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Title: CONTINUOUSLY VARYING MATERIAL PROPERTIES AND TALLIES FOR MONTE CARLO CALCULATIONS

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Continuously Varying Material Properties and Tallies for Monte Carlo Calculations

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Using a high-order Legendre polynomial representation for material density and tallies within each cell, Monte Carlo codes can model continuous variations in material properties and results. We have demonstrated the Monte Carlo techniques for sampling the free-flight distances and performing pathlength flux tallies for this continuous representation. Application to both fixed-source and eigenvalue problems illustrates the benefits of the continuous representation as compared to conventional stepwise approximations. With these new methods, Monte Carlo codes can now be developed which are continuous in energy, angle, space, material properties, and tallied results.

KEYWORDS: ***Monte Carlo, continuous materials, continuous tallies***

1. Introduction

Monte Carlo calculational methods for particle transport are highly regarded for their continuous treatment of particle energy and angular dependence, and for their very general geometric representations. However, the spatial variation of material properties and tallies have traditionally been modeled with a zero-th order description, i.e., constant over a geometric cell. Recent work [1,2,3] has shown that both of these limitations can be readily overcome, so that continuously varying spatial representations can be extended to material properties and tallies. In this work we provide a demonstration that it is now feasible to implement Monte Carlo codes with continuously varying particle energy and angular dependence, continuously varying material properties, and continuously varying tallies.

2. Description of the Methods

2.1 Continuously Varying Material Properties

Past work on Monte Carlo methods for problems with continuously varying spatial properties was based on the use of Woodcock tracking [4,5] (also called delta tracking, the pseudocollision method, and hole tracking). Woodcock tracking is a robust and ingenious method, but suffers from two drawbacks. First, it can be inefficient for cases where the material properties undergo large variations. Second, the use of Woodcock tracking precludes using tracklength estimators. Instead, tallies are made at pseudocollision points, resulting in an estimator that is intermediate between tracklength and collision estimators.

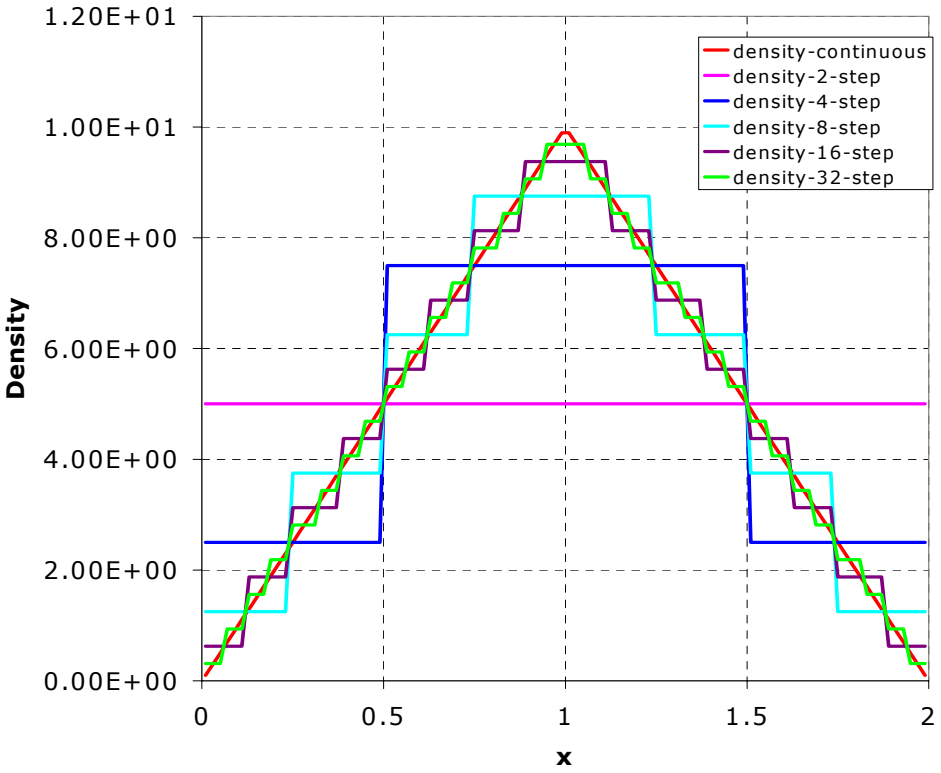

Figure 1. Density variation for Problem A: Continuous density and various stepwise approximations

