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Author(s): Betzler, Benjamin R.
Kiedrowski, Brian C.
Brown, Forrest B.
Martin, William R.

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CALCULATING α-EIGENVALUE SPECTRA WITH MONTE CARLO

Benjamin R. Betzler
Department of Nuclear Engineering and Radiological Sciences
University of Michigan
2355 Bonisteel Boulevard, Ann Arbor, MI 48109, USA
bbetzler@umich.edu

Brian C. Kiedrowski and Forrest B. Brown
X-Computational Physics Division, Monte Carlo Codes Group
Los Alamos National Laboratory
P.O. Box 1663, MS A143 Los Alamos, NM 87545
bckiedro@lanl.gov; fbrown@lanl.gov

William R. Martin
Department of Nuclear Engineering and Radiological Sciences
University of Michigan
2355 Bonisteel Boulevard, Ann Arbor, MI 48109, USA
wrm@umich.edu

ABSTRACT

The time-dependence of the neutron flux is investigated for continuous-energy infinite media and simple, one-speed, one-dimensional media using a transition rate matrix Monte Carlo tally based on a formulation of the α-eigenvalue problem. The research code TORTE calculates the α-eigenvalue spectra and shape eigenfunctions of these media. TORTE also performs the eigenfunction expansion, or modal expansion, necessary to analyze transient behavior of the neutron flux for an arbitrary initial source. These calculations compare well to time-dependent Monte Carlo calculations for infinite media and simple scattering slabs. For one-dimensional media, TORTE-calculated α eigenvalues and shape eigenfunctions compare well to those calculated in literature. Much of the work is verification with previous benchmarks, but we are able show some capabilities of this method.

Key Words: Monte Carlo, time eigenvalue, eigenfunction expansion, criticality

1 INTRODUCTION

The fission matrix method of estimating k eigenvalues and eigenvectors of a system using Monte Carlo techniques [1] discretizes the spatial domain and estimates transition probabilities between locations of fission events. For an adequately chosen spatial mesh, the eigenvalues and eigenvectors of the fission matrix match those of the k-eigenvalue problem of the underlying system. The fundamental k eigenvector matches the neutron flux for a steady-state, critical system. Time-dependent neutron behavior of a system is more adequately obtained using the α-eigenvalue problem, where eigenvalues describe the temporal behavior and eigenvectors describe the position, energy, and direction variation of the neutron distribution.

The transition rate matrix method [2] is the continuous-time analog of the discrete-time fission matrix method, where probabilities between states are calculated for a single fission

generation. The transition rate matrix contains rates defining transitions between states in continuous time. In the language of neutron transport, the eigenvalues of the transition rate matrix are the time-absorption or α eigenvalues, and the eigenvectors are discrete approximations of the eigenfunctions of the adjoint (backwards) transport equations.

For this paper, discrete states are defined over intervals in the energy spectrum for an infinite medium, and separately, over the position and direction domain for simple, one-dimensional media. The tallies needed to estimate elements of the transition rate matrix are defined. The standalone code TORTE calculates these tallies during a forward Monte Carlo simulation. For infinite media, observations of the convergence of α eigenvalue spectra are shown, and the accuracy of the calculated spectra in approximating the actual spectra is supported by agreement of the eigenfunction expansion solutions to time-dependent Monte Carlo calculations. For one-dimensional problems, calculated α eigenvalues and shape eigenfunctions compare well with benchmark solutions.

2 THEORY

Monte Carlo methods use probability and random numbers to perform direct simulation of neutron transport in systems. Solutions to the neutron transport equation are inferred through mean values of estimators, called tallies. These solutions describe the mean-value neutron behavior in the system with a precision dependent on the number of random numbers used in the calculation.

The common assumption for handling time dependence of the neutron flux, used in point kinetics and quasi-static methods, is that the temporal dimension is largely separable from the rest of phase space (position, energy, direction). Eigenfunction expansion uses this separation, but expands the neutron flux as a linear combination of the shape eigenfunctions multiplied by a time function. For a system with no external source for $t > 0$, this time function is an exponential, and ψ at any time t is described as

$$\psi(\mathbf{r}, E, \hat{\mathbf{\Omega}}, t) = \sum_{n=0}^{\infty} A_n \psi_n(\mathbf{r}, E, \hat{\mathbf{\Omega}}) e^{\alpha_n t}, \tag{1}$$

where α_n is the n-th eigenvalue, ψ_n is the corresponding shape eigenfunction, and A_n is an amplitude coefficient related to the neutron source. The fundamental eigenvalue α_0 is typically of most interest because it describes the asymptotic behavior of the system. The ψ_n contain information about the position, energy, and direction dependence, and are thus referred to as shape eigenfunctions. The combined value of $A_n\psi_n$ is sometimes known as the n-th kinetic mode. Completeness of the eigenfunctions has never been rigorously proven for a general system, but seems to work well empirically [3]. The delayed neutron precursor concentrations $C_m(\mathbf{r}, t)$ also follow this exponential time behavior.

