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A Deterministic-Monte Carlo Hybrid Method for Time-Dependent Neutron Transport Problems

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A new deterministic-Monte Carlo hybrid solution technique is derived for the time-dependent transport equation. This new approach is based on dividing the time domain into a number of coarse intervals and expanding the transport solution in a series of polynomials within each interval. The solutions within each interval can be represented in terms of arbitrary source terms by using precomputed response functions. In the current work, the time-dependent response function computations are performed using the Monte Carlo method, while the global time-step march is performed deterministically. This work extends previous work by coupling the time-dependent expansions to space- and angle-dependent expansions to fully characterize the 1D transport response/solution. More generally, this approach represents and incremental extension of the steady-state coarse-mesh transport method that is based on global-local decompositions of large neutron transport problems. An example of a homogeneous slab is discussed as an example of the new developments.

KEYWORDS: Time-dependent, neutron transport, response method, coarse mesh transport, hybrid, time-convolution

I. Introduction

A new solution method for the time-dependent transport equation is investigated. This work extends the work of Pounders and Rahnema1 where the infinite and semi-infinite transport equations were solved by expanding the transport solution in a polynomial series over finite time intervals. The transport solution itself is developed as a generic system response that is calculated in terms of arbitrary time-dependent source terms through the use of response functions. These new developments are ultimately aimed at extending the Coarse-Mesh Transport (COMET)2,3,4 method that has been previously developed for large-scale steady-state reactor problems. The current work presents a rigorous extension of the previous time-independent response-function-based methodology, where the precomputed response functions are calculated using a local Monte Carlo solution of the transport equation. An example problem is shown to highlight the time-stepping procedure that is new to this method.

II. Problem Statement

The one-dimensional time-dependent transport equation can be written1

\[
\frac{1}{v} \frac{\partial \psi(z, \mu, t)}{\partial t} + \mathbf{H} \psi(z, \mu, t) = q(z, \mu, t) \tag{1}
\]

with \( z \in [a, b] \) and the operator \( \mathbf{H} \) defined by

\[
\mathbf{H} \psi(z, \mu, t) = \mu \frac{\partial \psi(z, \mu, t)}{\partial z} + \sigma_{e}(z, \mu) \psi(z, \mu, t) \]

\[ - \sum_{g' = 1}^{G} \sigma_{\text{eff},g'}(z, t) \times \left( \int_{-1}^{1} f_{g',\mu'}(z, \mu' \rightarrow \mu, t) \psi_g(z, \mu', t) d\mu' \right) \tag{2} \]

Because the current work is principally focused on the time dependence of the transport problem, the quantity \( \psi(x, t) \) may denote a one-group, scalar-valued function and or a multigroup, vector-valued function otherwise.

Time-dependent boundary conditions are prescribed by

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\[ j^-(a, \mu, t) = B_a j^-(a, \mu^*, t), \]
\[ j^-(b, \mu^*, t) = B_b j^-(b, \mu, t), \]
\[ 0 \leq \mu \leq 1, \]
\[ -1 \leq \mu^* < 1, \]
\[ (3) \]

where \( j^- \) and \( j^- \) are the incoming and outgoing partial currents, respectively, and \( B_{a,b} \) are generic boundary operators. Additionally, an initial condition is prescribed on the angular flux at time \( t = 0 \):
\[ \psi(z, \mu, 0) = \psi^0(z, \mu) \]
\[ (4) \]

Equations (1)-(4) form a complete specification of the time-dependent transport.

### III. The Response Equations

In the current context, a response equation enables one to express the neutronic response of a system (e.g. outgoing partial current, angular flux, etc.) in terms of arbitrary source terms. For the problem considered here the neutron sources are represented by the boundary and initial conditions. The incoming partial currents used as boundary conditions are in fact already proper source terms and may be added directly to the right hand side of Eq. (1) provided that they appear as non-zero terms only on the mesh boundary.