In the present work, we assume a continuous representation of material properties within each geometric cell and consider only 1D slab geometries for demonstration purposes. We have chosen to use 5th order Legendre polynomials as basis functions within each cell to represent material properties. Since the Legendre polynomials (P_n) are orthogonal over the domain [-1,1], the spatial position within a cell k is first scaled from the range $x_k \le x \le x_{k+1}$ to the range [-1,1] according to

$$f_k(x) = 2 \cdot \left[\frac{x - x_k}{x_{k+1} - x_k} \right] - 1 \ . \tag{1}$$

The density within cell k is then assumed to vary according to

$$\rho_k(x) = \sum_{n=0}^{5} \frac{2n+1}{2} a_{k,n} P_n(f_k(x)), \tag{2}$$

and the macroscopic cross-sections within cell k vary as

$$\Sigma_{r,k}(x) = \frac{\rho_k(x)}{\rho_{0,k}} \cdot \Sigma_{r,k,0} \ , \tag{3}$$

where $\rho_{0,k}$ is the reference density used in computing $\Sigma_{r,k,0}$ and r denotes a specific reaction type. The expansion coefficients $a_{k,n}$ and cross-sections $\Sigma_{r,k,0}$ for each cell k are fixed for a problem, part of the input to the calculation. The density is permitted to be discontinuous at material boundaries.

