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Spatial homogenization method based on the inverse problem

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ABSTRACT

We present a method for deriving homogeneous multi-group cross sections to replace a heterogeneous region's multi-group cross sections; providing that the fluxes, the currents on the external boundary, the reaction rates and the integral of the fluxes are preserved. We consider one-dimensional geometries: a symmetric slab and a homogeneous cylinder. Assuming that the boundary fluxes are given, two response matrices (RMs) can be defined concerning the current and the flux integral. The first one derives the boundary currents from the boundary fluxes, while the second one derives the flux integrals from the boundary fluxes. Further RMs can be defined that connects reaction rates to the boundary fluxes. Assuming that these matrices are known, we present formulae that reconstruct the multi-group diffusion cross-section matrix, the diffusion coefficients and the reaction cross sections in case of one-dimensional (1D) homogeneous regions. We apply these formulae to 1D heterogeneous regions and thus obtain a homogenization method. This method produces such an equivalent homogeneous material, that the fluxes and the currents on the external boundary, the reaction rates and the integral of the fluxes are preserved for any boundary fluxes. We carry out the exact derivations in 1D slab and cylindrical geometries. Verification computations for the presented homogenization method were performed using two- and four-group material cross sections, both in a slab and in a cylindrical geometry.

1. Introduction

Reactor physics deals with the determination of criticality parameters and the associated flux- and power distributions in a composed volume. In order to solve large-scale neutron transport problems in a reasonable time, a wide range of approximations and numerical methods have been developed and are under development. Moreover, one can find even more stringent conditions in a simulator model, where real-time solution is needed. One of the most frequently utilized method is the homogenization, which is achieved by replacing a heterogeneous region by a homogeneous one. Selengut (1960) has formulated the following requirements against an equivalent homogeneous region: *"If this interchange can take place without distorting the flux in any way outside the two cells, we shall regard them as equivalent."*

The present paper gives a recipe for substituting a multi-region volume by a homogeneous one, so that the group currents and fluxes at the external boundary, the volume integrated group fluxes and cross sections remain the same for any given boundary flux.

The homogenization method presented below is originated from the inverse problem, which endeavors to determine the macroscopic cross sections of a simple geometry. We provide a given flux at the boundary of a slab or cylinder and detect the response. In this respect it is a question, if the measured values allow for reproducing the cross sections of a homogeneous material in the volume. In the present work, we discuss the problem in two basic geometries: in one-dimensional slab and cylinder. Symmetric boundary conditions are supposed. The materials are described by multi-group cross sections.

The present work is a part of a research aiming at providing homogenized cross sections for global reactor calculation with assemblies comprising a few homogeneous regions. The method can be extended to 2D geometries, which would increase its usability.

In Sections 2 and 3 we derive the necessary formulae between the response matrices and the few-group cross sections in the frame of the diffusion approximation. In the latter section, we reproduce the diffusion parameters from the known response matrices (RMs) in case of a homogeneous region, which is basically a solution to the inverse problem for a specific case.

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The results of Section 3 are applicable to heterogeneous regions as well, which is the foundation of our homogenization method, described in Section 4.

Numerical results of the homogenization method are presented in Section 5, in which the solution has been obtained for a two-region problem. Four- and two-group parameters of the homogenized and the composing materials are compared.

2. Multi-group response matrices in a homogeneous region

Consider the multi-group, source-free diffusion equation in a homogeneous one-dimensional region $x_l \leqslant x \leqslant x_r$:

$$-D_g\nabla^2\Phi_g(x)+\Sigma_{r,g}\Phi_g(x)-\sum_{g'\neq g}\Sigma_{g'\to g}\Phi_{g'}(x)-\chi_g\sum_{g'=1}^{N_G}\nu\Sigma_{fg'}\Phi_{g'}(x)=0,$$
$$g=1,2,\ldots,N_G. \tag{1}$$

Here N_G is the number of energy groups and g is the group index; D_g is the diffusion coefficient in group g; $\Sigma_{r,g}$ is the removal cross section in group g; $\Sigma_{g'\to g}$ is the scattering cross section from group g' to g; χ_g is the fission spectrum; $\nu\Sigma_{f,g}$ is the neutron production cross section by fission in group g and $\Phi_g(x)$ is the scalar neutron flux at x in group g. In the foregoing discussion the material in the region is described by its cross sections. The 1D region is either a slab or a cylinder in our case.[1] We only deal with subcritical regions.

