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# Assembly Discontinuity Factors for the Neutron Diffusion Equation discretized with the Finite Volume Method. Application to BWR

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#### ABSTRACT

The neutron flux spatial distribution in Boiling Water Reactors (BWRs) can be calculated by means of the Neutron Diffusion Equation (NDE), which is a space- and time-dependent differential equation. In steady state conditions, the time derivative terms are zero and this equation is rewritten as an eigenvalue problem. In addition, the spatial partial derivatives terms are transformed into algebraic terms by discretizing the geometry and using numerical methods. As regards the geometrical discretization, BWRs are complex systems containing different components of different geometries and materials, but they are usually modelled as parallelepiped nodes each one containing only one homogenized material to simplify the solution of the NDE. There are several techniques to correct the homogenization in the node, but the most commonly used in BWRs is that based on Assembly Discontinuity Factors (ADFs). As regards numerical methods, the Finite Volume Method (FVM) is feasible and suitable to be applied to the NDE. In this paper, a FVM based on a polynomial expansion method has been used to obtain the matrices of the eigenvalue problem, assuring the accomplishment of the ADFs for a BWR. This eigenvalue problem has been solved by means of the SLEPC library.

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#### 1. Introduction

Boiling Water Reactors (BWRs) are multi-physics systems where the energy released by nuclear fission is transformed into thermal energy. Since the fission rate can be determined by means of the neutron flux, the determination of the neutron flux distribution inside nuclear reactors is crucial to obtain the power distribution in a nuclear reactor core.

The neutron flux spatial distribution in BWR can be calculated by means of stochastic or deterministic methods. The latter ones solve the integral–differential neutron transport equation and they require typically less computational resources than the former ones. The deterministic method most widely used in Reactor Physics Analysis is the neutron diffusion theory, which is a simplification of the neutron transport theory based on Fick's Law, as discussed by many authors, such as Stacey (2001), due to its lowest computational resources. Nevertheless, the neutron diffusion theory applied to Nuclear Power Plants also has to cope with partial differential equations in heterogeneous media, and consequently numerical methods are required, since the analytical solution cannot be calculated in 3D. First, the time-dependent Neutron Diffusion Equation (NDE) is transformed into an eigenvalue problem to solve the neutron flux spatial distribution, as discussed in Section 2. Then, the spatial partial derivatives terms are transformed into algebraic terms by using numerical methods, as discussed also in Section 2.

Moreover, BWR are complex systems containing different components of different geometries and materials. Since the coefficients of the NDE. diffusion coefficients and cross-sections. depend on the materials, BWR are usually modelled as parallelepiped nodes each one containing only one homogenized material to simplify the solution of the NDE. It is usual that each of these nodes represents one fuel assembly, this homogenization should be based on assembly homogenization techniques (Smith, 1986). However, using homogenization of cross sections and diffusion coefficients in BWR requires techniques to correct this homogenization in order to accurately solve the NDE (Smith, 1986). One of these techniques most commonly used in BWR is that of the Assembly Discontinuity Factors (ADFs) Smith, 1986; Verdú et al., 2005, which are the ratio of the surface flux obtained from heterogeneous composition to that obtained from homogeneous composition. By means of this technique, the continuity of the heterogeneous flux has to be accomplished, which implies the discontinuity of the homogeneous flux if ADF is different from one.

As far as numerical methods are concerned, the most popular numerical techniques used to solve the NDE give accurate results