2.1 Transition Rate Matrix

The α eigenvalues and eigenfunctions are obtained from Monte Carlo simulation by discretizing the phase space into a collection of states and calculating transition rates between the

states. Each state represents particles (neutrons or precursors) that meet certain conditions. For infinite media, these states denote energy intervals or delayed neutron precursor groups. For one-dimensional media, these states denote a position and direction interval. In either case, the transition rate matrix $\mathbf{Q}$ has the form:

$$\mathbf{Q} = \begin{bmatrix} -q_1 & q_{12} & \cdots \\ q_{21} & -q_2 & \cdots \\ \vdots & \vdots & \ddots \end{bmatrix}. \tag{2}$$

The quantity q_i is the mean net removal rate from state i, and q_{ij} ($i \neq j$) is the mean rate that neutrons transition from state i into j. Note that q_i includes capture rates from state i, so the rows are not normalized to zero. Thus, there may be an overall net gain or loss in the neutron population, as is expected for a supercritical or subcritical system.

The $\mathbf{Q}$ for infinite and one-dimensional media differ greatly. For infinite media, $\mathbf{Q}$ is organized into four partitions describing transition rates between and within energy intervals and precursor groups. These transition rates are expressible in terms of cross sections. The top-left partition describes the transition of neutrons between energy intervals:

$$q_{ij} = \begin{matrix} v_i(\Sigma_{Ri} - \chi_{pi}\nu_{pi}\Sigma_{fi}), & i = j \\ v_i(\Sigma_{sij} + \chi_{pj}\nu_{pi}\Sigma_{fi}), & i \neq j \end{matrix}, \tag{3}$$

where v_i, Σ_{Ri}, Σ_{fi}, ν_{pi}, and χ_{pi} are the average speed, removal and fission cross sections, average prompt neutrons emitted per fission, and prompt fission emission probability for energy interval i; and Σ_{sij} is the scattering cross section from energy interval i to j. The top-right partition pertains to neutrons inducing fission resulting in the production of delayed neutron precursors:

$$q_{ij} = v_i\beta_j\nu_{di}\Sigma_{fi}, \tag{4}$$

where β_j is the delayed fraction for precursor group j and ν_{di} is the average delayed neutrons emitted per fission for energy interval i. The bottom-left partition represents the emission of neutrons from precursors:

$$q_{ij} = \chi_{ij}\lambda_i, \tag{5}$$

where χ_{ij} is the emission of neutrons from precursor group i into neutron energy interval j, and λ_i is the decay constant for precursor group i. Finally, the bottom-right partition represents precursor decay (removal):

$$q_{ij} = \begin{matrix} \lambda_j, & i = j \\ 0, & i \neq j \end{matrix}. \tag{6}$$

For one-dimensional media, $\mathbf{Q}$ is composed of two types of rates describing: (i) transitions between direction intervals for the same position interval (neutrons scattering from $\mu \to \mu'$) and (ii) transitions between position intervals for the same direction interval (neutrons moving to the next position interval at direction μ). The transition rate between direction intervals for the same position interval is represented by the scattering rate and fission rate:

$$q_{ij} = v_i(\Sigma_{sij} + \chi_j\nu_i\Sigma_{fi}), \tag{7}$$

where Σ_{sij} is the scattering cross section from direction interval i to j and χ_j is the prompt fission emission probability for direction interval j. For this paper, isotropic scattering and prompt fission neutron emission is assumed. The transition rate between position intervals for the same direction interval is represented by the rate that neutrons travel through the position interval:

$$q_{ij} = \frac{v_i}{d_{ij}}, \tag{8}$$

where d_{ij} is the average distance traveled before exiting to position interval j. The diagonal q_i elements are the total removal rate from state i.