The equation above can be written in the following condensed form:

$$\mathbf{\nabla}^2\mathbf{\Phi}(x)+\mathbf{D}^{-1}\mathbf{\Sigma}\mathbf{\Phi}(x)=0, \tag{2}$$

where $\mathbf{D}$ is an N_G order diagonal matrix containing the diffusion coefficients and $\mathbf{\Sigma}$ is the multi-group cross-section matrix of the same order. The elements of $\mathbf{\Sigma}$ can be calculated from the few-group cross sections: $\Sigma_{gg'}=-\delta_{gg'}\Sigma_{r,g}+(1-\delta_{gg'})\Sigma_{g'\to g}+\chi_g\nu\Sigma_{f,g'}$ (the diagonal and off-diagonal elements of $\mathbf{D}^{-1}\mathbf{\Sigma}$ are positive and negative, respectively). In a homogeneous region, the analytical solution of Eq. (2) is the linear combination of the eigenvectors of $\mathbf{D}^{-1}\mathbf{\Sigma}$ and the corresponding eigenfunctions of the Laplacian:

$$\mathbf{\Phi}(x)=\mathbf{T}\langle\mathcal{K}(B_g x)\rangle\mathbf{c}+\mathbf{T}\langle\mathcal{L}(B_g x)\rangle\mathbf{d}, \tag{3}$$

where $\mathbf{c}$ and $\mathbf{d}$ are constant vectors of N_g elements,[2] matrix $\mathbf{T}$ is composed of the eigenvectors ($\mathbf{t}_g$) of $\mathbf{D}^{-1}\mathbf{\Sigma}$, B_g is the eigenvalue of the Laplace operator, $\mathcal{K}$ and $\mathcal{L}$ are the even and odd eigenfunctions of the Laplace operator, respectively. The diagonal matrices of N_G order are denoted in angle brackets:

$$\langle\mathcal{K}(B_g x)\rangle=\begin{bmatrix}\mathcal{K}(B_1\cdot x) & 0 & \cdots & 0\\ 0 & \mathcal{K}(B_2\cdot x) & \cdots & 0\\ \vdots & \vdots & \ddots & \vdots\\ 0 & 0 & \cdots & \mathcal{K}(B_{N_G}\cdot x)\end{bmatrix}. \tag{4}$$

The eigenpairs B_g^2 and $\mathbf{t}_g$ are determined by the material parameters of the diffusion equation (2):

$$\mathbf{D}^{-1}\mathbf{\Sigma}\mathbf{t}_g=B_g^2\mathbf{t}_g,\quad g=1,2,\ldots,N_G. \tag{5}$$

The boundary values determine $\mathbf{c}$ and $\mathbf{d}$.

Let the boundary condition be symmetric, then $\mathbf{\Phi}(x_l)=\mathbf{\Phi}(x_r)=\mathbf{\Phi}_l$. In this case, only the even part of the solution is kept

$$\mathbf{\Phi}(x)=\mathbf{T}\langle\mathcal{K}(B_g x)\rangle\mathbf{c}. \tag{6}$$

To eliminate $\mathbf{c}$ from the previous equation, we can write

$$\mathbf{c}=\langle\mathcal{K}(B_g x_l)\rangle^{-1}\mathbf{T}^{-1}\mathbf{\Phi}_l, \tag{7}$$

supposing that $\mathbf{T}$ is invertible. This assumption restricts the cross-section matrix of a homogeneous region, see Appendix B for more details. Substituting $\mathbf{c}$ into the expression of the flux gives

$$\mathbf{\Phi}(x)=\mathbf{T}\langle\mathcal{K}(B_g x)\rangle\langle\mathcal{K}(B_g x_l)\rangle^{-1}\mathbf{T}^{-1}\mathbf{\Phi}_l=\mathbf{T}\left\langle\frac{\mathcal{K}(B_g x)}{\mathcal{K}(B_g x_l)}\right\rangle\mathbf{T}^{-1}\mathbf{\Phi}_l. \tag{8}$$

The net neutron current is defined as

$$\mathbf{J}(x)=-\mathbf{D}\frac{d\mathbf{\Phi}(x)}{d}x=-\mathbf{D}\mathbf{T}\left\langle\frac{\mathcal{K}'(B_g x)}{\mathcal{K}(B_g x_l)}\right\rangle\mathbf{T}^{-1}\mathbf{\Phi}_l, \tag{9}$$

where a comma denotes the derivative. The even eigenfunctions ($\mathcal{K}$) of the Laplace operator are the cosine function and the Bessel function of the first kind (J_0) in slab and cylindrical geometries, respectively. We present the derivations in the aforementioned geometries.

