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Uncollided Flux Techniques for Discrete-Ordinate Radiation Transport Solutions in Rattlesnake

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Contents

1 Introduction

The fast-neutron hodoscope at the Transient Reactor Test Facility has been used to detect fuel motion within test samples inserted in the center of the reactor core. The hodoscope system was been built to support nuclear reactor safety testing by providing a mechanism to detect when fuel motion is induced under simulated accident conditions. Optical detection methods cannot be used due to opacity of fuel capsules and pressure vessel walls. However, those materials are transparent to fast neutrons leaving the test fuel(s). The hodoscope uses collimators and two sets of detectors located outside the reactor core for fast neutron measurements. Thus, it relies on fast neutrons born in the test sample to travel significant distances (3m) through air to reach the detector. The detector configurat is illustrated in Fig. 1.

However, this quite simple means of experiment visualization presents a challenge to most neutron transport methods. Even high order deterministic methods are limited due to angular discretization issues and ray effects; the number of discrete angles required to overcome this problem is prohibitively large. On the other hand, Monte Carlo methods require unreasonable amounts of time to obtain adqueate statistical responses at the location of the hodoscope detectors, unless a biasing technique is used. Other approaches must be taken to better simulate neutron streaming in the hodoscope. Note that such a treatment is not necessary in TREAT core transient modeling; other approaches have been developed to account for streaming effects. [1]

This report reviews uncollided flux techniques (first and last collision methods) to be implemented in the S_N solver of the Rattlesnake code in order to mitigate ray effects in modeling the TREAT reactor+hodoscope system. Angular discretization techniques (S_N and P_N) for the transport equation are notoriously poor at capturing accurately streaming effects. The uncollided component of the angular flux solution is the most anisotropic part and it can be difficult for discrete-ordinate methods to accurately represent; this phenomena is well-known and termed “ray effects”. However, it has long been recognized that an analytical or semi-analytical treatment of the uncollided flux, coupled with a discrete-ordinate treatment of the collided flux, can yield dramatic improvements in accuracy and computational efficiency. In this report, we present an algorithm for semi-analytical calculation of the uncollided flux. The algorithm seeks to compute

1. The existing uncollided flux at each point in a collect of point on the surface of the problem domain, with the angular flux reported for each “source point”. The direction is from the source point to the surface point. The source points are chosen