In both formulations, the quantities are elements of the matrix from the adjoint α-eigenvalue problem. The adjoint eigenvalues $\alpha^\dagger$ are the complex conjugates of the forward eigenvalues α, but because the matrix is real, if an eigenvalue is complex, its complex conjugate is also an eigenvalue. Thus, the forward and adjoint eigenvalue spectra contain the same eigenvalues. Still, the forward eigenvectors must be obtained by taking $\mathbf{Q}^\top$, exchanging the speeds v_i and v_j, and finding the eigenvectors of the resultant matrix.

2.2 Monte Carlo Tallies

The Monte Carlo simulation tallies the elements of $\mathbf{Q}$ during a k-eigenvalue calculation using the power iteration technique. Technically, when the system is not exactly critical, the spectrum is incorrect; this effect is assumed to be negligible. During the simulation, reaction rate tallies are used to estimate the q_{ij}'s.

All elements are combinations of removal rates and probabilities. For infinite media:

$$\lambda_i = \tau_{Ri}^{-1} = (\text{average decay time from precursor group } i)^{-1},$$

$$v_i\Sigma_{Ri} = \tau_{Ri}^{-1} = (\text{average removal time from energy interval } i)^{-1},$$

$$v_i\Sigma_{fi} = v_i\Sigma_{Ri}\frac{\Sigma_{fi}}{\Sigma_{Ri}} = \tau_{Ri}^{-1}\left(\frac{\text{\# of fissions caused by neutrons in energy interval } i}{\text{\# of removals from energy interval } i}\right),$$

$$v_i\Sigma_{sij} = v_i\Sigma_{Ri}\frac{\Sigma_{sij}}{\Sigma_{Ri}} = \tau_{Ri}^{-1}\left(\frac{\text{\# of scatters from energy interval } i \text{ into interval } j}{\text{\# of removals from energy interval } i}\right).$$

For one-dimensional media, where a state is a direction interval in a position interval:

$$v_i\Sigma_{fi} = \tau_i^{-1}\left(\frac{\text{\# of fissions caused by neutrons in state } i}{\text{\# of removals from state } i}\right),$$

$$v_i\Sigma_{sij} = \tau_i^{-1}\left(\frac{\text{\# of scatters from state } i \text{ into state } j}{\text{\# of removals from state } i}\right),$$

$$\frac{v_i}{d_{ij}} = \tau_i^{-1}\left(\frac{\text{\# of removals to state } j}{\text{\# of removals from state } i}\right),$$

where τ_i is the average removal time from state i.

2.3 Eigenfunction Expansion Coefficients

The expansion coefficients A_n determine the contribution of the n-th shape eigenfunction to the flux solution. While the eigenvalues α_n and their corresponding shape eigenfunctions ψ_n are only dependent on the system configuration, the expansion coefficients A_n depend on initial source characteristics $S(\mathbf{r}, E, \hat{\mathbf{\Omega}}, t)$ as well:

$$A_n = \frac{\left\langle \psi_n^\dagger, S_0 \right\rangle}{\left\langle \psi_n^\dagger, v^{-1}\psi_n \right\rangle + \sum_m \left\langle C_{m,n}^\dagger, C_{m,n} \right\rangle}, \tag{9}$$

where the brackets denote integration over all relevant phase space variables, and the † denotes adjoint shape eigenfunctions. The initial source S_0 may be used to model a pulsed source or an initial condition (such as an initial flux and precursor distribution) for time-dependent analysis.

3 INFINITE-MEDIUM CONTINUOUS-ENERGY RESULTS

TORTE is a standalone research code written in FORTRAN using LAPACK [4] for matrix eigenvalue functions. It performs k-eigenvalue power iteration calculations with multigroup or continuous-energy nuclear data (read from ENDF/B-VII.0 [5] or ENDF/B-VII.1 [6]). For scattering, TORTE handles free gas and continuous $S(\alpha, \beta)$, but is limited in that it does not treat high-energy inelastic scattering. During the power iteration, TORTE collects the aforementioned tallies for the q_{ij} and calculates the α eigenvalues and eigenfunctions after the run is completed. Code physics and multigroup problems agree well with expected distributions and analytical solutions [2]. Here, the discussion is limited to continuous-energy media.

3.1 Convergence Behavior

In a Monte Carlo simulation, as the number of particle histories increases, the uncertainty in results decrease. Extending this to TORTE, the tallies for the q_{ij} decrease in uncertainty as more particle histories are used, in turn resulting in better solutions for the α eigenvalue spectrum and eigenfunctions. The fundamental α eigenvalue and shape eigenfunction converge first, and in general, the lower eigenvalues and shape eigenfunctions converge faster than higher ones.