We basically utilize two RMs: $\boldsymbol{R}_C$ that determines the net neutron current ($\mathbf{J}$) at the boundary from $\mathbf{\Phi}_l$, and $\boldsymbol{R}_F$ that determines the volume integral of the neutron flux ($\overline{\mathbf{\Phi}}=\int_0^{x_l}\mathbf{\Phi}(x)dx$) from $\mathbf{\Phi}_l$. We have therefore the following definitions:

$$\mathbf{J}_l=\boldsymbol{R}_C\mathbf{\Phi}_l, \tag{10}$$
$$\overline{\mathbf{\Phi}}=\boldsymbol{R}_F\mathbf{\Phi}_l. \tag{11}$$

Considering the symmetric 1D homogeneous region described in the beginning of this section, the first response matrix can be expressed from the right hand side of Eq. (9) as:

$$\boldsymbol{R}_C=-\mathbf{D}\mathbf{T}\left\langle\frac{\mathcal{K}'(B_g x_l)}{\mathcal{K}(B_g x_l)}\right\rangle\mathbf{T}^{-1}. \tag{12}$$

Integrating the expression of the flux in Eq. (8):

$$\overline{\mathbf{\Phi}}=\int_0^{x_l}\mathbf{\Phi}(x)dx=\mathbf{T}\left\langle\frac{1}{\mathcal{K}(B_g x_l)}\int_0^{x_l}\mathcal{K}(B_g x)dx\right\rangle\mathbf{T}^{-1}\mathbf{\Phi}_l$$
$$=\mathbf{T}\left\langle\frac{\mathcal{H}(B_g)}{\mathcal{K}(B_g x_l)}\right\rangle\mathbf{T}^{-1}\mathbf{\Phi}_l, \tag{13}$$

where $\mathcal{H}(B_g)=\int_0^{x_l}\mathcal{K}(B_g x)dx$. Comparing Eqs. (13) and (11) gives the second response matrix

$$\boldsymbol{R}_F=\mathbf{T}\left\langle\frac{\mathcal{H}(B_g)}{\mathcal{K}(B_g x_l)}\right\rangle\mathbf{T}^{-1}. \tag{14}$$

Substituting the corresponding eigenfunctions of the Laplacian into $\mathcal{K}$, $\mathcal{K}'$ and $\mathcal{H}$ in the above expressions yields the flux, current and the RMs in case of the slab and cylindrical geometries.

Further response matrices can be utilized to describe the reaction rates. Consider an arbitrary reaction m, characterized by its few group cross-section matrix $\mathbf{\Sigma}_m$, which is constant over the homogeneous region. The connection between the reaction rate of m over the region and the boundary flux is

$$\overline{\mathbf{\Sigma}_m\mathbf{\Phi}}=\boldsymbol{R}_m\mathbf{\Phi}_l. \tag{15}$$

Expressing the left hand side of the previous equation with the use of Eq. (14) gives

$$\overline{\mathbf{\Sigma}_m\mathbf{\Phi}}=\int_0^{x_l}\mathbf{\Sigma}_m\mathbf{\Phi}(x)dx=\mathbf{\Sigma}_m\overline{\mathbf{\Phi}}=\mathbf{\Sigma}_m\mathbf{T}\left\langle\frac{\mathcal{H}(B_g)}{\mathcal{K}(B_g x_l)}\right\rangle\mathbf{T}^{-1}\mathbf{\Phi}_l=\mathbf{\Sigma}_m\boldsymbol{R}_F\mathbf{\Phi}_l, \tag{16}$$

and thus the RM of a reaction m can be written as

$$\boldsymbol{R}_m=\mathbf{\Sigma}_m\boldsymbol{R}_F. \tag{17}$$

[1] A derivation, similar to the one given below, can also be given for 1D spherical geometry.

[2] Bold letters indicate vectors or matrices. The fluxes, currents are collected into vectors by energy groups.