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ABSTRACT

A fully variational finite element method is developed for solving the one-speed neutron transport equation using a heterogeneous coarse-mesh grid with a mesh size of the order of a fuel assembly size. The method requires no homogenization of the coarse-mesh. It is derived and tested in slab geometry typical of a highly heterogeneous BWR core in one-dimension. The fine-mesh solution such as the fuel pin flux and power is reconstructed readily using the coarse-mesh solution and the basis functions. Preliminary results indicate that in slab geometry, the fine-mesh solutions can be reproduced from the coarse-mesh solution. It is shown that the method is very accurate for solving practical problems.

INTRODUCTION

In designing the next generation of power reactors, a computational tool that can accurately solve for the neutron flux and power distributions within these highly heterogeneous systems would be highly desirable. For the present-day commercial reactors such a code would also be very desirable, because it would allow for the designer to reduce the safety margin leading to a substantial economic saving.

Presently, the only methods capable of computing the power (flux) distributions very accurately throughout a large system such as a nuclear reactor core are the Monte-Carlo or fine-mesh transport theory methods. The main drawback of these methods is their prohibitive large computational time.

The current deterministic transport methods (Lewis and Miller, 1993) that are capable of generating a very accurate solution in a small system, like Monte Carlo methods are computationally too inefficient to use for reactor core analysis. This is due to the huge number of fine spatial meshes and discrete directions required for an accurate solution.

Methods have been developed that can handle homogeneous coarse meshes accurately. For example, the nodal discrete ordinates methods (Badruzzaman, 1990) use finite spatial moments algorithms in conjunction with discrete ordinates for the angular

direction. The use of the polynomial basis functions limits the intranodal complexity that can be handled. For the recent progress in variational nodal methods applied to large-scale transport problems, the reader is referred to Lewis and Palmiotti (2000).

A transport based asymptotic method that uses a two spatial scales expansion was developed by Zhang, Rizwan-uddin and Dorning (1997). Although it allows for an accurate pin power reconstruction and provides a systematic homogenization theory, the method seems to be too complex to implement for routine calculations. The method assumes periodic boundary condition in the single assembly calculations needed to generate homogenized cross sections

Starting from a variational principal, in this paper, we discretize the transport equation using discontinuous finite elements in space and discrete ordinates in angle. This method is distinguished from the present methods in its class by the form of the basis functions. The discontinuous basis functions are generated by fixed source calculations in the unique single assemblies (coarse-meshes) in the system. In the classical finite element approach, polynomials ("hat" functions) are used as the basis functions and the mesh is assumed to be homogeneous (have constant properties`). The method presented in this paper is an extension of the method developed for solving the diffusion equation by Nichita and Rahnema (1998).

A variational principle that incorporates the discontinuities at the interface between two coarse meshes is first presented. The principal is then used to generate a system of algebraic equations that has as unknowns the values of the angular fluxes at the interfaces between elements. No homogenization is required. The fine mesh solution is reconstructed by a linear superposition of the basis functions. The method is developed for slab geometry in one-group.

VARIATIONAL PRINCIPLE

Assume a one-dimensional system divided into N subsystems, called "elements". The term "nodes" will be used to denote the interface (point) between two adjacent elements. For this system we propose the following functional:

$$\boldsymbol{F}(\Psi) = \sum_{i=1}^{N} \boldsymbol{F}_i \tag{1}$$

where the "elemental" functionals are given by:

$$\boldsymbol{F}_i \equiv \begin{cases} \langle H\Psi_1, \Psi_1 \rangle_1 - \left\langle m\Psi_1^l, \Psi_1^l \right\rangle^+ + \frac{1}{2}\left\langle m\left(\Psi_1^r - \Psi_2^l\right), \left(\Psi_1^l + \Psi_2^r\right)\right\rangle^+, & i = 1 \\ \langle H\Psi_i, \Psi_i \rangle_i - \frac{1}{2}\left\langle m\left(\Psi_i^l - \Psi_{i-1}^r\right), \left(\Psi_i^l + \Psi_{i-1}^r\right)\right\rangle^- + & \\ \frac{1}{2}\left\langle m\left(\Psi_i^r - \Psi_{i+1}^l\right), \left(\Psi_i^r + \Psi_{i+1}^l\right)\right\rangle^+, & i \neq 1, N \\ \langle H\Psi_N, \Psi_N \rangle_N + \left\langle m\Psi_N^r, \Psi_N^r \right\rangle^- - \frac{1}{2}\left\langle m\left(\Psi_N^l - \Psi_{N-1}^r\right), \left(\Psi_N^l + \Psi_{N-1}^r\right)\right\rangle^-, & i = N \end{cases} \tag{2}$$