This observed behavior shows that the method converges to a solution, but the ability of that solution to approximate the actual α-eigenvalue spectrum of the problem is related to the number of energy intervals used to formulate $\mathbf{Q}$. Consider a very subcritical, graphite-moderated medium with an 80:1 C:UO_2 molecular ratio and 4.25% enriched uranium. Several TORTE runs have numbers of equal-lethargy intervals ranging from $G = 80$ to $G = 3000$ between $E_0 = 20$ MeV and $E_G = 1 \times 10^{-11}$ MeV. All runs were performed with 100×10^6 particles and calculated $k = 0.86962 \pm 0.00015$. The fundamental eigenvalue is limited by the slowest decaying delayed precursor group, $\alpha_0 = -0.012526$ s^{-1}. Fig. 1 shows the calculated α-eigenvalue spectrum for selected numbers of energy intervals.

All cases converge to the same mentioned fundamental α_0 matching the slowest decaying delayed neutron precursor. All cases also agree for the first few (largest) eigenvalues, but above that, significant differences appear. The cases with the fewest energy bins differ the most from the

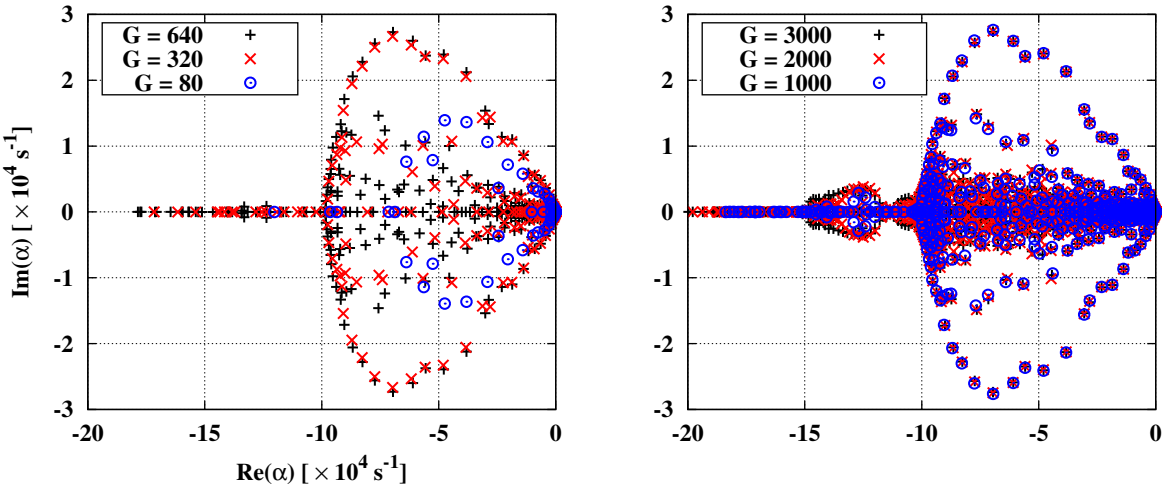

Figure 1: The α-eigenvalue spectrum for the subcritical graphite problem.

other calculations (Fig. 1, left). But, as the number of energy intervals increases, the bulk of the spectrum remains unchanged and seems to converge with additional eigenvalues appearing closer to the real axis (Fig.1, right). This is empirical evidence that as the energy intervals increase, the solution more closely approaches the actual α-eigenvalue spectrum. When fewer energy intervals are used, the higher α eigenvalues are an approximation to the higher portion of the actual α-eigenvalue spectrum. Thus, many of the most negative eigenvalues of the lower energy interval cases ($G = 80$) are between those of higher energy interval cases ($G = 640$). This is supported by similar observations of the fission matrix method for k-eigenvalues [1]. One complication of analyzing specific α eigenvalues is the presence of lines in the spectrum [3]. These lines appear during calculations in areas of the spectrum where specific eigenvalues continue to change as the number of energy intervals is increased. This change is due to numbers of eigenvalues grouping to form lines in the spectrum.

3.2 Eigenfunction Expansion

Using the same subcritical graphite problem, TORTE performs eigenfunction expansion to obtain a time-dependent solution for the neutron flux as a result of a pulsed source with no initial delayed neutron precursors (no delayed neutron background). All modes are included during the expansion. For any of the cases $G = 80$ through $G = 3000$, the expanded solutions are indistinguishable on a log-log plot, except for the resolution of resonances that an increased number of energy intervals provides. This serves to support the notion that the spectrum calculated with fewer energy intervals is an approximation to the larger spectrum. Using the $G = 3000$ case, Fig. 2 compares the expanded solution with a true, time-dependent Monte Carlo calculation performed with a censusing technique. To increase the statistics for the time-dependent Monte Carlo run, only $G = 320$ equal-lethargy intervals was used.