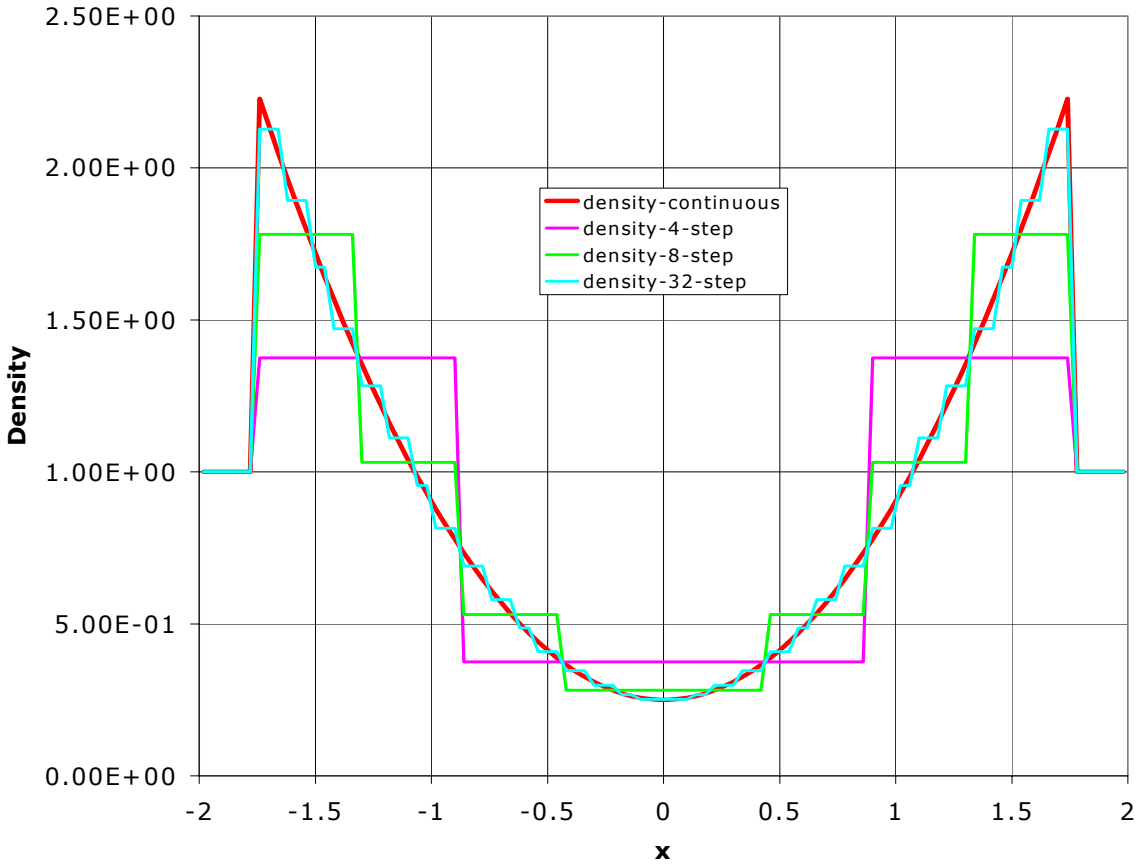

Figure 2. Density variation for Problem B: Quadratic variation for center fissionable region and various stepwise approximations

Figures 1 and 2 illustrate the density variations used in the example problems A and B in this paper. Problem A is a slab of thickness 2 cm where the density varies linearly between 0 at the outer boundary and 10 in the center, as shown in Figure 1. In conventional Monte Carlo codes, the density variation would be modeled by a stepwise approximation, where the geometry is divided into smaller cells which each have a different uniform density. Figure 1 shows the mass-preserving approximations using 2, 4, 8, 16, and 32 steps. Problem B is a fissionable slab bordered on both sides by a reflector. Within the fissionable region, the density increases quadratically toward the outer edges, suggestive of a reactor core which has depleted more in the higher flux central region. Figure 2 shows the density variation along with several stepwise approximations.

Eqs. 1-3 specify the continuously varying material properties within each cell. The cross-sections at any collision point can then be readily computed and nearly all of the procedures used in normal Monte Carlo codes can be used without change. The notable exception is random sampling of the particle free-flight distance to the next interaction. Because of the varying cross-section along the flight path special procedures must be used. Rather than resort to Woodcock tracking, we sample particle flight paths using the direct numerical scheme reported in [1] and as a result can make all of the normal tracklength tallies. We have previously shown that this approach is computationally efficient. With this approach to the

Monte Carlo sampling, it is possible to explicitly represent continuous material density gradients without resorting to step-wise approximations.

To apply the direct sampling procedure from [1], Eqs. 1-3 are used for the cross-section variation along the flight path s. The optical distance $\tau_k(s)$ for cell k is also required, as given by

$$\tau_k(s) = \int_x^{x+s} \Sigma_{t,k}(x+s)ds = \int_x^{x+s} \Sigma_{t,k,0} \cdot \frac{1}{\rho_{k,0}} \cdot \left[\sum_{n=0}^{5} \frac{2n+1}{2} a_{k,n} P_n(f_k(x+s)) \right] ds$$

$$= \frac{x_{k+1} - x_k}{2} \cdot \left\{ \frac{a_{k,0}}{2} [f_k(x+s) - f_k(x)] \right. \tag{4}$$

$$\left. + \sum_{n=1}^{5} \frac{a_{k,n}}{2} [P_{n+1}(f_k(x+s)) - P_{n-1}(f_k(x+s)) - P_{n+1}(f_k(x)) + P_{n-1}(f_k(x))] \right\}$$

where the relation $\int P_n(x) = [P_{n+1}(x) - P_{n-1}(x)]/(2n+1)$ was used in the integration. Given Eqs. 1-4, the free-flight distance is sampled using the direct numerical method described in [1], with a Newton iteration scheme utilized in solving the nonlinear equation for the flight distance.