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#### Nomenclature

- neutron flux of the g energy group
- $\frac{\phi_g}{J_g}$ neutron current of the g energy group
- neutron velocity of the g energy group  $v_{g}$
- neutron diffusion coefficient of the g energy group  $D_{g}$
- $\Sigma_{a,g}$ absorption macroscopic cross-section of the g energy group
- scattering macroscopic cross-section from the first to  $\Sigma_{s,1\rightarrow 2}$ the second energy group
- $v\Sigma_{f,g}$ Nu-fission macroscopic cross-section of the g energy group
- fraction of delayed neutrons of the precursors of group *i*  $\beta_i$ total fraction of delayed neutrons β
- decay constant of the precursors of group *i*
- $\lambda_i$  $C_i$ concentration of delayed neutrons precursors of group *i*
- S<sub>j</sub> V area of the face *j*
- volume of the cell i
- $D_{\sigma}^{i}$ neutron diffusion coefficient of the g energy group for the cell *i*
- $\phi_{g,i}$ neutron flux of the g energy group for the cell *i*
- neutron flux of the g energy group for the face j, corre- $\phi_{g,i,j}$ sponding to the cell *i*
- $\phi_{g,i,j}^{\text{het}}$ heterogeneous neutron flux of the g energy group for the face *i*, corresponding to the cell *i*
- Assembly Discontinuity Factor of the g energy group for ADF<sub>g,i,j</sub> the face *j*, corresponding to the cell *i*

 $\Sigma_{a.g}^{i}$ absorption macroscopic cross-section of the g energy group for the cell *i*  $\Sigma_{s,1\rightarrow 2}^{i}$ scattering macroscopic cross-section from the first to the second energy group for the cell *i* eigenvalue k  $v\Sigma_{f,g}^{i}$ Nu-fission macroscopic cross-section of the g energy group for the cell *i* Nfaces number of faces of each cell coefficient multiplying the term *t* of the polynomial  $a_{g,i,t}$ expansion of the flux of g energy group for the cell *i* 

- term *t* of the polynomial expansion of the flux
- $\begin{array}{c} p_t(x,y,z) \\ \bar{p_t}^{V_i} \end{array}$ volume averaged value of the term *t* of the polynomial expansion of the flux for the cell *i*
- $\bar{p_t}^{S_{ij}}$ surface averaged value of the term *t* of the polynomial expansion of the flux for the cell *i* and its face *j*
- $\overrightarrow{\nabla} p_t S_{ij}$ surface averaged value of the gradient of the term *t* of the polynomial expansion of the flux for the cell *i* and its face *i*
- X-component of the unit vector which is normal to face *j*  $u_{ijx}$ and in the outgoing direction of cell *i*
- Y-component of the unit vector which is normal to face *i*  $u_{iiv}$ and in the outgoing direction of cell *i*
- Z-component of the unit vector which is normal to face *j*  $u_{ijz}$ and in the outgoing direction of cell *i*
- its value is +1 or -1 depending on the normal to face *j*  $u_{i,i}$ and the outgoing direction of cell *i*

in structured meshes. However, the application of these methods in unstructured meshes dealing with complex geometries is not straightforward and it may cause problems of stability and convergence of the solution, as discussed by Hoffmann and Chiang (Hoffmann and Chiang, 2000). In contrast, the Finite Volume Method (FVM) is easily applied to unstructured meshes. In addition, the application of the FVM to the NDE is feasible, as discussed by Bernal et al. (2014, 2015) and Theler (2013).

In this paper, the FVM based on a polynomial expansion method (Bernal et al., 2015) has been used to discretize the steady state of the NDE to obtain the matrices of the eigenvalue problem. This eigenvalue problem has been solved by means of the SLEPc library, which is appropriate to solve eigenvalue problems in which the associated matrices are sparse, such as those arising after the discretization of partial differential equations (Hernández et al., 2005; Román et al., 2015).

This polynomial expansion method can accurately solve nuclear reactors in coarse meshes (Bernal et al., 2015). However, two modifications have been performed in order to solve the neutronics in a BWR. First, the accomplishment of the continuity of the heterogeneous flux at the faces of the fuel assemblies, which is imposed by means of the ADF. Second, the reduction of the number of equations used by this method, due to the high number of nodes used to model BWRs. Nevertheless, this reduction should not decrease the accuracy of the results.

The outline of the paper is as follows. Section 2 explains the method applying the ADF to the NDE equation discretized with the FVM. Section 3 describes the characteristics of the BWR used to assess the methodology and their results. Finally, Section 4 summarizes the conclusions about the results.