The eigenfunction-expanded solution is able to preserve much of the detail in the energy spectrum and matches well with the time-dependent Monte Carlo calculation throughout the transient. At $t = 0.1$ ms, the neutrons have just begun to slow down from the initial 14.1 MeV

pulse strength of 10^{15}. A noisy behavior is observed in the eigenfunction expansion for this short time period $t < 0.3$ ms. This is at least in part due to the inability of the eigenfunction expansion to accurately model such a sharp source. In cases where smoother sources are used, this behavior is less pronounced, but still exists, suggesting some other contributions to this discrepancy. The time-dependent Monte Carlo calculation has no issues handling these incredibly short time periods. At $t = 0.5$ ms, the slowing neutrons form a distinct flux packet as they collide with the graphite moderator. Both solutions match very well, with the time-dependent Monte Carlo solution having issues with low-probability high energy neutrons born from fast fissions. At $t = 10$ ms, the flux packet decreases in size as the fast neutron flux has decreased considerably. Dips in the spectrum because of ^{238}U capture resonances are resolved in the eigenfunction expansion solution due to the large number of energy intervals used. The time-dependent Monte Carlo solution also has dips due to resonances, but they are less detailed. At $t = 250$ ms, the flux packet continues to decrease as the spectrum begins to assume the shape of the prompt fundamental shape eigenfunction. Noise present in the higher energies of the time-dependent

