then used to construct a functional expansion of the thermal flux in the pin cell, shown in Figure 2a for a 2 million history simulation. For comparison, a 2 million history MCNP5 benchmark eigenvalue calculation was performed using 400 mesh tally regions (20 in the x-direction, 20 in the y-direction) to obtain a direct estimate of the thermal flux distribution over the x-y plane of the pin cell. The results of this simulation are shown in Figure 2b.

By averaging the functional expansion over each of the mesh tally regions defined in the MCNP5 reference solution a quantitative comparison of the two methods was obtained. Figure 3 shows a density plot of the relative difference between the FET and mesh tally approximations across the x-y plane of the fuel pin. The two methods agree well in the center of both the fuel region and the coolant channels and show only slight ~1% disagreement in the behavior of the flux near the fuel-water material interface. This disagreement is due to truncation error which results from approximating a piecewise smooth function with a finite series Legendre expansion. Although low order Legendre expansions demonstrate excellent convergence behavior for approximating analytically smooth functions, such expansions are less robust when applied to functions that are discontinuous or have discontinuous derivatives. In the case of the PWR pin cell, the scalar flux has a discontinuity in its first derivative at the fuel-water interface and, therefore, the FET requires higher order moments to accurately resolve the spatial variation near this interface.

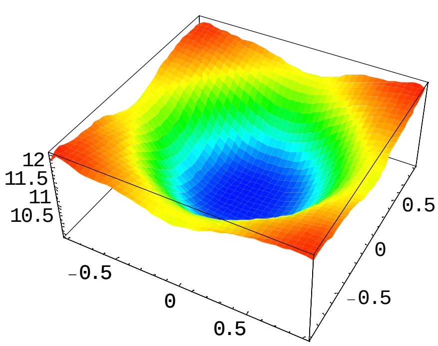

Figure 2a. 9x9 Legendre expansion tally for thermal neutron flux across the fuel pin obtained in a 2 million history simulation.

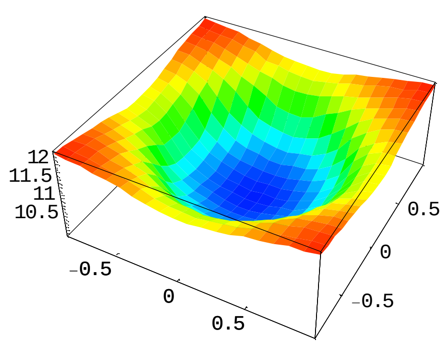

Figure 2b. MCNP5 20×20 mesh tally for thermal neutron flux across the fuel pin obtained in a 2 million history simulation.

To better assess the effect of truncation error on the FET, a series of tests were run to measure the average relative error of the FET (as compared to the MCNP5 benchmark solution) as a function of both Legendre expansion order and number of starting particles. The results of these tests, shown in Figure 4, demonstrate that the functional expansion of the flux converges towards the benchmark solution as the number of histories and the number of terms in the Legendre expansion becomes larger. The observed convergence with increasing Legendre order for a fixed number of histories indicates that both statistical and truncation errors need to be considered with any Monte Carlo functional expansion technique. Simply increasing the number of histories used in a simulation will only reduce the statistical error associated with the estimation of each expansion coefficient. In order to obtain an accurate pointwise scalar flux estimate over the entire spatial domain it is necessary to increase the number of terms in the Legendre expansion and thereby reduce the truncation error associated with approximating a function by a finite series of polynomials. A comparison of run times between the Legendre expansion and mesh tallying methods, given in Table 1, for obtaining 2-D spatial information about a scalar flux distribution indicates that estimating a functional expansion of the flux is comparable to the run time with the mesh tally.