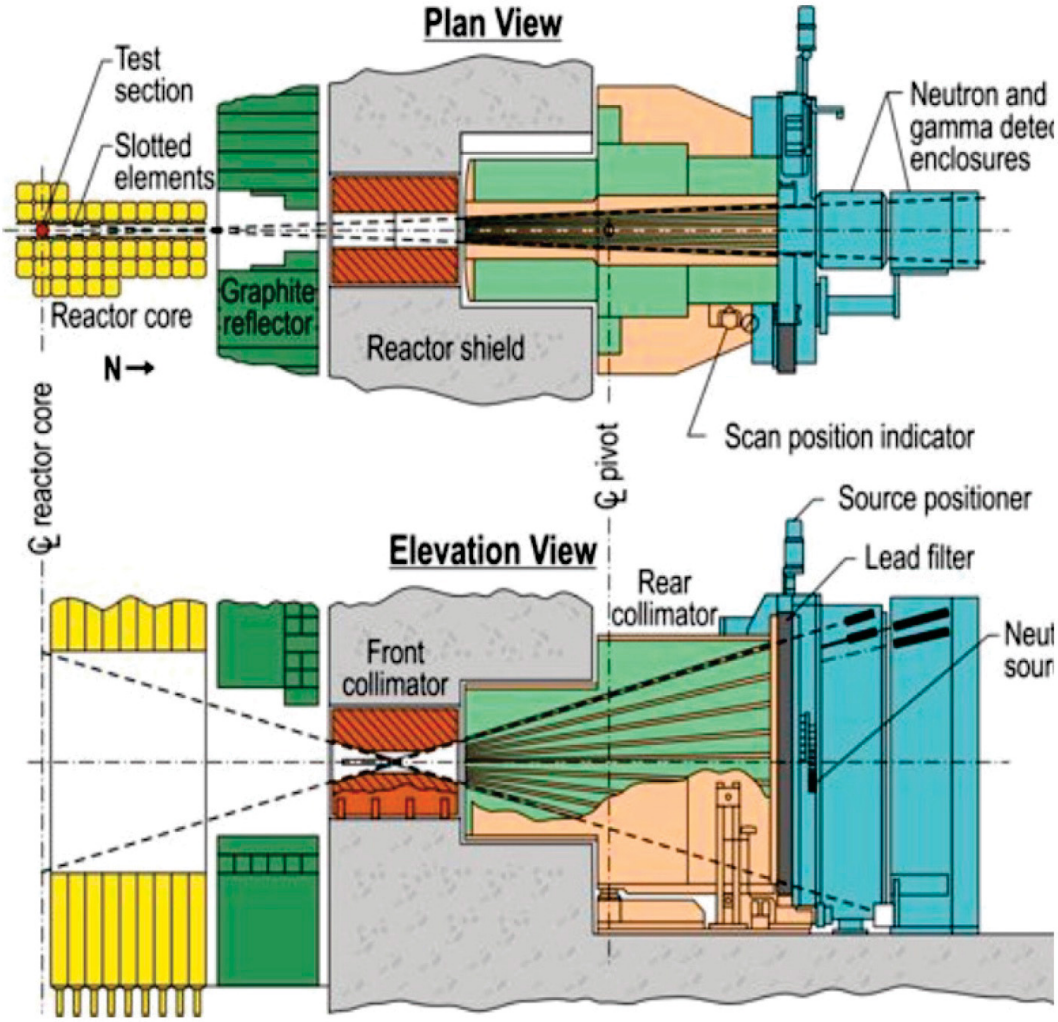

Figure 1: Plan and elevation views of a cross-section of the reactor, showing the relative orientation of the core, a test item, reactor structural materials, and components of the 1.2-m collimator hodoscope at TREAT [2].

to be spatial quadrature points that integrate the source volume.

2. Spatial and angular distributions of the uncollided flux in every cell in the problem. These provide all of the information necessary to form the first-collision source in each cell.

The proposed algorithm is tailored for parallel efficiency given a spatial domain decomposition.

1.1 Basic Approach

For simplicity, we describe the uncollided flux technique using a single-speed description. Generalization to multigroup is straightforward. We recall the one-group transport equation below:

$$\vec{\Omega}\cdot\vec{\nabla}\Psi(\vec{r},\vec{\Omega})+\sigma_t(\vec{r})\Psi(\vec{r},\vec{\Omega})=\sum_{\ell}\frac{2\ell+1}{4\pi}\sigma_{s,\ell}(\vec{r})\sum_{m=-\ell}^{\ell}\Phi_{\ell,m}(\vec{r})Y_{\ell,m}(\vec{\Omega})+q(\vec{r},\vec{\Omega})\,, \tag{1}$$

where $\Psi(\vec{r},\vec{\Omega})$ is the angular flux at position $\vec{r}$ and in direction $\vec{\Omega}$, $Y_{\ell,m}(\vec{\Omega})$ is the spherical harmonic function of degree ℓ and order m, $\Phi_{\ell,m}$ is the flux moment of degree ℓ and order m

$$\Phi_{\ell,m}(\vec{r})=\int_{4\pi}d\Omega\Psi(\vec{r},\vec{\Omega})Y_{\ell,m}(\vec{\Omega})\,.$$

It helps to introduce an operator notation for brevity:

$$L\Psi=H\Psi+q\,. \tag{2}$$

where L is the streaming and total interaction operator and H the scattering operator. Typically, the transport equation is solved iteratively (index k)

$$L\Psi^{(k+1)}=H\Psi^{(k)}+q\,. \tag{3}$$

Let us now introduce a decomposition of the angular flux into collided and uncollided components:

$$\Psi=\Psi^{u}+\Psi^{c}$$

Then, Equation 2 can be re-cast as

$$L^{RT}\Psi^{u}=q \tag{4a}$$

$$L^{S_N}\Psi^c = H\Psi^c + H\Psi^u \tag{4b}$$

where we have emphasized how the transport operator L will be solved in each case. The subscript RT denotes ray-tracing while S_N stands for discrete-ordinate techniques.