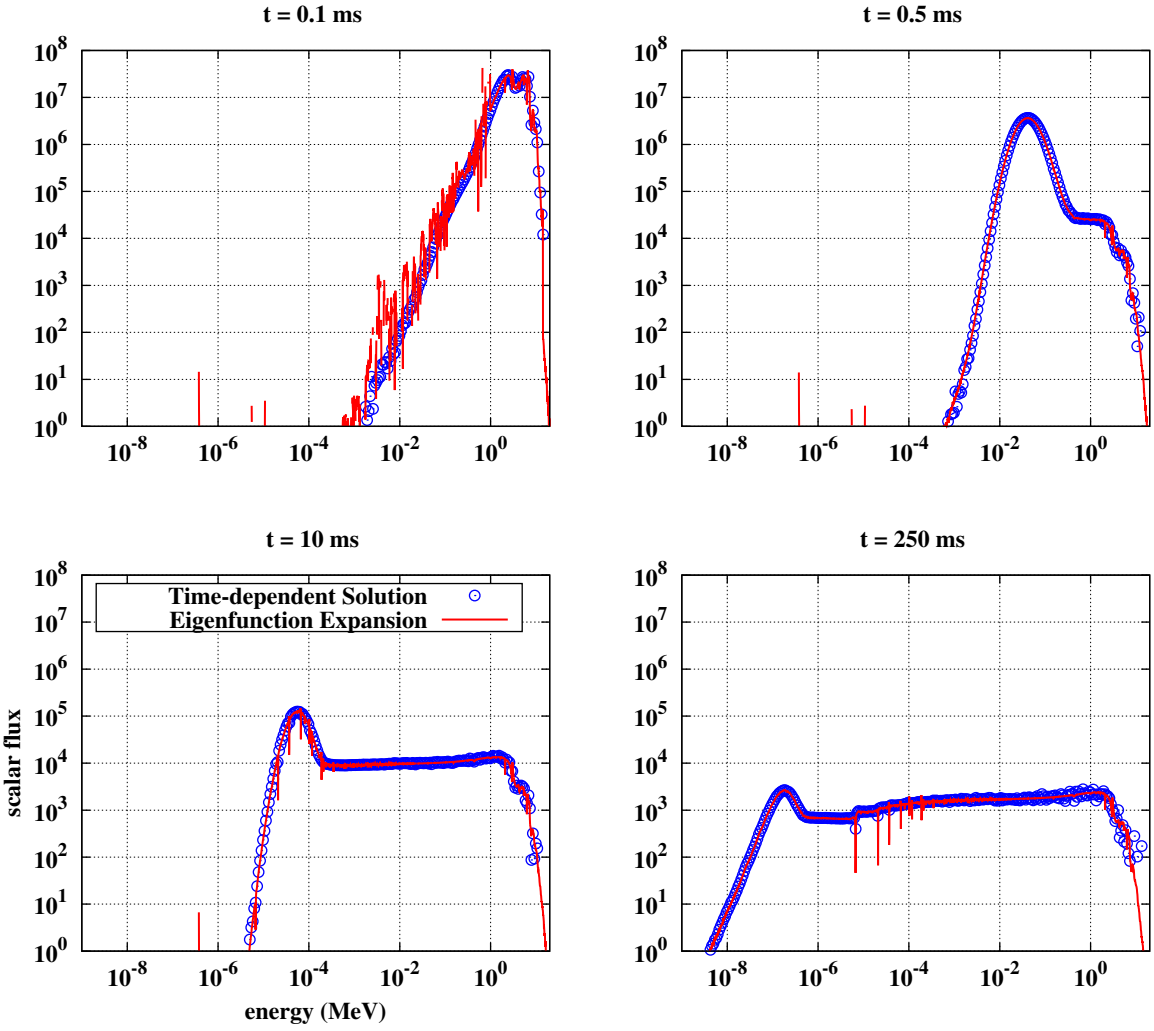

Figure 2: Snapshots of a transient for the subcritical graphite problem.

solution is due to the decreasing neutron population leading to the decreasing fission rate necessary to replenish the fast flux. The spectrum converges to the prompt fundamental shape eigenfunction on the order of a few seconds. Not long after, delayed fission neutrons will dominate the spectrum and it will decrease according to the delayed precursor decay constants. This is difficult to calculate with time-dependent Monte Carlo because of the very low probability ($> 1\%$) of a fission resulting in the emission of a delayed neutron precursor. The delayed neutron shape eigenfunctions are generally very similar to that of the prompt fundamental shape eigenfunction.

4 ONE-DIMENSION RESULTS

TORTE was edited to include the spatial variables needed to perform one-dimensional Monte Carlo transport. The k-eigenvalue power iteration and tally scheme is similar, but the code is one-speed ($v = 1$ cm/s) and total fission cross sections are set to unity $\Sigma_t = 1$ cm^{-1}. Thus, the resulting calculations are dimensionless. Isotropic scattering and fission emission are assumed. The code is set up for one-dimensional finite slabs of thickness Δ with vacuum boundary conditions at $x = 0$ and $x = \Delta$, as any reflecting boundary condition eliminates higher shape eigenfunctions from the solution. Good literature on α-eigenvalues for simple geometries provide a benchmark to which the transition rate matrix method may be compared. The Green's Function Method (GFM) [7] is capable of calculating the α-eigenvalue and shape eigenfunctions of scattering or multiplying one-dimensional media. The next sections discuss some verification work.

4.1 Non-multiplying Medium

Initial tests show that the transition rate method adapts well to a simple scattering slabs. Instead of a k-eigenvalue calculation, TORTE uses a collision (c) eigenvalue iteration to obtain a neutron source within the slab. Fig. 3 compares the eigenfunction expansion to the

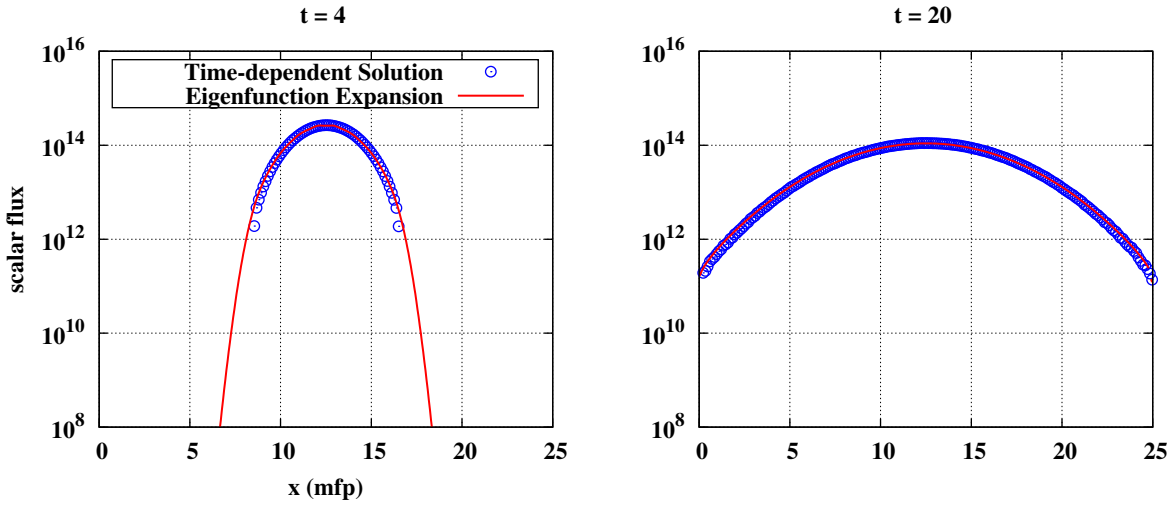

Figure 3: Snapshots of a transient in a scattering slab.