The following scalar product notations have been used:

$$\langle f,g\rangle_i \equiv \int_i dx \int_{-1}^{1} dx f(x,m) g(x,-m),\ \langle f,g\rangle^+ \equiv \int_0^1 dm f(m) g(-m),\ \langle f,g\rangle^- \equiv \int_{-1}^{0} dm f(m) g(-m).$$

The function Ψ_i is the restriction of the trial function Ψ at element *i*, while Ψ_i^l and Ψ_i^r are the corresponding restrictions at the left and right nodes of element *i*, respectively. The operator *H* is given as

$$H = L + C - S - \frac{1}{k} F \tag{3a}$$

with *L*, *C*, *S* and *F* as the leakage, collision, scattering and fission operators, whose action upon a differentiable function *f* is defined by:

$$Lf(x,m) \equiv m \frac{\partial}{\partial x} f(x,m) \tag{3b}$$

$$Cf(x,m) \equiv s(x) f(x,m) \tag{3c}$$

$$Sf(x,m) \equiv \frac{1}{2} s_s(x) \int_{-1}^{1} dm' f(x,m') \tag{3d}$$

$$Ff(x,m) \equiv \frac{1}{2} n s_f(x) \int_{-1}^{1} dm' f(x,m') \tag{3e}$$

The notation above is standard. A one-group problem with isotropic scattering was considered.

We note that the above functional allows the use of trial functions that do not necessarily satisfy the coarse-mesh interface continuity and external boundary condition.

It is easy to see that the functional in Eq. (1) is a variational principle for the transport equation (4) below since the functional and its first variation vanish when evaluated with the solution of the homogeneous transport equation:

$$Ly(x,m) + Cy(x,m) = Sy(x,m) + \frac{1}{k} Fy(x,m) \tag{4a}$$

The solution to Eq. (4a) satisfies the interface continuity conditions holding at the common boundary between elements *i* and *i*+1:

$$y_i^r = y_{i+1}^l, \qquad i = 1,\ldots,N-1 \tag{4b}$$

and a void condition at the external boundary:

$$\begin{aligned} y_1^l &= 0, \quad m > 0 \\ y_N^r &= 0, \quad m < 0 \end{aligned} \tag{4c}$$

HETEROGENEOUS FINITE ELEMENT METHOD

The angular flux in an isolated element (fuel assembly) can be reproduced if the boundary conditions and the volumetric sources are identical to those when the element belonged to the whole system (Case and Zweifel, 1967). Therefore, to find the angular flux distribution in the isolated element, we have to solve a fixed source transport problem within the element with an incoming boundary flux that reproduces the conditions at the element's boundary when it belonged to the whole system and with a

fission cross section modified by the system's eigenvalue. Since the incoming boundary angular flux and the eigenvalue of the system are not known, some approximations will be necessary.

If the discrete ordinates technique is used, the angular flux for a specific element can be reconstructed from basis functions by linear superposition. These functions can be chosen as the angular fluxes produced by a unit source in a given direction. If slab geometry is assumed, one can write the angular flux in element *i*, for direction *m* as:

$$\Psi_{im}(x) = \sum_{m'} x_{im'} \Psi_{i,m' \to m}(x) \tag{5}$$

The summation is over all M discrete ordinates used. The negative ($m_m < 0$) directions will be labeled with negative *m*, while the positive ones will be labeled with a positive *m*. The coefficients $x_{im'}$ are the values of the incoming angular fluxes at the boundary of the element (nodal values for this 1-D case) and $\Psi_{i,m' \to m}(x)$ is the response given by a unit incoming flux in direction *m'* into direction *m* for element *i*.