#### 2. Material and methods

The time-dependent multigroup neutron diffusion approximation most widely used for commercial nuclear reactors is that of 2-energy groups (Stacey, 2001), exhibited in Eq. (1). In this equation, the neutron current can be calculated by using Fick's Law, expressed in Eq. (2).

$$\frac{1}{\nu_{1}} \frac{d\phi_{1}(\vec{r},t)}{dt} = -\nabla\left(\vec{J}_{1}(\vec{r},t)\right) - \left(\Sigma_{a,1}(\vec{r}) + \Sigma_{s,1\rightarrow2}(\vec{r})\right)\phi_{1}(\vec{r},t) \\
+ (1-\beta)\left(\nu\Sigma_{f,1}(\vec{r})\phi_{1}(\vec{r},t) + \nu\Sigma_{f,2}(\vec{r})\phi_{2}(\vec{r},t)\right) + \sum_{i}\lambda_{i}C_{i} \\
\frac{1}{\nu_{2}} \frac{d\phi_{2}(\vec{r},t)}{dt} = -\nabla\left(\vec{J}_{2}(\vec{r},t)\right) - \Sigma_{a,2}(\vec{r})\phi_{2}(\vec{r},t) + \Sigma_{s,1\rightarrow2}(\vec{r})\phi_{1}(\vec{r},t) \\
\frac{dC_{i}}{dt} = \beta_{i}\left(\nu\Sigma_{f,1}(\vec{r})\phi_{1}(\vec{r},t) + \nu\Sigma_{f,2}(\vec{r})\phi_{2}(\vec{r},t)\right) - \lambda_{i}C_{i}; \quad i = 1, \dots, 6 \quad (1)$$

$$\vec{J}_{g}(\vec{r},t) = -D_{g}\vec{\nabla}\phi_{g}(\vec{r},t)$$
(2)

In steady state conditions, the time-dependent terms are zero and Eq. (1) is rewritten as the eigenvalue problem expressed by Eq. (3). If one applies the FVM to Eqs. (3) and (2), Eqs. (4) and (5) are obtained (Bernal et al., 2014).

$$0 = -\nabla \left( \overrightarrow{J}_{1}(\overrightarrow{r}) \right) - \left( \Sigma_{a,1}(\overrightarrow{r}) + \Sigma_{s,1\rightarrow2}(\overrightarrow{r}) \right) \phi_{1}(\overrightarrow{r}) + \frac{1}{k} \left( \upsilon \Sigma_{f,1}(\overrightarrow{r}) \phi_{1}(\overrightarrow{r},t) + \upsilon \Sigma_{f,2}(\overrightarrow{r}) \phi_{2}(\overrightarrow{r}) \right) 0 = -\nabla \left( \overrightarrow{J}_{2}(\overrightarrow{r}) \right) - \Sigma_{a,2}(\overrightarrow{r}) \phi_{2}(\overrightarrow{r}) + \Sigma_{s,1\rightarrow2}(\overrightarrow{r}) \phi_{1}(\overrightarrow{r})$$
(3)

$$\sum_{j} (S_{j}u_{i,j}J_{1,i,j}) + (\Sigma_{a,1}^{i} + \Sigma_{s,1\rightarrow 2}^{i})\phi_{1,i}V_{i} = \frac{1}{k} (\upsilon\Sigma_{f,1}^{i}\phi_{1,i} + \upsilon\Sigma_{f,2}^{i}\phi_{2,i})V_{i}$$
$$\sum_{j} (S_{j}u_{i,j}J_{2,i,j}) + \Sigma_{a,2}^{i}\phi_{2,i}V_{i} - \Sigma_{s,1\rightarrow 2}^{i}\phi_{1,i}V_{i} = 0$$
(4)

$$J_{g,ij} = -D_g^i \overrightarrow{\nabla} \phi_{g,ij} \tag{5}$$

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