The initial condition, on the other hand, is a flux term and may not be directly added to the transport equation. Pounders and Rahnema\(^1\) have shown, however, that an equivalent source term is given by
\[ v^{-1} \psi^0(z, \mu) \delta(t). \]
\[ (5) \]

The local problem transport equation can therefore be written
\[ v^{-1} \frac{\partial \psi(z, \mu, t)}{\partial t} + H \psi(z, \mu, t) = q(z, \mu, t) + j^-(a, \mu, t) \delta(z-a)H(\mu) \]
\[ + j^-(b, \mu, t) \delta(z-b)H(1-\mu) + v^{-1} \psi^0(z, \mu) \delta(t). \]
\[ (6) \]

subject to free surface (vacuum) boundary conditions and zero initial flux conditions because the original conditions have been incorporated as explicit source terms.

Due to the linearity of the transport equation, the solution of Eq. (6) can be expressed as a linear combination of the responses arising from four distinct source terms:
\[ \psi(x, t) = R[z, \mu, t; q(z', \mu', t')] \]
\[ + R[z, \mu, t; j^-(a, \mu, t')] \delta(z' - a)H(\mu') \]
\[ + R[z, \mu, t; j^-(b, \mu, t')] \delta(z' - b)H(1-\mu') \]
\[ + R[z, \mu, t; v^{-1} \psi^0(z', \mu') \delta(t')]. \]
\[ (7) \]

where the response functions, \( R \), return the value of the flux at \( (z, \mu, t) \) resulting from a given source term. It can be shown, but is beyond the scope of this paper, that the response functions are linear in the source term argument, i.e. for scalars \( a \) and \( b \)
\[ R[z, \mu, t; aq_1 + bq_2] = \]
\[ aR[z, \mu, t; q_1] + bR[z, \mu, t; q_2]. \]
\[ (8) \]

This fact will be used later. A similar response equation can be derived for the outgoing partial currents or any other functional of the angular flux.

Once the response functions have been determined (or approximated), this approach provides a means for efficiently solving large-scale neutron transport by reducing the problem to one of determining consistent boundary sources. Namely, given an initial condition and in initial guess for the boundary sources, one calculates the time-dependent exiting partial currents leaving the system. These exiting partial currents can then be used to update the boundary source terms, and the process is iterated until convergence.

To implement the method numerically, all that remains is to express the source and response terms in a discrete manner. An initial steady-state implementation of this coarse-mesh response method used a discrete ordinates representation of the angular flux. Because of memory limitations for large systems, a later steady-state implementation utilized shifted Legendre polynomial expansions of the source and response terms; this approach will be extended here to time-dependent problems.

### IV. Numerical Solution

#### 1. Source and Response Approximation

As in previous work, the space and angle dependence of the source terms are approximated by expansions in products of shifted Legendre polynomials. Writing the problem space-angle domain as \( \mathcal{R} = [a, b] \times [-1, 1] \) and the positive angular half-space as \( \Omega^+ = [0, 1] \), the expansions become
\begin{equation}
q(z, \mu, t) \approx \sum_{q=0}^{S} \sum_{r=0}^{S} q_{q,r}(t) \tilde{P}_{q,r}^{S}(z, \mu),
\end{equation}

\begin{equation}
\psi^0(z, \mu, t) \approx \sum_{q=0}^{S} \sum_{r=0}^{S} \psi_{q,r}^0(t) \tilde{P}_{q,r}^{S}(z, \mu), (9)
\end{equation}

\begin{equation}
j^-(a, \mu, t) \approx \sum_{q=0}^{S} j_{q}^-(a, t) \tilde{P}_{q}^{S}(\mu).
\end{equation}

where the superscripts of the basis functions represent the domain of orthogonality and the coefficients are defined

\begin{equation}
q_{q,r}(t) = \frac{(2q-1)(2r-1)}{2(z_n - z_m)} \left\{ \tilde{P}_{q,r}^{S}(z, \mu), q(z, \mu, t) \right\}_n,
\end{equation}

\begin{equation}
\psi_{q,r}^0(t) = \frac{(2q-1)(2r-1)}{2(b-a)} \left\{ \tilde{P}_{q,r}^{S}(z, \mu), \psi_0^0(z, \mu) \right\}_n, (10)
\end{equation}

\begin{equation}
j_{q}^-(a, t) = (2q-1) \left\{ \tilde{P}_{q}^{S}(\mu), j_{-}(a, \mu, t) \right\}_n.
\end{equation}