Now, use Eq. (5) as the trial function in the variational principle given by Eq. (1). By setting to zero the derivative of the resulting quadratic form in x yields the following eigenvalue matrix equation:

$$\sum_{i'=1}^{N} \sum_{m'} \hat{H}_{im,i'm'} x_{i'm'} = \frac{1}{k} \sum_{i'=1}^{N} \sum_{m'} \hat{F}_{im,i'm'} x_{i'm'} \quad i = 1,...,N, \; m = -\frac{M}{2},...,\frac{M}{2} \tag{6}$$

The matrix $\hat{H}$ is an algebraic sum of four matrices corresponding to the leakage, collision, scattering and interface (or external boundary) terms:

$$\hat{H} \equiv \hat{L} + \hat{C} - \hat{S} + \hat{I} \tag{6a}$$

The matrix elements are given by:

$$\hat{L}_{im,i'm'} = d_{ii'} \sum_{m''} w_{m''} m_{m''} \int_{i'} \left[\frac{\partial \Psi_{i',m \to m''}(x)}{\partial x} \Psi_{i,m' \to -m''}(x) + \frac{\partial \Psi_{i',m' \to m''}(x)}{\partial x} \Psi_{i,m \to -m''}(x) \right] dx \tag{7a}$$

$$\hat{C}_{im,i'm'} = d_{ii'} \sum_{m''} w_{m''} \int_{i'} s_{i'}(x) \left[\Psi_{i,m \to m''}(x) \Psi_{i,m' \to -m''}(x) + \Psi_{i,m' \to m''}(x) \Psi_{i,m \to -m''}(x) \right] dx \tag{7b}$$

$$\hat{S}_{im,i'm'} = d_{ii'} \sum_{m''} \sum_{m'''} \frac{1}{2} w_{m''} w_{m'''} \int_{i'} s_{si'}(x) \left[\Psi_{i',m \to m''}(x) \Psi_{i,m' \to -m'''}(x) + \Psi_{i',m' \to m''}(x) \Psi_{i',m \to -m'''}(x) \right] \tag{7c}$$

$$\hat{F}_{im,i'm'} = d_{ii'} \sum_{m''} \sum_{m'''} \frac{1}{2} w_{m''} w_{m'''} \int_{i'} n s_{fi'}(x) \left[\Psi_{i',m \to m''}(x) \Psi_{i,m' \to -m'''}(x) + \Psi_{i',m' \to m''}(x) \Psi_{i',m \to -m'''}(x) \right] \tag{7d}$$

In the above equations, $d_{ii'}$ is the Kröneker delta function. The matrix elements for the interface and boundary terms are nonzero for $i' = i, \; i \pm 1$ only:

$$\hat{I}_{igm,ig'm'} = \begin{cases} -\sum_{m''<0} w_{m''} m_{m''} \left[\Psi^{l}_{1,m\to m''} \Psi^{l}_{1,m'\to -m''} + \Psi^{l}_{1,m'\to m''} \Psi^{l}_{1,m\to -m''} \right], & i = 1 \\ 0, & i \neq 1, N \\ \sum_{m''>0} w_{m''} m_{m''} \left[\Psi^{r}_{N,m\to m''} \Psi^{r}_{N,m'\to -m''} + \Psi^{r}_{N,m'\to m''} \Psi^{r}_{N,m\to -m''} \right], & i = N \end{cases} \tag{7e}$$

$$\hat{I}_{igm,i+1g'm'} = -\sum_{m''} w_{m''} m_{m''} \Psi^{r}_{i,m\to m''} \Psi^{l}_{i+1,m'\to -m''}, \qquad i \neq N \tag{7f}$$

$$\hat{I}_{igm,i-1g'm'} = -\sum_{m''} w_{m''} m_{m''} \Psi^{r}_{i-1,m'\to m''} \Psi^{l}_{i,m\to -m''}, \quad i \neq 1 \tag{7g}$$

The superscripts l and r refer again to the left and right boundaries of element i, respectively. Also, w_m and m_m are the weight and the cosine for direction m, respectively.

The matrix $\hat{H}$ is block tridiagonal, each block of dimension $M \times M$, while $\hat{F}$ is block diagonal with N blocks on its main diagonal.

Equation (6) is first solved for the unknowns x and eigenvalue k and then the angular fluxes are reconstructed throughout the domain on a fine mesh basis using Eq. (5).

IMPLEMENTATION

The matrix elements of Eq. (6) can be computed once the basis functions are known. To generate the basis functions, one has to assume a value for the multiplication constant of the system. If the exact value $\tilde{k}$ were known, one would be able to reproduce the exact angular flux in every element by using a reconstruction as in Eq. (5). Since this value is not known, a priori an approximation ($k^{(0)}$) should be used. These approximate basis functions are used to compute the matrix elements of Eq. (6). The resulting eigenvalue matrix equation is then solved to obtain the eigenvalue of the system, $\hat{k}^{(1)}$. Next the new eigenvalue $\hat{k}^{(1)}$ is used to generate new basis functions, which in turn are used to solve Eq. (6) for the next iterate of the eigenvalue, $\hat{k}^{(2)}$. The process is continued until convergence is achieved.