time-dependent Monte Carlo solution for a $\Delta = 25.0$ slab subject to an isotropic source of strength 10^{15} in the center of the slab at $x = 12.5$. This solution was calculated with $N = 401$ position intervals and $L = 8$ angular intervals to obtain fine results. The eigenfunction expansion solution approximates the actual solution well throughout the transient, but has some issues in the region ahead of the neutron pulse where there should be zero neutrons. The smooth shape of the eigenfunction expansion solution is unable to approximate such a sudden change. In this case, the initial source is in the center of the slab, so the asymmetric (odd-numbered) eigenfunctions are not important to the solution. This is preserved during the eigenfunction expansion as the coefficients for the odd-numbered shape eigenfunctions are orders of magnitude smaller than coefficients of even-numbered ones.

4.2 Multiplying Medium

The transition rate method also adapts to multiplying slabs. Consider a five region problem consisting of fuel ($\nu = 3.5$, $\Sigma_f = 0.2$, $\Sigma_s = 0.8$), moderator ($\Sigma_s = 0.8$, $\Sigma_\gamma = 0.2$), and absorber ($\Sigma_s = 0.1$, $\Sigma_\gamma = 0.9$). The total cross section Σ_t for all materials is set to unity. The outer regions on left and right are fuel ($\Delta = 1$), the center region is absorber ($\Delta = 5$), and the regions between are moderator ($\Delta = 1$). The two fuel regions are loosely coupled due to the large absorber in between; very few neutrons born in one fuel region will reach the other. Also, the first two k eigenvalues and α eigenvalues are very close to one another. These factors potentially complicate the rate of convergence.

With $N = 270$ position intervals and $L = 12$ angular intervals, TORTE calculated $k = 0.9900929 \pm 0.0000321$, $\alpha_0 = -0.006157484$, and $\alpha_1 = -0.006447668$. These compare well to the GFM-calculated $k = 0.9900716$, $\alpha_0 = -0.006156369$, $\alpha_1 = -0.006440766$, though they do not match exactly. TORTE also calculates a whole spectrum ($NL \times NL$) of higher eigenvalues and shape eigenfunctions not included in the GFM analysis. The first two shape eigenfunctions compare well to GFM calculations. Fig. 4 compares the TORTE-calculated fundamental and first shape eigenfunction to those calculated by the GFM [7]. The shape eigenfunctions calculated by

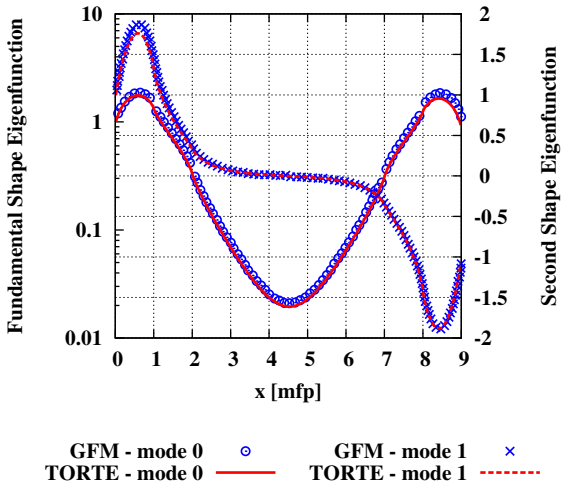

Figure 4: The first two shape eigenfunctions of the five-region problem.