2.2 Continuously Varying Tallies

Monte Carlo tallies are typically made for spatial bins, with just the zero-th moment of the tally information provided (i.e., the mean value for the bin, along with its standard deviation). Higher-order components of the tallies are readily obtained, either as just the higher moments within a cell or in terms of arbitrary basis functions. A few reported past studies have made use of such treatments for special purposes [6], and recent work has focused on practical implementations in 1D and 2D geometry [2,3]. To demonstrate that continuously varying tallies can be incorporated into standard Monte Carlo algorithms, we have chosen a 5th order Legendre polynomial representation for cell fluxes in 1D geometry. This can readily be extended to other sets of basis functions. Using the coordinate scaling from Eq. 1, a continuous flux within spatial cell k can be represented as

$$\phi_k(x) = \sum_{n=0}^{5} \frac{2n+1}{2} \cdot b_{k,n} \cdot P_n(f_k(x)) , \tag{5}$$

where cell k covers the range $x_k \le x \le x_{k-1}$ and the coefficients $b_{k,n}$ are defined by

$$b_{k,n} = \frac{2}{x_{k+1} - x_k} \cdot \int_{x_k}^{x_{k+1}} \phi_k(x) P_n(f_k(x)) dx \tag{6}$$

The coefficients are estimated by pathlength tallies during the Monte Carlo simulation by tallying the $N+1$ quantities

$$F_{k,n}(x,\mu,d) = \begin{cases} \dfrac{wd}{f_k(x+d\mu) - f_k(x)} \cdot \displaystyle\int_{f_k(x)}^{f_k(x+d\mu)} P_n(x')dx' & \text{if } \mu \neq 0 \\ wd \cdot P_n(f_k(x)) & \text{if } \mu = 0 \end{cases} \tag{7}$$

for each flight path of length d in cell k, where x is the coordinate at the start of the path and μ is the direction cosine for the flight. Using the relation $\int P_n(x) = [P_{n+1}(x) - P_{n-1}(x)]/(2n+1)$, the tally quantities given by Eq. 7 can be evaluated as

$$F_{k,n}(x,\mu,d) = \begin{cases} \dfrac{wd}{f_k(x+d\mu) - f_k(x)} \cdot [\, P_{n+1}(f_k(x+du)) - P_{n-1}(f_k(x+du)) \\ \qquad -P_{n+1}(f_k(x)) + P_{n-1}(f_k(x))\,]/(2n+1) & \text{if } \mu \neq 0 \\ wd \cdot P_n(\, f_k(x)\,) & \text{if } \mu = 0 \end{cases} \tag{8}$$

Since $N+1$ quantities must be tallied for each flight (i.e., 6 quantities for a 5th order Legendre representation), the computation time will be larger than for conventional Monte Carlo with zero-th order tallies. However, the conventional approach would require subdividing the geometry into much finer cells in order to spatially resolve the flux variations, and that would also require significant additional computation for the Monte Carlo tracking. With continuous representations of the tally information, it is not necessary to subdivide the geometric cells so finely; fewer cells may be used due to the higher-order information content of the continuous tallies. Which approach is faster, stepwise approximation vs. the Legendre representation, will depend on the complexity of the geometry and the particular computer code implementation. The examples in the next section illustrate the tradeoffs.

3. Results

We have demonstrated the feasibility of using continuously varying material properties and tallies by means of a 1D Monte Carlo code which includes anisotropic scattering, 5th order Legendre basis functions for material properties, and 5th order Legendre basis functions for flux tallies. We have used this code first to verify that the continuous representation was implemented correctly, through comparisons with the normal step-wise constant approximation to varying materials. In addition, we have investigated a number of deep penetration problems and eigenvalue problems to examine the benefits of a continuous representation.