The maximum number of fixed source transport calculations for a given multiplication constant will be M for each unique fuel assembly (coarse mesh), i.e. one for each direction. Making use of the assembly's symmetry, the number of calculations can be reduced. A library of basis functions for different k's can be precomputed to avoid the calculation of new basis functions during the iteration process.

The simplest iteration strategy that can be used is:

$$k^{(j)} = \hat{k}^{(j)} \qquad j = 1,2,... \tag{10}$$

This means that the eigenvalue used to generate the next set of basis functions is simply the eigenvalue that resulted from solving the system given by Eq. (6).

It is known that the homogeneous (eigenvalue) transport equation admits, in the class of continuous functions, a unique solution (up to a multiplicative constant) that

corresponds to the physical (actual) eigenvalue of the system. Therefore, the solution (angular flux) reconstructed from the basis functions with the x's obtained by solving Eq. (6) must be discontinuous. Since the variational principle is not chosen to minimize the errors in the flux distribution, these can be larger than first order. Therefore, an alternative method to find the flux should be provided. The coefficients x found as the eigenvector of Eq. (6) can be further used to generate a solution "as continuous as possible". By taking the average of the corresponding angular fluxes at the left and right of the interfaces of the element as the new value of x, one can initiate an iterative procedure. The value of x at iteration $(j+1)$ is given by:

$$x_{im}^{(j+1)} = \begin{cases} \dfrac{\Psi_{im}^{r,(j)} + \Psi_{i+1,m}^{l,(j)}}{2}, & m_m < 0 \\ \dfrac{\Psi_{im}^{l,(j)} + \Psi_{i-1,m}^{r,(j)}}{2}, & m_m > 0 \end{cases} \qquad (11)$$

We designate the set of x's resulting directly from solving Eq. (6) by $x^{(0)}$ and call them the "initial" values. The converged x's resulting from the "interface" iteration as described above are called the "asymptotic" values. This procedure of "smoothing" the solution is found to lead to very good results in computing the assembly and pin powers (fission reaction rates). The smoothing is necessary not only when a guess close enough to the exact eigenvalue is not available, but also whenever a perturbation (real or numerical) is affecting the basis functions.

NUMERICAL RESULTS

The method described above was tested by solving the transport equation in a 7-bundle benchmark configuration typical of the Boiling Water Reactor (BWR) core in one-dimension. This configuration is highly heterogeneous both from an intra-assembly (large flux gradient within each assembly) and assembly-to-assembly point of views (large k_∞ mismatch: 1.2414 for type 1 assembly vs. 0.7912 for type 2). The core and assembly configurations are described in detail in Rahnema and Nichita (1997) and reproduced in Fig. 1 below. The water gap at the periphery of each assembly has a thickness of 1.158 cm while the fuel pins are 3.231 cm thick for an assembly length of 15.6 cm. The resulting length of the core is 109.2 cm. The one-group cross sections are given in Table 1. A void boundary condition was assumed at external boundaries of the core. The calculations were performed using an S4 discrete ordinates approach.

The scalar flux from the fine mesh calculations is plotted in Fig. 2. When the exact (fine mesh) eigenvalue is used to generate the basis functions, $\Psi_{i,m'\to m}$, an *exact* reproduction of the fine mesh results is obtained (including the angular fluxes).

Fuel Assembly Configuration:

