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A HYBRID DIFFUSION/TRANSPORT METHOD

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ABSTRACT

A hybrid diffusion/transport method is presented in this paper. The traditional diffusion theory is used for regions where the diffusion approximation is valid, while response functions pre-computed by a local transport solver are used for non-multiplying regions or regions with strong heterogeneities, where diffusion theory breaks down. The two methods are coupled through the 0^{-th} and 1^{st} moments of the partial angular flux on the interface between the diffusion and transport nodes (coarse meshes). The hybrid method was implemented and tested on a one dimensional BWR benchmark problem. This test has shown that the hybrid method can achieve high accuracy while maintaining a computational efficiency comparable to the pure diffusion methods.

Key Words: Transport theory, Diffusion theory, Hybrid method, Reactor core simulation

1. INTRODUCTION

Diffusion theory is one of the most widely-used methods to obtain whole reactor core solutions (neutron flux distribution) because of its computational efficiency. Whole core diffusion methods are based on a number of approximations on the energy and angular phase space distribution. Consequently, these methods yield relatively accurate results provided the reactor is not strongly heterogeneous and that the nodes are diffusive and not highly absorbing. However, in the presence of strong material discontinuities, near external boundaries (preferential neutron leakage) and in highly absorbing regions, diffusion theory assumptions break down requiring a direct high order (i.e. transport) treatment.

To overcome the diffusion theory weakness, a hybrid diffusion/transport method is developed in this paper. In this approach, a local transport solver based on the incident flux response expansion method is used in nodes in which diffusion theory breaks down, while the conventional diffusion theory is still used in the rest of the core. The diffusion and transport nodes are coupled through the first two moments of the interface angular flux.

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The paper is organized as follows. The hybrid method is presented in section 2. Section 3 describes the numerical implementation and benchmark results and concluding remarks are found in section 4.

2. HYBRID DIFFUION/TRANSPORT METHOD

2.1. Incident Flux Response Expansion Method

In addition to the usual weaknesses of diffusion theory, coarse mesh macroscopic cross section development is a challenge for non-multiplying region due to the lack of source neutrons (fission). These problems can easily be addressed if one uses a response based transport method in nodes (coarse meshes) where diffusion theory breaks down or accurate cross sections are not easily attainable (i.e., a non-multiplying node). In this paper we use the incident flux expansion method of references [1-5] in transport nodes. In this method, a whole core problem is first divided into a number of non-overlapping local problems (nodes). As a result, the global solution can be obtained by iteratively generating local solutions to each node via pre-computed response functions. These response functions are local transport solutions (e.g., node-average flux, outgoing partial currents, fuel pin power distribution and absorption rate in control material) due to a unit incoming flux or current. An example of such response functions is the surface-to-region response function, which is essentially the local solution to the following problem

$$\mathbf{H}R_{is}^{m}(w_i)=\frac{1}{k}\mathbf{F}R_{is}^{m}(w_i), \tag{1}$$

with the boundary condition

$$R_{is}^{m}(w_i^-)=\begin{cases}\Gamma_m, & \text{for } w_i^-\cap w_{is}^-\\ 0, & \text{otherwise.}\end{cases} \tag{2}$$

Here Γ_m (m = 0, 1, ..., ∞) is a complete set of orthonormal functions on w_{is}^- with $\int dw_{is}^-\,\Gamma_m\Gamma_n=\delta_{mn}$, where "$s$" indexes the interfaces and boundary segments that comprise the boundary of coarse-mesh V_i, and δ is the Kronecker delta, and the phase-space variables are denoted by:

$$w\equiv\left(\vec{r},\hat{\Omega},E\right) \tag{3}$$

The operators **H** and **F** are defined as

$$\mathbf{H}\psi(\vec{r},\hat{\Omega},E)\equiv\hat{\Omega}\cdot\vec{\nabla}\psi+\sigma_t(\vec{r},E)\psi-\int_0^{\infty}\int_{4\pi}\sigma_s(\vec{r},\hat{\Omega}',E'\to\hat{\Omega},E)\psi(\vec{r},\hat{\Omega}',E')d\hat{\Omega}'dE', \tag{4}$$

$$\mathbf{F}\psi(\vec{r},\hat{\Omega},E) \equiv \frac{\chi(\vec{r},E)}{4\pi}\int_0^\infty \nu\sigma_f(\vec{r},E')\int_{4\pi}\psi(\vec{r},\hat{\Omega}',E')d\hat{\Omega}'dE', \tag{5}$$