Problem A is a fixed-source Monte Carlo problem with a monodirectional beam source impinging on a slab, with vacuum boundaries. The cross-sections for unit density were Σ_T=1.00, Σ_S=0.99, and Σ_A=0.01. The material in the slab has a linear variation in density from 0 at the outer edges to 10 in the center. The density variation for this problem is shown in Fig. 1. With the continuous Legendre representation of the material density, the density variation may be modeled exactly using only 2 geometric cells. Also shown in Fig. 1 are several stepwise approximations to the density variation, using 2, 4, 8, 16, or 32 steps of constant density. Fig. 3 shows the results of running Monte Carlo calculations with 50,000 histories each. For the continuous tallies, a 5th order Legendre representation was used in each of the 2 geometric cells. For the stepwise cases, uniform tallies were made for each region of constant density. It is clear from Fig. 3 that the stepwise approximations converge to the continuous results as the number of subdivisions for geometry and tallies increases. It is not clear *a priori*, however, how fine the subdivisions must be to yield acceptably accurate results. A conscientious Monte Carlo practitioner would have to run this problem with increasingly finer mesh cells until the results did not appear to change. Using the continuous representation, only 1 calculation is necessary, assuming that the basis functions for density and tallies are sufficiently high-order and complete.

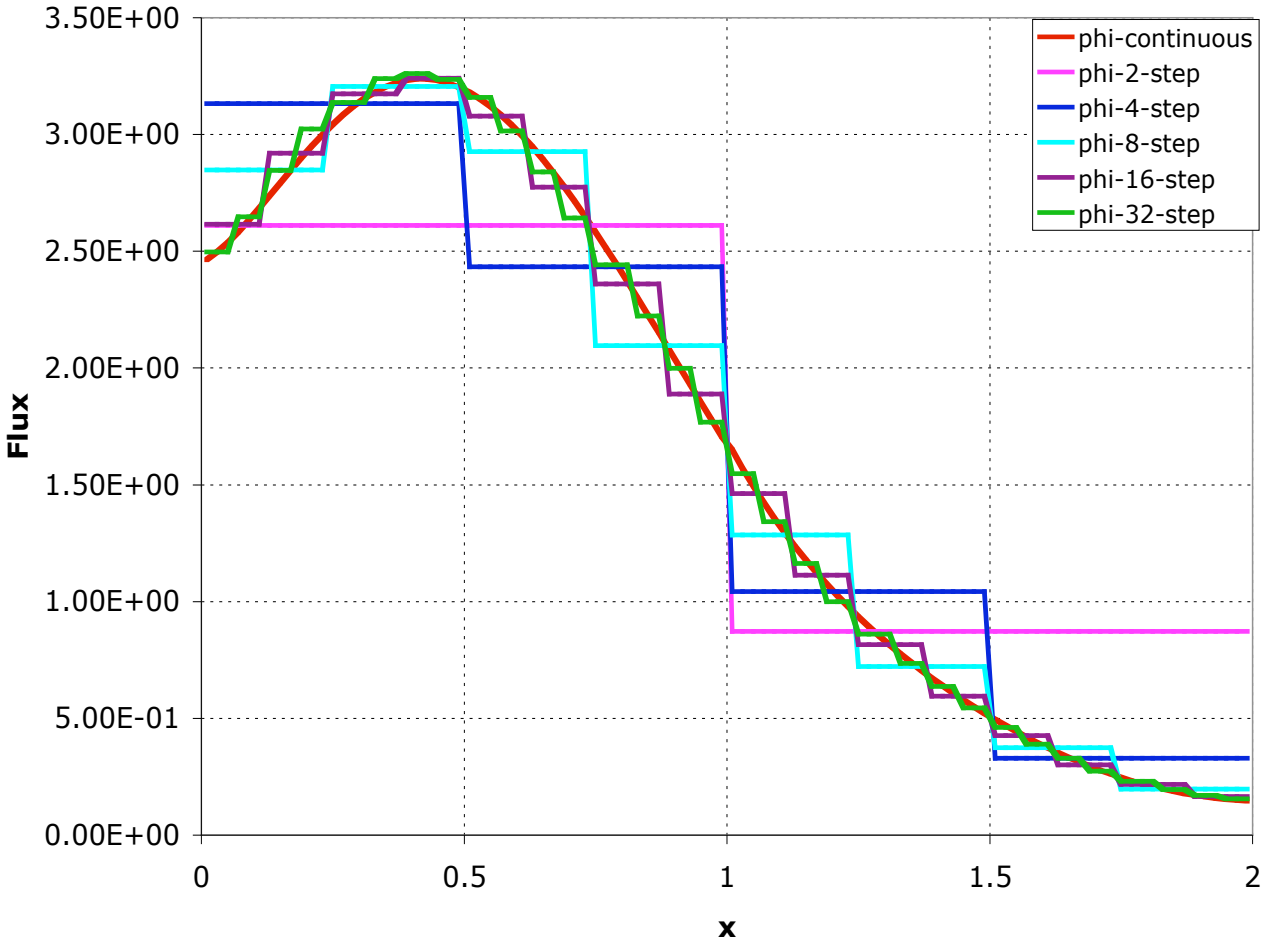