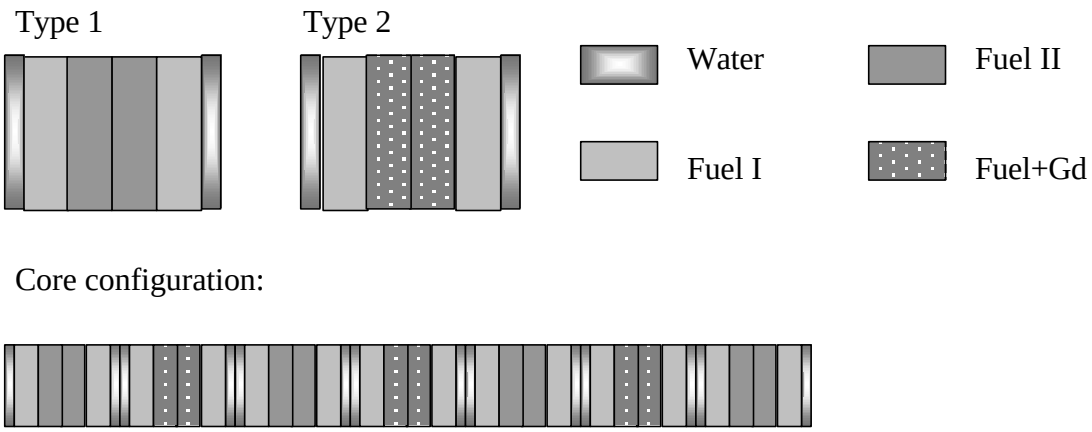

Figure 1. Assembly and the Core Configurations

Table 1. Material Properties

Material	s	ns_f	s_s
Water	0.1890	0.0	0.1557
Fuel I	0.2263	0.042850	0.2006
Fuel II	0.2252	0.034500	0.1994
Fuel IIg (with gadolinium)	0.2173	0.006122	0.1902

Since in general the system (core) eigenvalue is not known a priori, an iteration procedure as described in the previous section is initiated with a guess for *k*. Tables 2 and 3 summarize the results for two situations when one starts out with a guess for the eigenvalue that is ±10% of the exact (fine mesh value), $\tilde{k} = 1.0085$. In these tables, the iteration counter is *j* and the second column contains the difference between the eigenvalue used to generate the basis functions and the exact value, $\Delta k^{(j)} = 100 \cdot (k^{(j)} - \tilde{k})$. The next column shows the eigenvalue resulted by solving Eq. (6) and its absolute error, $\Delta \hat{k}^{(j)} = 100 \cdot (\hat{k}^{(j)} - \tilde{k})$. The remaining columns list the errors in the bundle (average) and fuel pin fission reaction rates using the initial and asymptotic fluxes labeled in the tables as "I" and "A", respectively. Both the maximum and RMS errors are computed.

To eliminate the interpolation errors in the basis functions, an exact calculation for these functions was performed each time using the "guess" value for the multiplication constant.