(Not that the \( j^- (b, \mu, t) \) is not shown for brevity because its expansion is identical to the expansion of \( j^- (a, \mu, t) \) except for the sign of \( \mu \)). Inserting these approximations into Eq. (7), multiplying both sides of the equation by one of the \( \tilde{P}_{q,r}^{S}(z, \mu) \), and integrating over the phase space yields a relationship between the source and response coefficients:

\begin{equation}
\psi_{q,r}^0(t) = R^E_{q,r,\rightarrow q',r'} \left[ t; q_{q',r'}(t') \right] + R^S_{q,r,\rightarrow q',r'} \left[ t; j_{q'}^- (z, t') \right] + \psi_{q,r}^0 \left[ t; \delta(t') \right] (11)
\end{equation}

where definitions of the surface, \( R^S_{q,r,\rightarrow q',r'}[t; \tau] \), and volume, \( R^E_{q,r,\rightarrow q',r'}[t; \tau] \), response functions follow directly from the sequence of operations described above. The difference between this expression and those described in previously referenced steady-state work is that, except for the initial condition term, the polynomial coefficients remain an argument of the response functions because of their dependence on time. As a result the response functions are still dependent on the global solution and the desired decoupling is not obtained.

If the time domain is partitioned into a number of contiguous finite intervals then one could apply the same sequence of operations detailed above in the time variable: (1) expand the source terms in a series of shifted Legendre polynomials over a given time interval, (2) multiply both sides of the resulting equation by one of the polynomials, and (3) and integrate over the time interval. If one applied such a procedure, say using an \( S \)-order expansions in time, then calculation of the response functions would be completely independent of the global solution. The number of response function computations, however, would increase by a factor of \( (S+1) \) because the calculation of each response function represents the solution of a local transport problem with polynomial source. A method will now be described that produces all of the necessary time-dependent response functions without increasing the computational burden over that of the steady-state problem.

2. Source Convolution

Given some source function, \( q(t) \), and an arbitrary response function acting on the source, \( R[t, q(t')] \), over the interval \([0, T]\), then it can be shown that

\begin{equation}
R[t, q(t')] = \int_0^T R[t - \tau, \delta(t')] q(\tau) d\tau, 0 \leq t \leq T. (12)
\end{equation}

The response function term, \( R[t - \tau, \delta(t')] \), in this expression is simply the system response at time \( t - \tau \) resulting from a pulsed (delta) source at time 0. Eq. (12) states the convolution of an arbitrary source term against the pulsed-source response function is equivalent to the response that results from the original source term. (This fact becomes more apparent when thinking about the problem in terms of Green’s functions, since the notion of response functions and Green’s functions are very closely related.)

Following the work of \( ^6 \) and \( ^1 \), we expand the pulsed-source response function and the time-dependent source term in series of shifted Legendre polynomials over the interval \([0, T]\)

\begin{equation}
R[t - \tau, \delta(t')] \approx \sum_{S=0}^{S} R_{q,r}^0 \tilde{P}_{q,r}^{S}(t - \tau), (13)
\end{equation}

\begin{equation}
q(\tau) \approx \sum_{S=0}^{S} \sum_{r=0}^{S} \tilde{P}_{q,r}^{S}(\tau), (14)
\end{equation}

where, as above, the expansion coefficients are defined with respect to the Legendre orthogonality conditions. Inserting these approximations into Eq. (12) yields

\begin{equation}
R[t, q(t')] \approx \sum_{S=0}^{S} \sum_{r=0}^{S} R_{q,r}^0 \tilde{P}_{q,r}^{S}(t - \tau) \tilde{P}_{q,r}^{S}(\tau) d\tau, 0 \leq t \leq T \end{equation}