If the incoming/outgoing fluxes/currents are expanded in terms of the orthonormal functions Γ_m, the expansion coefficient (i.e. partial current moment) of the outgoing partial current from a coarse mesh can be calculated as below.

$$J_s^{+,m} = \sum_{s',m'} R_{s's}^{m'm} J_{s'}^{-,m'}\ , \tag{6}$$

where $J_s^{\pm,m}$ is the mth expansion coefficient (moment) of the outgoing/incoming current across surface "*s*" and $R_{s's}^{m'm}$ is the surface-to-surface response function.

It should be pointed out that Equation (1) is a fixed source problem in which the fission source, if present, is scaled by $1/k$. As a result, the response functions R_{is}^m and $R_{s's}^{m'm}$ implicitly depend on the global eigenvalue k in multiplying nodes. Usually the response functions are pre-computed at a set of pre-defined eigenvalues and a linear interpolation is used to calculate the response at an arbitrary eigenvalue. Recently, a perturbation method [6] has been developed to calculate the response functions at an arbitrary eigenvalue as a first order perturbation from the reference value. This method has been shown to be computationally more efficient while maintaining the same accuracy as the interpolation approach.

Because of the local nature of the incident flux response expansion method, a variety of methods such as discrete ordinates, Monte Carlo or even diffusion theory can be used to solve Equation (1). The choice of the method depends on the physics of the sub-volume (node) under consideration and what level of approximations is deemed sufficient. For this reason, the incident flux response method is very suitable for developing hybrid methods, by which different methods are coupled naturally through partial currents including higher moments crossing mesh interfaces.

2.2. Diffusion to Transport Coupling

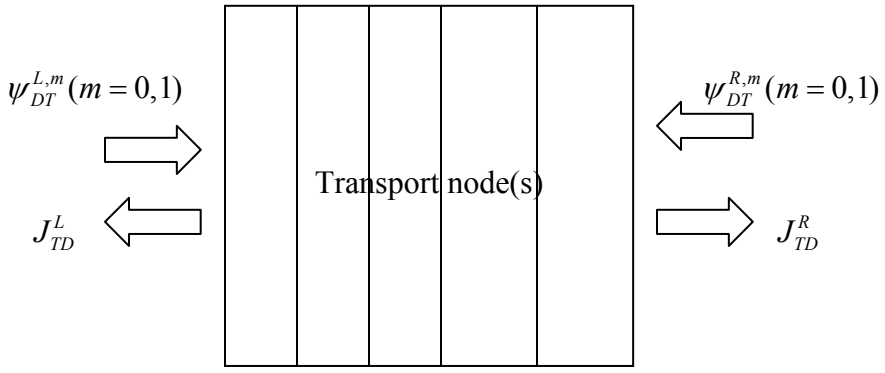

Figure 1. Coupling diffusion nodes to transport nodes

When coupling the diffusion nodes to the transport nodes, the scalar fluxes and net currents on the interface between the diffusion and transport nodes are provided by the diffusion module. These quantities will then be used as the isotropic (the 0^{th} moment) and linear anisotropic (the 1^{st} moment) components of the incoming angular flux impinging on the transport node, i.e.

$$\psi_{DT}^{0}\left(\hat{\Omega}\right)=\frac{\phi_{DT}}{4\pi} \tag{7}$$

and

$$\psi_{DT}^{1}\left(\hat{\Omega}\right)=\frac{3J_{DT}}{4\pi}\left(\hat{\Omega}\cdot\vec{n}_{DT}\right) \tag{8}$$

where ϕ_{DT} and J_{DT} are the scalar flux and the net current on the diffusion-transport interface calculated by the diffusion module, $\vec{n}_{DT}$ represents the outward normal on the diffusion-transport interface.