Figure 3. Flux results for Problem A: Beam into slab with linearly-varying density, continuous tally and various stepwise approximations

Problem B is an eigenvalue calculation for a slab reactor with finite reflector. The cross-sections for unit density were Σ_T=0.25, Σ_S=0.24, and Σ_A=0.01 for the reflector, and Σ_T=2.00, Σ_S=0.125, and Σ_A=1.025, Σ_F=0.85, and ν=2.4 for the core. The material in the core had a quadratic density as shown in Fig. 2, varying from 0.25 at the center to 2.25 at the core edges. This is suggestive of a reactor later in life, where more depletion has occurred in the higher-flux central region. Fig. 2 also shows stepwise approximations to this density with 4, 8, and 32 steps of constant density per material. Fig. 4 shows the results of Monte Carlo eigenvalue calculations performed with 5000 histories per cycle. For each case, 175 cycles were run, with the first 25 discarded, for a total of 750,000 active histories per calculation. For the stepwise approximations, zero-th order tallies were made over each of the constant-density cells. For the continuous tallies, only 3 cells were used, with 5th order Legendre representations in the single cell representing the core and in the 2 reflector cells. It is seen in Fig. 4 that the stepwise approximations converge to the continuous tally results, with 32 steps per material needed for close accuracy. As for Problem A, a conscientious Monte Carlo practitioner would have to run a series of cases refining the mesh cells until results converged. Only 1 run is needed with the continuous density and tallies.