1.1.1 Uncollided Flux Equation

The uncollided flux equation (Equation 4a)

$$L^{RT}\Psi^u = q \quad \text{or} \quad \vec{\Omega}\cdot\vec{\nabla}\Psi^u(\vec{r},\vec{\Omega}) + \sigma_t(\vec{r})\Psi^u(\vec{r},\vec{\Omega}) = q(\vec{r},\vec{\Omega}),$$

can be re-written, along a given direction $\vec{\Omega}$, as

$$\frac{d\Psi^u(\vec{r},\vec{\Omega})}{ds} + \sigma_t(\vec{r})\Psi^u(\vec{r},\vec{\Omega}) = q(\vec{r},\vec{\Omega}), \tag{5}$$

where $\vec{r} = \vec{r}_0 + s\vec{\Omega}$ and $\vec{r}_0$ is an origin point (i.e., a source point). Equation 5 can be solved analytically for simple geometries or semi-analytically using ray-tracing, for more complicated geometries.

1.1.2 Collided Flux Equation

Once Equation 5 has been solved, the uncollided flux solution Ψ^u is thus available throughout the domain and the first collision source q^{1st} can be computed as follows:

$$q^{1st}(\vec{r},\vec{\Omega}) = H\Psi^u = \sum_\ell \frac{2\ell+1}{4\pi}\sigma_{s,\ell}(\vec{r}) \sum_{m=-\ell}^{\ell} \Phi^u_{\ell,m}(\vec{r})Y_{\ell,m}(\vec{\Omega}) \tag{6}$$

where Φ^u denote the flux moments computed from the uncollided angular flux Ψ^u. Then, one simply needs to solve Equation 4b, the equation for the collided component Ψ^c:

$$L^{S_N}\Psi^c = H\Psi^c + H\Psi^u = L^{S_N}\Psi^c = H\Psi^c + q^{1st}. \tag{7}$$

Note that Equation 7 is similar in nature to Equation 1. An iterative technique (Source Iteration) is employed:

$$L^{S_N}\Psi^{c,(k+1)} = H\Psi^{c,(k)} + q^{1st}.$$

Equation 7 gives the collided component of the angular flux. Standard discrete-ordinates methods are used to solve Equation 7.

1.1.3 From First-collision Source Treatment to Last-collision Source Treatment

The above uncollided flux treatment addresses ray effect issues in the uncollided flux solution. However, ray effects can also occur in the collision flux solution, for instance, when there is a large distance from a small scatter source to a detector (e.g., neutrons streaming in a duct). TREAT's fuel motion monitoring system, with about 3m distance between the hodoscope and the centere of the core, clearly falls into this category. In a manner analogous to the uncollided flux treatment, a last collided flux treatment can be employed to remove ray effects in a detector response. The last collision source treatment is simply expressed as the original transport equation, where the first-collided source due to the uncollided angular flux and the collided source (obtained from a discrete ordinate solution) are known (they come from the ray-tracing and the discrete-ordinate solution, previously described):

$$L^{RT}\Psi^{last} = H\Psi^{c} + H\Psi^{u} + q = q^{last}\,, \tag{8}$$

That is, instead of using $\Psi^{c} + \Psi^{u}$ as the final angular flux at the detector locations, we perform one more ray-tracing using the total source q^{last} and then employ Ψ^{last} as the final answer. Note, we can also solve for the last collision angular flux $\Psi^{c,last}$ as follows

$$L^{RT}\Psi^{c,last} = H\Psi^{c} + H\Psi^{u} = q^{c,last}\,. \tag{9}$$

Equation 9 is simply obtained by subtracting Equation 8 and Equation 4a. Then

$$\Psi^{last} = \Psi^{c,last} + \Psi^{u}\,.$$

1.2 Parallel Aspects of the Traditional Uncollided Flux Treatment

Most uncollided-flux algorithms track directly form each source point to a set of a few points in each cell of the domain. The source volume assigned to each source point is effectively treated as vanishingly small, so that the angular flux at any other spatial point is treated as a δ-function in the direction $\vec{\Omega}$ subtended by the two points. This traditional algorithm does not scale well given a spatial domain decomposition: the process (or processor) that owns a source point must execute $\mathcal{O}(N)$ work given N spatial cells. If the process that owns the source point has knowledge of the entire domain, its works grows proportionally to N. When sources are localized (in this case the very localized fuel sample(s) located within the experimental vehicle in TREAT or the detectors in the hodoscope for the case of the last-collision source treatment), then many processes not owning any source points stay

idle. A simple workaround would be for processes not owning source points to ray-trace once a ray enters their subdomains (this would be mandatory is the mesh is truly parallel and not reproduced on any one processor). However, there are two deficiencies with this approach:

1. The algorithm is partially sequential. Processes not owning a source point stay idle until a ray has reached them.

2. As one moves further away from the source point, the ray density decreases, which can cause inaccuracies.

However, independent research for development of a MOOSE-based method of characteristics solver has developed a MOOSE application for parallel domain decomposed ray tracing: SQUID. This work is at present unpublished, but is available in the MOOSE open source repository [3]. The following section provides more detail about this application.