The local solutions (response functions) in the transport node are computed using a Monte Carlo method. This choice is motivated by the high accuracy and geometric flexibility of the Monte Carlo method. Computational efficiency is not of concern here since all of the local response function calculations are pre-computed in a few unique nodes (e.g., assembly/bundle types, controlled and reflector nodes). Response Monte Carlo calculations are in general efficient because they are fixed source calculations in small systems with vacuum boundary conditions.

2.3. Transport to Diffusion Coupling

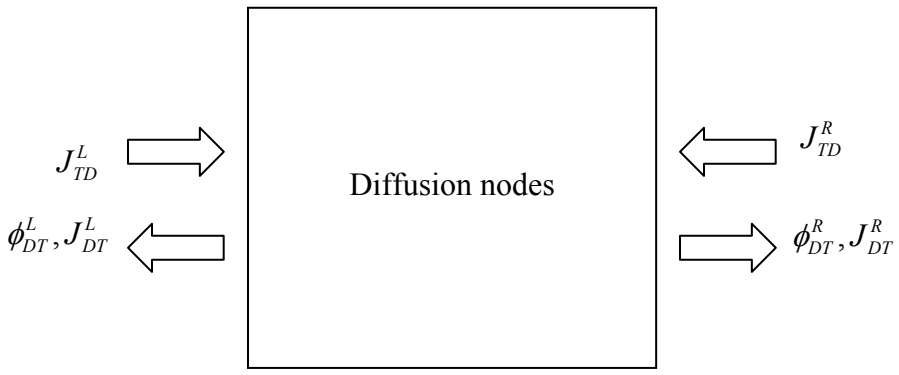

Figure 2. Coupling transport nodes to diffusion nodes

On the interface between diffusion and transport nodes, the coupling quantities must be consistent with both the diffusion and transport methods. When coupling transport nodes to diffusion nodes, the partial current from a transport node to a diffusion node is treated as an external surface current impinging on the boundary of the diffusion nodes (i.e. be treated as boundary conditions) and traditional diffusion methods are used within the diffusions nodes.

It should be pointed out that the transport module can provide the higher moments of the partial currents to the diffusion nodes, but these quantities cannot be incorporated into diffusion theory, which is a second order differential equation and only two boundary conditions are required. As a result, transport effects are taken into account only through the partial currents from the transport nodes once entering diffusion nodes, while the component of transport effects in the higher moments is lost. For this reason, in order to maintain the overall high accuracy of the hybrid method, diffusion theory must be used only in nodes where the transport effects are negligible.

2.4. Two-level Iterations

An iterative algorithm in the following two levels is developed to solve the hybrid diffusion/transport equations: outer iterations on the eigenvalue and inner iterations on the incoming/outgoing fluxes crossing interfaces. The numerical procedure of the iterative algorithm is outlined as follows:

1) Make an initial guess of the global eigenvalue k_0 (normally k_0=1) and the incoming partial currents from the transport nodes.
2) Update the matrices in the diffusion module and solve the linear system.
3) Calculate the new global eigenvalue, scalar fluxes and net currents on the interfaces between diffusion and transport nodes.
4) Use Eqs. (7) and (8) to determine the isotropic and linear anisotropic components of fluxes transmitted from a diffusion node to a transport node.
5) Equation (6) is used in the sweep to update the outgoing partial currents from a transport node to a diffusion node.
6) Outer iterations – Repeat steps 2) – 5) until the global eigenvalue is converged.

3. NUMERICAL RESULTS

The hybrid method has been implemented into a 1-D fine-mesh diffusion code, in which some of nodes can be selectively treated by transport using response expansion coefficients. The transport nodes must be pre-determined so that the response function library is generated in the pre-computation phase. The accuracy of the hybrid method has been evaluated by comparison to the MCNP reference solution for a 1-D BWR benchmark problem.