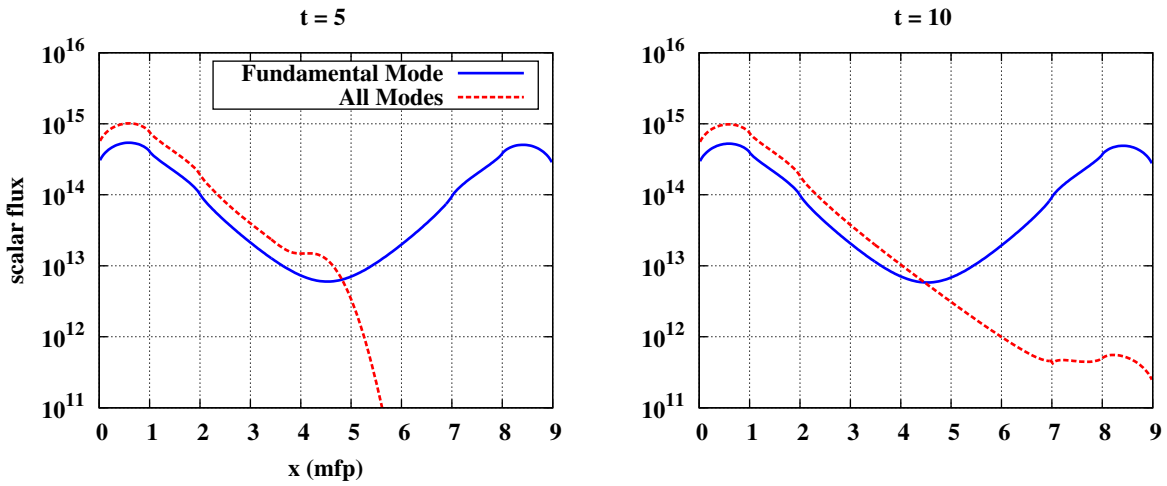

Figure 5: Snapshots of a transient in the five-region problem.

TORTE do not match exactly. This is in part due to the loose coupling between the two regions.

Fig. 5 shows an example of the eigenfunction expansion applied to this multiplying medium, with a rightward incident source from the left vacuum at $x = 0$. It compares the fundamental mode solution to the full expansion including all higher modes, not just the two shown in Fig. 4. For this case, no time-dependent Monte Carlo solutions were obtained. The behavior of the flux throughout the transient is very smooth, even at short times, but there are issues at the front of the propagating flux shape where the actual flux should drop abruptly to zero. At $t = 5$ the neutrons entering from the left have penetrated to the absorbing center of the problem, where a small bump forms at the front of the spectrum. Small inflections at $x = 1$ and $x = 2$ show the change in materials from fuel to moderator to absorber. There is a smooth drop off after $x = 5$ in the solution, but there should be zero neutrons anywhere $x > 5$ considering the speed of neutrons and the time. At $t = 10$, the neutrons have arrived at the other end of the slab and begin to fission in the opposite fuel material. Inflections points again show the change in materials at the right end of the slab. The flux shape still has a long way to go before approaching the fundamental mode.

4.3 Discussion

The transition rate matrix method is able to preserve information about one-dimensional scattering and multiplying media, yielding an accurate expanded solution. The quality of the solution depends on the number of position and direction intervals, N and L, used in the formulation of $\mathbf{Q}$. As more intervals are used, the ability of the calculated α eigenvalues and shape eigenfunctions to approximate the actual ones increases, though this dependence is still to be investigated. The resulting $\mathbf{Q}$ is a $NL \times NL$ matrix and has potential to be very large. However, for these problems the matrix is very sparse, with only $N(L \times L) + NL$ nonzero elements. Thus, sparse matrix storage is important for using this method for larger problems.

The eigenfunction expansion is able to approximate the time-dependent behavior of the scalar flux within the slabs. The expansion for the scattering slab compares well to the time-dependent Monte Carlo solution, where issues arise when attempting to model irregular

spectrum shapes. The expansion for the five region multiplying medium shows how different the spectra behaves in comparison to the fundamental mode. Before the higher modes decay, the fundamental mode is an incorrect solution for the time dependent flux.

5 CONCLUSIONS & FUTURE WORK

A transition rate matrix, the continuous-time analog of the fission matrix, accurately computes α eigenvalues and eigenvectors in infinite and one-speed, one-dimensional media. These can be applied to model transient behavior of the energy spectrum for infinite media or of the spatial dependence in one-dimensional media. A standalone research code TORTE performs these calculations with continuous-energy nuclear data for infinite media and one-speed one-dimensional slabs. TORTE is able to approximate the actual α-eigenvalue spectrum for infinite media. The eigenfunction expansion results compare very well to time-dependent Monte Carlo solutions.

Future work will focus on further verifying one-dimensional multiplying media with previous work and time-dependent Monte Carlo solutions. Also, studying the effect of position and direction interval choices on numerical convergence and eigenvalue accuracy is important. Incorporating this methodology for continuous-energy slabs can be seen as a combination of the two previous sections, where for each direction interval in a spatial interval, there is a given energy distribution.

6 ACKNOWLEDGMENTS

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