This equation can be reformed into the following simpler expression:

\begin{equation}
R[t, q(t')] \approx \sum_{S=0}^{S} q_{r} \sum_{S=0}^{S} R_{q,r} \tilde{P}_{q,r}^{S}(t), 0 \leq t \leq T (15)
\end{equation}

where the \( \tilde{R}_{q,r} \) are linear combinations of the original \( R_{q,r} \) coefficients. Applying this approximation to each of the response terms in Eq. (11), multiplying both sides of the
result by one of the $P_{\nu}^{(0,\ell)}(t)$ polynomials, and integrating over the time interval results in an expression of the form

$$
\psi_{q,r,s} = \sum_{s'=0}^{s} q_{r',s'} \overline{R}_{q,r,s}^{\nu} + \sum_{s'=0}^{s} \sum_{a} \overline{R}_{q,r,s}^{\nu}(a)(\overline{R}_{q,r,s}^{\nu}(a)(\tau_{s'+1})
$$

Although the response function coefficients appear somewhat cumbersome, their calculation is relatively straightforward and is the topic of the next section.

3. Monte Carlo Calculation of Response Coefficients

The response function calculations are characterized by the following:

1. All response function calculations are independent of the global problem solution;
2. The response functions associated with one mesh are independent of the response functions associated with all other mesh;
3. Each response function calculation is a fixed-source, free-surface problem with a delta initial condition;
4. The shape of the source for each calculation is polynomial and determined by the shifted Legendre basis;
5. Each response function calculation returns a set of response coefficients corresponding to all of the polynomial response moments.

The response functions can in theory be computed using any transport method, but in the current and previous work the Monte Carlo method has been used because of its high accuracy, robustness with respect to physics and geometry, and the capability of sampling from continuous distributions. Polynomial sampling and the tallying of polynomial moments have been presented previously, and it is based on this experience that the current response function calculations have been implemented. The Monte Carlo code MCNP5 was modified to perform these functions and was used to generate all response functions for the examples found in the next section.

It is important to note that because all response function calculations are independent of the global problem solution, they can be precomputed and stored in a database for future use. This separation of the computational burden has been shown to be very efficient for large reactor calculations.

V. Numerical Example

In this section, a fixed-source slab problem is examined using the time-dependent response-based method—COMET. The slab initially has no neutrons, and at time $t=0$ a uniform, isotropic source is “turned on” and remains on for the duration of the problem, eventually evolving to a steady-state distribution. The slab is ten mean-free-paths in width with vacuum boundary conditions and is not fissionable; the ratio of the scattering to the total cross section is 0.9. This problem was chosen because there is an analytical solution available in the literature. This problem tests both the time-stepping procedure and the convolution approximation. The COMET results are compared against the analytic solution and a discrete ordinates solution with 32-point quadrature, implicit time differencing and finite differencing in space.

The problem is solved using two time step widths. Figure 1 shows the analytical, COMET and discrete ordinates ($S_{32}$) flux solutions as a function of space at 1.0, 2.5, 5.0, 7.5 and 10 mean-free-times. This COMET solution was generated using a $5^0$ order angular expansion, $10^0$ order spatial expansion and $10^0$ order time expansion. It can be seen that the solutions differ the most near the slab boundaries, particularly at early times. It should be noted that $t=10$, where the agreement is relatively poor, the results shown represent the beginning of the second time step, not the end of the first.

Figure 2 shows the same results but with a COMET solution using a time step width of ~30 mean-free-times. The agreement between COMET and discrete ordinates in this case shows improved agreement at later times and similar agreement at early times. This difference seems to indicate that the presence of end-point effects in the polynomial solution, since the agreement, in both space and time, deteriorates near interval endpoints. Furthermore, these effects do not diminish if the polynomial expansion order is increased. This end-point effect can be observed in Figure 3 at $t=10$ mft, where the two polynomial time intervals meet.

Figures 4 and 5 show the evolution of the flux as it progresses to steady-state for time-step widths of 10 and ~30 mean-free-times.
VI. Conclusion

A new time-dependent, coarse-mesh transport method has been presented. The method uses Monte Carlo-computed response functions to construct polynomial solutions over coarse space and time grids. Although delayed neutrons have not been explicitly accounted for presently, they could easily be incorporated the external source term. In the future this method will be applied to more realistic, heterogeneous reactor problems.

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