The 1-D simplified BWR benchmark configuration is shown in Figure 3. The core consists of a 91.0336-cm fuel region divided into 28 nodes and two 1.1176-cm water reflectors. To increase heterogeneity, 4% Gadolinium is added to the four rightmost fuel nodes (nodes 26 - 29). Vacuum boundary condition is imposed on the left and right external boundaries. The macroscopic cross sections for each material are shown in Table I.

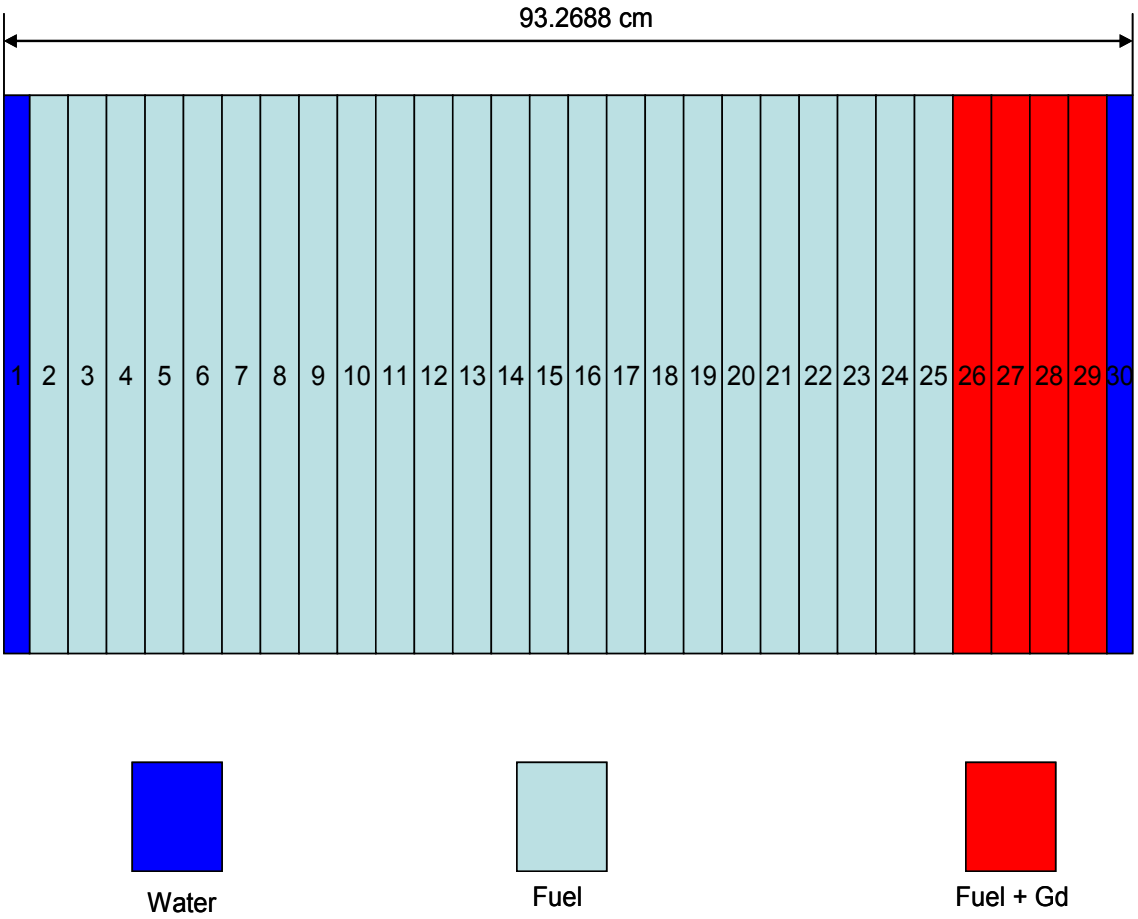

Figure 3. 1-D BWR core configuration

Table I. 2-Group macroscopic cross sections (cm^{-1}) for a BWR benchmark

Material	Fuel	Fuel + Gd	Water
σ_{tr}^{1}	3.12115E-01	3.21412E-01	2.86323E-01
σ_{tr}^{2}	9.35057E-01	1.33731E+00	1.19936E+00
$\sigma_{s}^{1\to1}$	5.149970E-01	5.233490E-01	5.936410E-01
$\sigma_{s}^{1\to2}$	1.664570E-02	1.500030E-02	2.853770E-02
$\sigma_{s}^{2\to1}$	3.300580E-03	1.350790E-02	1.203230E-03
$\sigma_{s}^{2\to2}$	1.178710E+00	9.310470E-01	1.636710E+00
$\nu\sigma_{f}^{1}$	6.148650E-03	8.280660E-03	0
$\nu\sigma_{f}^{2}$	1.066940E-01	1.027460E-01	0

The MCNP code [7] was used to perform two-group reference Monte Carlo calculations in the above 1-D BWR core. Twenty five million active particles were followed. The reference (Monte Carlo) core eigenvalue is 1.08697±0.00006. The maximum and average uncertainties of the node-averaged flux are 0.44% and 0.05%, respectively. The reference calculations took approximately 4.5 hours (not including 4 hours for source convergence).

