

A Boundary Element - Response Matrix Method for 3D Neutron Diffusion and Transport Problems

V. Giusti¹ and B. Montagnini¹

Abstract: An application of a 3D Boundary Element Method (BEM), coupled with the Response Matrix (RM) technique, to solve the neutron diffusion and transport equations for multi-region domains is presented. The discussion is here limited to steady state problems, in which the neutrons have a wide energy spectrum, which leads to systems of several diffusion or transport equations. Moreover, the number of regions with different physical constants can be very large. The boundary integral equations concerning each region are solved via a polynomial moment expansion and, taking advantage of suitable recurrence formulas, the multi-fold integrals there involved are reduced to single or double integrals. The usual unknowns (the boundary particle density and its normal derivative) are here replaced by the partial currents entering or leaving each computational cell. The intuitive physical meaning of such quantities facilitates the application of the response matrix technique. Only eigenvalue (criticality) problems will be here considered. As it regards the transport equation, the use of the so called Simplified Spherical Harmonics method (SP_N) allows, through suitable approximations, to cast the problem into a system of differential elliptic equations of the diffusion type, which can still be solved by BEM.

Keywords: Response matrix, Neutron diffusion, Neutron transport, 3D criticality problems, Simplified spherical harmonics.

1 Introduction

The computational procedures based on the Boundary Element Method (BEM) here presented have been devised for the calculation of the nuclear reactor cores, an application field that, although subject to heavy criticisms, is still a valid option in order to contrast the persisting, and even increasing, use of coal, oil and gas. Getting aside from these considerations, it should also be noted that several computational techniques of neutron transport can be applied, with minor changes,

¹ Dipartimento di Ingegneria Civile ed Industriale, Università di Pisa, Pisa, ITALY.

to other fields as, for instance, radiation transfer or, via the linearized Boltzmann equation, the theory of the highly rarefied gases.

An exhaustive collection of historical references on the application of BEM to neutronic problems is outside the aim of this paper. Thus we limit ourselves to list some relevant works. The first paper, with a rather complete account of the basic theory, goes back to Koskinen (1965). At the beginning of the eighties, further developments [Itagaki (1985); Itagaki and Brebbia (1991)] gave a strong impulse to BEM, owing to the introduction of the Multiple Reciprocity Method (MRM) [Novak and Neves (1994); Itagaki (1995, 2000, 2002); Ozgener (1998); Ozgener and Ozgener (2000); Cavdar and Ozgener (2004)]. Despite of its elegance, MRM has not completely ruled out other classical methods for systems of second order partial differential equations (also discussed in some of the aforementioned papers), e.g. the diagonalization method and, as a second step, the decoupling of the global problem into two levels [Purwadi, Tsuji, Narita, and Itagaki (1997, 1998); Chiba, Tsuji, and Shimazu (2001a,b); Maiani and Montagnini (1999, 2004); Cossa, Giusti, and Montagnini (2010)]. As regards the latter subject, it can be observed that a link, although not explicit, should exist between our physically intuitive approach in [Maiani and Montagnini (1999, 2004); Cossa, Giusti, and Montagnini (2010)] and the more abstract techniques of hierarchical decomposition of matrices that are now extensively used in other fields (e.g. Brancati, Aliabadi, and Benedetti (2009)), although examples can be found also in the neutron field [Purwadi, Tsuji, Narita, and Itagaki (1997, 1998); Chiba, Tsuji, and Shimazu (2001a,b)]. The necessity of summarizing in a limited space how BEM can be used for the neutron diffusion and transport problems has forced us to converge, very strictly, towards our own specific approach. This resulted in a short review of some ideas of ours, to the prejudice of the other Authors' ones. The references quoted above should suffice, however, to start a more complete bibliographical research.

The main purpose of this paper is to give a quick account of BEM as applied to steady state reactor calculations, in which the interest is focused on the determination of the multiplication constant, k (the ratio of two successive neutron generations) and local and global distribution of the neutron population.

Section 2 introduces the simplest model, based on diffusion theory, and gives a general outline of the problems to be solved. Section 3 deals with the setting of the Boundary Integral Equations (BIE) in the so called partial current form, while the related numerical methods are described in section 4. In this section emphasis is given to the analytical procedures that were introduced in order to obtain a fast computation of the boundary integrals of a single reactor fuel cell. Section 5 outlines the calculations referring to the reactor core, viewed as the global cell system. Section 6 introduces the Simplified Spherical Harmonics method, as a first step to

proceed from the diffusion theory approach towards an approach fully based on the linear Boltzmann equation (or transport equation). Numerical results are reported in section 7 and the conclusion are drawn in section 8. An appendix has been written in order to give the reader a summary of some basic topics of neutron theory.