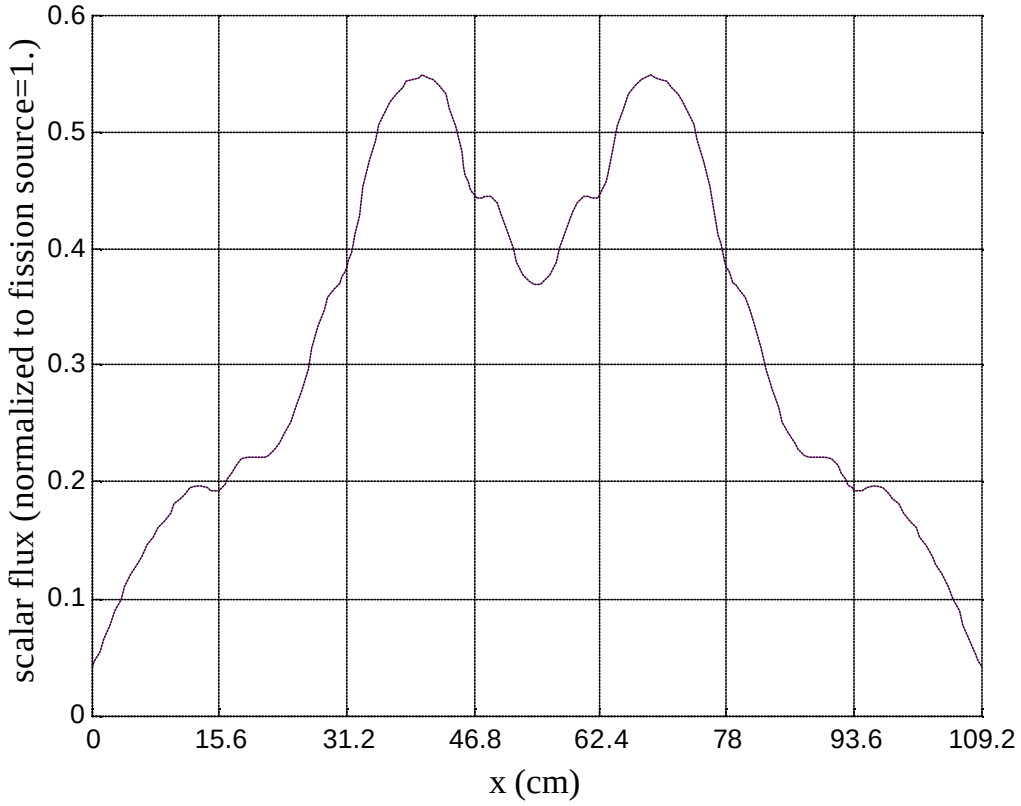

Figure 2. The Scalar Flux in the Core

Table 2. Iterative Process with $\Delta k^{(0)} = 10\%$

j	$\Delta k^{(j-1)}$ (%)	$\hat{k}(j)$	$\Delta\hat{k}(j)$ (%)	RMS bundle (%)		Max bundle (%)		RMS pin (%)		Max pin (%)	
				I	A	I	A	I	A	I	A
1	**10.00**	**0.9957**	**-1.27**	**20.5**	**2.7**	**27.1**	**3.7**	**20.9**	**3.4**	**27.2**	**6.1**
2	**-1.27**	**1.0125**	**0.41**	**57.2**	**0.4**	**87.7**	**0.6**	**57.6**	**0.5**	**87.8**	**0.9**
3	**0.41**	**1.0084**	**-0.01**	**6.7**	**0.1**	**10.1**	**0.2**	**6.7**	**0.2**	**10.1**	**0.3**
4	**-0.01**	**1.0085**	**0.00**	**0.4**	**0.0**	**0.7**	**0.0**	**0.5**	**0.0**	**0.7**	**0.0**

Table 3. Iterative Process with $\Delta k^{(0)} = -10\%$

j	$\Delta k^{(j-1)}$ (%)	$\hat{k}(j)$	$\Delta\hat{k}(j)$ (%)	RMS bundle (%)		Max bundle (%)		RMS pin (%)		Max pin (%)	
				I	A	I	A	I	A	I	A
1	-10.00	1.0165	0.80	24.8	4.0	39.4	5.5	25.0	4.9	40.2	8.6
2	0.80	1.0081	-0.04	10.2	0.3	15.4	0.3	10.3	0.3	15.4	0.6
3	-0.04	1.0085	-0.00	1.2	0.0	1.8	0.0	1.2	0.0	1.8	0.0

DISCUSION AND CONCLUSIONS

For the configuration considered, the iteration scheme described by Eq. (10) reproduced the fine mesh results including the assembly (bundle) averaged and the fine mesh power distributions after 3-4 iterations. It is interesting to note the monotonically decreasing trend in the "asymptotic" values and their smaller values as opposed to those of the "initial" errors. The reduction in the ratio of the computational effort for the coarse mesh method to that for the fine-mesh discrete ordinates method is proportional to the ratio of the number of fine to coarse meshes used in the two methods. The price paid for the substantial gain in the calculational speed is the precomputation of the library of basis functions. The effort required for the minimization of the errors in the flux (and fission reaction) distributions is negligible.

The error in the initial eigenvalue as used in the benchmark problem to generate the basis functions is much larger than normal. In general, estimations within 1% should be available for a critical system (operating reactor).

The maximum asymptotic errors in both the assembly and pin powers (fission density) are of the order of the error in the eigenvalue used to generate the basis functions. The dependence of these errors on $\Delta k^{(j-1)}$ is quasilinear.

In conclusion, a computationally efficient and accurate method to solve the transport equation in discrete ordinates form is developed in this paper. The new technique is based on a new fully variational heterogeneous finite element method. It is shown that in one-dimensional geometry, the method reproduces the fine mesh solution. This was demonstrated by considering a benchmark problem typical of a heterogeneous BWR core in slab geometry. The computation time is only a fraction of the time required to solve the fine mesh transport equation. A library of elemental basis functions for different eigenvalues, for each type of assembly is needed to achieve the desired computational efficiency. Two to three iterations were sufficient to achieve a very good accuracy (less than one tenth of a percent in eigenvalue) when the initial guess for the eigenvalue was 10% from the exact (fine mesh) value. A method for smoothing the discontinuity in the solution (expansion coefficients) was suggested. This smoothing process leads to excellent results with negligible computational effort.

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