For the hybrid calculation, the diffusion method was used in nodes 2 to 25, while the transport method was used in the reflectors (nodes 1 and 30) and fuel+Gd nodes (nodes 26 to 29). MCNP was used to pre-compute response function for each unique coarse mesh (a reflector node and a fuel+Gd node). Each response function was computed using 20 million particles with each calculation taking 5 minutes. A pure diffusion calculation was also performed in this core. The flux and eigenvalue convergence criteria were set at 1×10^{-6} for both the hybrid and pure diffusion methods. The eigenvalues predicted by the different methods and CPU times are listed in Table II. The node-average fluxes computed by the pure diffusion method and the hybrid method are also compared to a direct 2-group MCNP calculation in Table III and Figures 4 and 5. Additionally, the root mean square flux error, mean relative error and the maximum error in the flux are presented in Table III.

Table II. Comparison of eigenvalue and CPU times

Method	Eigenvalue	CPU Time
MCNP	1.08697	271 minutes
Pure diffusion	1.08643	0.069 seconds
Hybrid method	1.08682	0.083 seconds

Table III. Relative flux error statistics for the node-averaged flux in the 1-D benchmark

Method	Pure Diffusion	Hybrid Method
Flux AVG (%)	0.73	0.21
Flux RMS (%)	1.22	0.31
Flux MRE (%)	0.80	0.23
Flux MAX (%)	10.8	1.5

AVG: Average relative error

$$avg\ RE = \frac{\sum_{N}|e_n|}{N}$$

where N is the number of regions and e_n is the calculated per cent error for the n-th region.