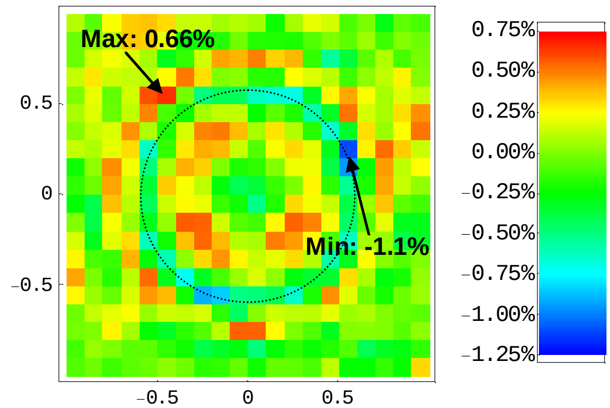

Figure 3. Relative residual error between 9x9 FET and 20x20 mesh tally approximations. The location of the fuel pellet is illustrated by the dashed line. Note that the FET slightly under predicts the flux at the fuel-water interface.

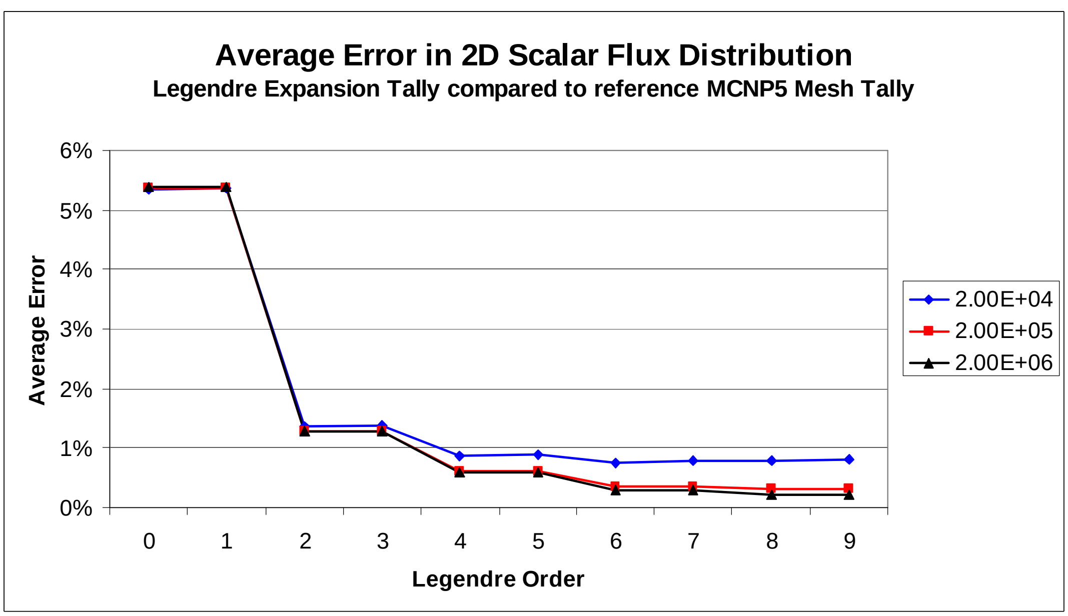

Figure 4. Relative error between the Legendre expansion tally and the 2 million history MCNP5 reference mesh tally solution, averaged over all 400 mesh regions.

Table 1. Comparison of run times between 9th order Legendre functional expansion tally (FET) and MCNP5 20×20 mesh tally for estimating the spatial distribution of thermal flux over a 2-D fuel pin.

Run Time Comparison (minutes)		
Histories	**MCNP4c FET**	**MCNP5 Mesh Tally**
2.00E+04	0.77	0.87
2.00E+05	6.53	8.23
2.00E+06	64.83	75.84

4. Conclusion

In conclusion, we have developed a set of unbiased Monte Carlo track length estimators for the Legendre moments of a scalar flux distribution over a two dimensional region. These estimators have been incorporated into a modified version of MCNP4c and benchmarked against a lattice of realistic PWR type pin cells. The results of the benchmark tests show that, for all cases studied, the method provides accurate functional estimates of the spatial flux distribution when compared to reference solutions obtained from a conventional Monte Carlo mesh tally method.

Acknowledgements

The first author would like to acknowledge the educational support provided by the Naval Nuclear Propulsion Fellowship Program sponsored by Naval Reactors Division of the U.S. Department of Energy.

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