2 SQUID: A Parallel Ray-Tracing Application for Domain-Decomposed Geometries

2.1 Overview

SQUID is a recently created MOOSE-based application developed by MIT & INL to perform ray-tracing in parallel for domain-decomposed geometries. SQUID is currently used in reactor physics applications based on the Method of Characteristics (MOC) where ray tracing is typically performed in Constructive Solid Geometries (CSG).

2.2 Enhancements Required for the Uncollided Flux Treatment

Currently, SQUID ray-traces through a domain described usig CSG and computes the angular flux attenuation using a given direction $\vec{\Omega}$, a starting point $\vec{r}_0$, and a termination distance

D:

$$\Psi^u(\vec{r}_0 + s\vec{\Omega}, \vec{\Omega}) = \Psi^u(\vec{r}_0, \vec{\Omega}) \exp\left(- \int_0^s ds' \sigma_t(\vec{r}_0 + s'\vec{\Omega}) \right) + \int_0^s ds'' \left(q(\vec{r}_0 + s''\vec{\Omega}, \vec{\Omega}) \exp\left(- \int_{s''}^s ds' \sigma_t(\vec{r}_0 + s'\vec{\Omega}) \right) \right) \quad (10)$$

for $0 \leq s \leq D$. In the uncollided flux treatment approach, $\vec{r}_0$ will be any quadrature point location within the external source volume (or surface if the external source is defined as a surface source). The direction $\vec{\Omega}$ will be determined as

$$\vec{\Omega} = \frac{\vec{r} - \vec{r}_0}{\|\vec{r} - \vec{r}_0\|}$$

where $\vec{r}$ is a spatial quadrature point in any cell of the domain. $D = \|\vec{r} - \vec{r}_0\|$.

Note that the external source term, q, and the total cross section can be arbitrarily space-dependent. In MOC techniques, however, the source is often constant or linear per cell and the cross section is cell-wise constant. At first, the fast neutron source burst from the experimental vehicle in TREAT will be treated as piece-wise constant per spatial cell. If it is important that the fast neutrons' spatial variation within a finite element cell be accounted for, a numerical quadrature integration along each ray segment will need to be implemented in SQUID. The same remark applies to the spatially-dependent cross section. They are typically constant per cell in MOC calculations. However, in multiphysics applications, cross sections may spatially vary within the cell.

Algorithmically, this can be presented as follows:

Algorithm 1 Ray-tracing for uncollided flux algorithm

```
1: procedure RAY-TRACING FOR ALL SOURCE POINTS
2:     for each src_qpt ∈ N_src do
3:         Perform the ray-trace procedure (see below)
4:     end for
5: end procedure
```

```
1: procedure RAY-TRACING FOR A GIVEN SOURCE POINT src_qpt
2:     for each cell K ∈ N_K do
3:         for each quadrature point qpt on outgoing faces of K, i.e., qpt ∈ N_qpt(∂K^+) do
4:             This pair (src_qpt, qpt) define a ray
5:             for each segment i in the ray do
6:                 Compute the uncollided angular flux
7:                 Accumulate the contribution of the uncollided angular to the flux moments
8:             end for
9:         end for
10:    end for
11: end procedure
```

The contribution of the uncollided angular to the flux moments in each spatial cell is discussed in the next Section.
Enhancements needed to SQUID are:

1. Ray-tracing on a parallel FEM mesh;

2. Ray-tracing that accounts for source and cross-section variations within a cell.

3 Finite-element Evaluation of the First-collided Scattering Source

Ray-tracing provides an estimation of the angular flux distribution. This must then be converted into a first-collided source distribution (Equation 6)

$$q^{1st}(\vec{r},\vec{\Omega}) = H\Psi^u = \sum_\ell \frac{2\ell+1}{4\pi}\sigma_{s,\ell}(\vec{r}) \sum_{m=-\ell}^{\ell} \Phi^u_{\ell,m}(\vec{r})Y_{\ell,m}(\vec{\Omega})\,.$$