RMS: Root Mean Square Error

$$RMS = \frac{\sqrt{\sum_{N} e_n^2}}{N}$$

MRE: Mean Relative Error

$$MRE = \frac{\sum_{N} |e_n| \cdot p_n}{N \cdot p_{avg}}$$

MAX: Maximum Error

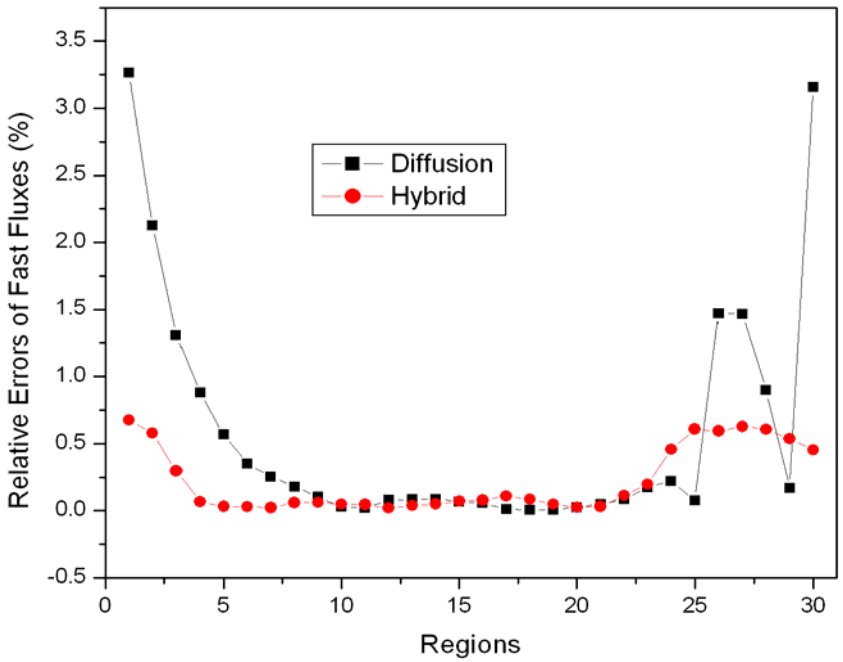

Figure 4. Relative error of the node-averaged fast flux for each region

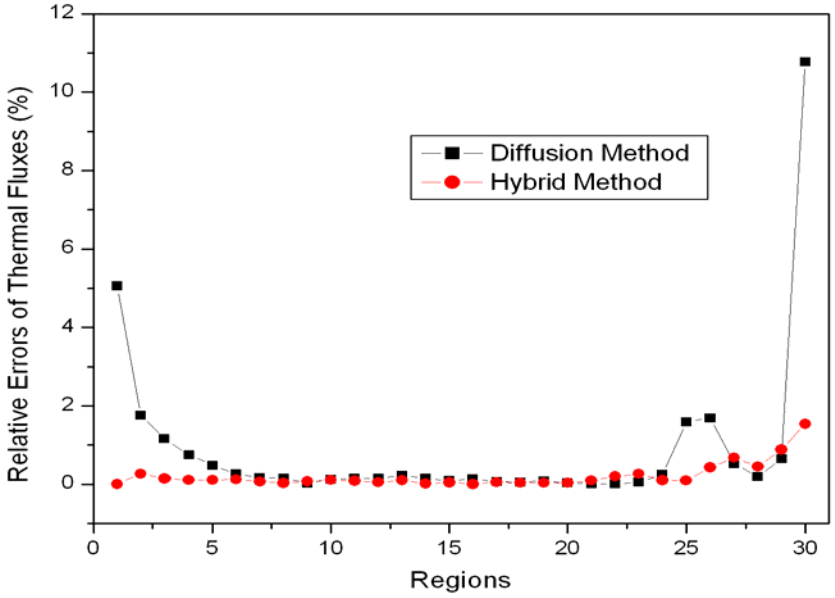

Figure 5. Relative error of the node-averaged thermal flux for each region

It is clear from Tables II and III that the results of the hybrid method agree much better with MCNP than those of the pure diffusion method. This is especially obvious in the water reflectors and fuel+Gd nodes, where the maximum relative error in the flux predicted by the diffusion method is about 11%. The maximum relative error reduces to 1.5% when the hybrid method is used.

5. CONCLUSIONS

A hybrid diffusion/transport method has been developed to solve highly heterogeneous reactor core problems. In this approach, the Monte Carlo method is used to generate the local transport solutions (response functions) to nodes in which the diffusion approximation breaks down, while the diffusion method, which is reformulated to accommodate the responses from the adjacent transport nodes, is used in the rest of core. The hybrid method was implemented and tested on a 1-D BWR benchmark problem. The comparison of the hybrid solutions with the MCNP and pure diffusion calculations indicates that the hybrid method can achieve accuracy comparable to the Monte Carlo method, while maintaining a computational efficiency comparable to the pure diffusion theory.

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