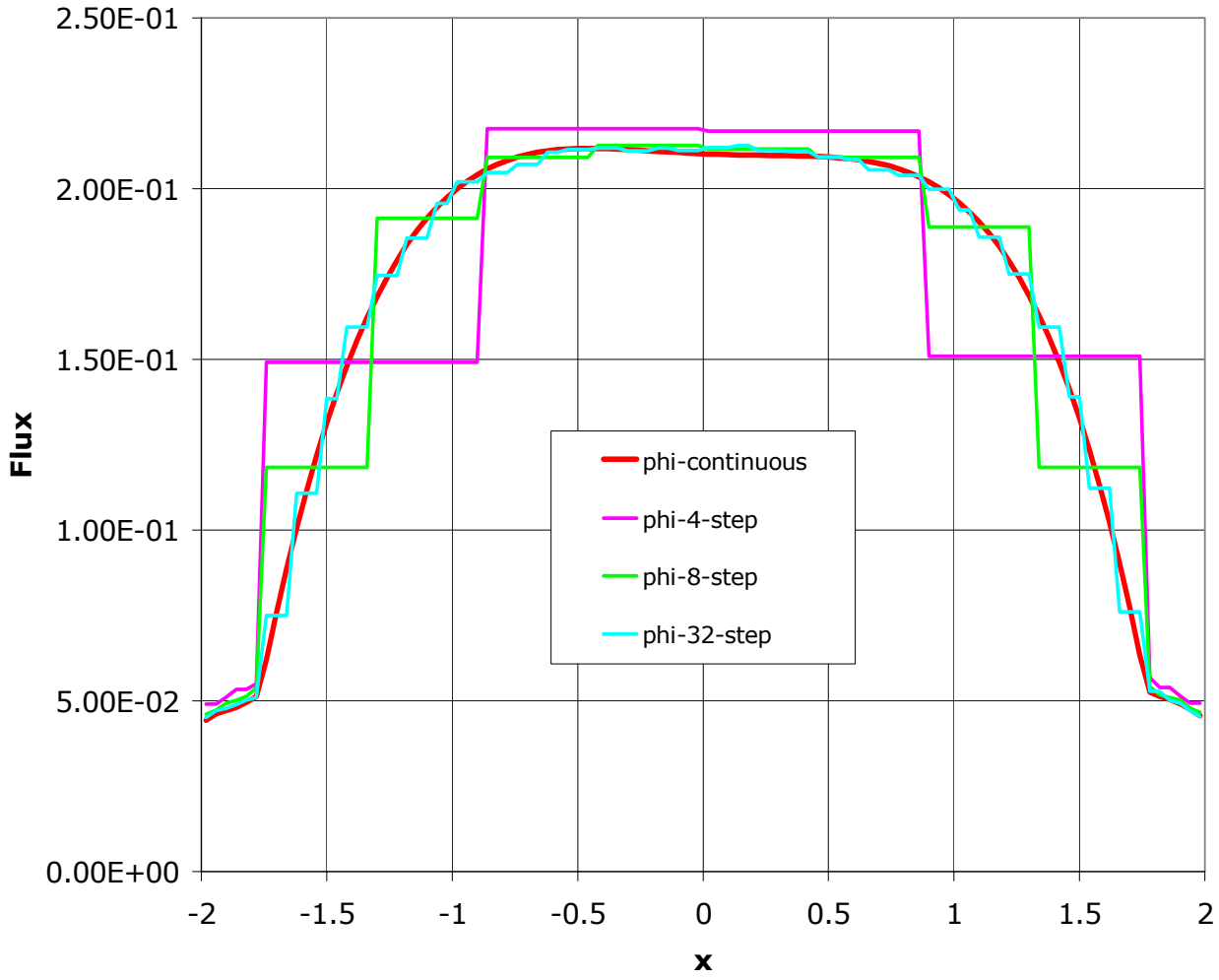

Figure 4. Flux results for Problem B: Quadratic density variation, continuous tallies and various stepwise approximations

A comparison of running times for Problem B serves to illustrate the tradeoff in computation time between fewer cells with high-order density and tallies vs. more cells with zero-th order density and tallies:

Continuous (3 cells)	102 sec
4-step (12 cells)	117 sec
8-step (24 cells)	130 sec
32-step (96 cells)	283 sec

For this problem, the continuous representation uses less computer time, despite the added complexity of the 5th order representation, due to the smaller number of tracking operations and cell boundary crossings.

4. Conclusions

In this work we have provided a demonstration that it is now feasible to implement Monte Carlo codes with continuously varying particle energy and angular dependence, continuously varying material properties, and continuously varying tallies. All of the production Monte Carlo codes available today make use of a zero-th order approximation for representing material densities and cell flux tallies. We have demonstrated that using high-order basis functions to represent the density and tallies (e.g., 5^{th} order Legendre polynomials) can greatly reduce the difficulty in modeling problems with varying density and tallies, can significantly reduce the number of cells required, and for complex problems may even reduce the computation time. Future challenges include the significant effort needed for practical implementation of these methods into production Monte Carlo codes and the investigation of methods for depleting materials using the continuous representations.

Acknowledgements

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