The key aspect here is the computation of the moments of the uncollided angular flux

$$\Phi^u_{\ell,m}(\vec{r}) = \int_{4\pi} d\Omega\, \Psi^u(\vec{r},\vec{\Omega})Y_{\ell,m}(\vec{\Omega})$$

These should be obtained using only the information available from the ray-tracing process. Assume that the uncollided angular flux can be represented as an expansion in spatial basis functions in each cell K and that the only angular information needed are the speherical harmonic expansion of the first-collision source.

$$\Psi^u(\vec{r},\vec{\Omega}) = \sum_n C_n^{m2d} \sum_j \Phi^u_{jn}\varphi_j(\vec{r})Y_n(\vec{\Omega})$$

for $\vec{r} \in K$. We have replaced, for brevity, the spherical harmonics subscripts (ℓ,m) with n, knowing that this is a bijection from n to the pair (ℓ,m). The φ_j's are the FEM basis function over element K; $1 \leq j \leq N_{\text{Dofs}}(K)$ where the number of degrees of freedom in cell K, $N_{\text{Dofs}}(K)$, is determine by the type of element and the FEM order of approximation. A Galerkin approach would seek the flux moments coefficients by enforcing the following:

$$\int_K d^3r \int_{4\pi} d\Omega\, \varphi_{j'}(\vec{r})Y_{n'} \left(\sum_n C_n^{m2d} \sum_j \Phi^u_{jn}\varphi_j(\vec{r})Y_n(\vec{\Omega}) - \Psi^u(\vec{r},\vec{\Omega}) \right) = 0$$

for all j' and n'. A least-square version of this uses approximations to the above space-angle integrals. These approximations are based on the requirements that the only information available stems from the ray-tracing procedure.

For each cell K, we assign subvolumes with each ray that cuts cell K. Recall that a given ray iq starts at source point i and extends to a quadrature point q located on the outgoing faces for cell K. Each subvolume associated with a given ray also has a solid angle denoted Δw_{iq}.

From these observations, the following linear system is posed for each cell K in order to determine the FEM expansion coefficients for the flux moment associated with the spherical harmonic function $Y_{n'}(\vec{\Omega})$, $(0 \leq n' \leq ANISO)$:

$$A\Phi^u_{n'} = y_{n'}$$

where

$$A_{j'j} = \sum_i \sum_q \Delta w_{iq} \int_{s_{inc,iq}}^{s_{out,iq}} ds\, s^2 \varphi_{j'}(\vec{r}(s))\varphi_j(\vec{r}(s))$$

$$y_{n'} = \sum_i \sum_q \Delta w_{iq} \int_{s_{inc,iq}}^{s_{out,iq}} ds\, s^2 \varphi_{j'}(\vec{r}(s)) \int_{4\pi} d\Omega\, \Psi^u(\vec{r}(s),\vec{\Omega}) Y_{n'}(\vec{\Omega})$$

where $s_{inc,iq}$ and $s_{out,iq}$ denote the entry/exit locations in cell K for ray iq. The element volume d^3r is been changed to $ds\, s^2 \Delta w_{iq}$ (from the definition of the solid angle). Note that we have summed over all source points i. Also note that the FEM basis functions φ need to be evaluated along the rays. The spatial integrals contains an integrand of degree $2p+2$ where p is the FEM basis degree. Therefore, we choose a Gauss-Lobatto quadrature of order $P = p+3$ to numerically performed these integrals (recall that a Gauss-Lobatto quadrature of order P exactly integrates a polynomial of degree $2P-3$). By using a Gauss-Lobatto quadrature, the entry and exit points of the ray, $s_{inc,iq}$ and $s_{out,iq}$, are used in the numerical evaluation of the integrals.

4 Conclusions

Modeling neutron transport from the center of the core to the fast neutron hodoscope at the Transient Reactor Test Facility presents challenges to numerical simulation. Accurate calculation of such streaming effects will be important in simulating the hodoscope response for an experiment loaded in the center of the core. This report has summarized the findings of research to overcome this issue, namely, an algorithm for semi-analytical calculation of the uncollided flux source. Key to implementation within Rattlesnake is an algorithm that provides parallel efficiency for a given spatial domain decomposition - SQUID. To continue to develop first and last collision source terms, follow-up research will build off of SQUID and apply if for streaming resolution calculations. In this report, the theory of this implementation has been developed. In follow-up work in FY-2017, this theory will be added to Rattlesnake and tested against available benchmarks.

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