2 The simplest model: problem setting

The simplest model to be used for the calculation of a reactor core is based on a system of diffusion equations, one for each energy (or speed) group, g say, with $g = 1, \dots, G$, in which the neutron population can be divided. In the case of steady state conditions, what is to be determined is the density, $\rho_g(\mathbf{r})$, of the particles belonging to the energy group g at the point \mathbf{r} of the body where the diffusion process occurs. One can make use, equivalently, of the neutron *traffic* $\phi_g(\mathbf{r}) = v_g \rho_g(\mathbf{r})$, v_g being the mean neutron speed in the group g . The latter quantity allows for a more direct evaluation of the reaction rates, although the name *traffic* is usually, but improperly, substituted by the name *flux*, despite of the confusion that may follow. The equation system in order to obtain the ϕ_g 's is as follows

$$\begin{aligned} \nabla \cdot D_g(\mathbf{r}) \nabla \phi_g(\mathbf{r}) - \Sigma_{a,g}(\mathbf{r}) \phi_g(\mathbf{r}) + \sum_{g'=1}^G \Sigma_{s,gg'}(\mathbf{r}) \phi_{g'}(\mathbf{r}) \\ + \frac{\chi_g}{k} \sum_{g'=1}^G v_{g'} \Sigma_{f,g'}(\mathbf{r}) \phi_{g'}(\mathbf{r}) = 0 \quad (g = 1, \dots, G), \end{aligned} \quad (1)$$

where D_g , $\Sigma_{a,g}$, $\Sigma_{s,gg'}$ and $v_g \Sigma_{f,g}$ are, respectively, the diffusion coefficient, the absorption cross section, the scattering cross section from group g' to group g and the fission cross section times v_g , the number of secondary neutrons emitted by such fissions. Finally, χ_g is the fraction of secondary neutrons whose energy is within the group g , while k represents the multiplication constant, which plays the rôle of eigenvalue of the equation system, and is equal to one at criticality.

The commonly used conditions on the reactor boundary are vanishing conditions for each ϕ_g or, preferably, for the incoming particle flux (see section 3).

The main difficulties as regards the application of BEM to such problems are: (i) the problem domain is, in general, a 3D domain, (ii) the number of equations, G , is rather large, (iii) the reactor core is divided into regions that are physically homogeneous (or can be considered homogeneous after applying suitable averaging procedures), but such regions might be thousands.

The lucky circumstance is that the regions, or 'cells' (as we will refer to them from now on) have a rather simple shape: usually right prisms with a rectangular, hexagonal or triangular base, arranged accordingly to a regular lattice.

As pointed out above the calculation procedure can be divided into two steps or levels:

- the first level: one considers the neutrons entering each cell from the boundary, which is accomplished by assigning a suitable combination of ϕ_g and its normal derivative. Making use of BEM it is then possible to determine those neutrons which leave the cell and will therefore be considered as entering the adjacent ones;
- the second level: on the basis of the ingoing and outgoing particles, an iterative procedure is established in order to determine the neutron distribution over the global reactor system as well as the multiplication constant k .

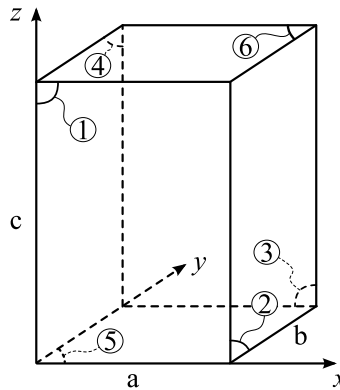


Figure 1: Face numbering on the rectangular node.

3 The first level: solution of the diffusion equation system for a single cell

Let us consider a single cell, V say, with a shape of a prism with rectangular base and sides a , b and c (Fig. 1) and homogeneous physical properties (thus the quantities D_g , $\Sigma_{a,g}$, etc. are constant inside V). Equation system 1 can be written in a compact matrix form:

$$-\nabla_{\mathbf{r}}^2 \boldsymbol{\phi}(\mathbf{r}) + \mathbf{Q} \boldsymbol{\phi}(\mathbf{r}) = \mathbf{0}, \tag{2}$$

where $\boldsymbol{\phi}(\mathbf{r}) = [\phi_1(\mathbf{r}), \dots, \phi_G(\mathbf{r})]$ and \mathbf{Q} is a $G \times G$ matrix in which all the physical quantities of the cell are embedded. The k eigenvalue refers to the global physical system and is kept fixed during the present single cell calculations, so that it can be momentarily understood. It is assumed that \mathbf{Q} has G distinct eigenvalues, λ_h . Then, the corresponding eigenvectors $\boldsymbol{\xi}_h \equiv [\xi_{1h}, \dots, \xi_{Gh}]$ constitute a basis of the space \mathbb{C}^G and denoting by $\boldsymbol{\Xi}$ the (non-singular) matrix having these eigenvectors as

its columns and by $\mathbf{\Xi}^{-1}$ its inverse, the matrix \mathbf{Q} is diagonalized

$$\mathbf{\Xi}^{-1}\mathbf{Q}\mathbf{\Xi} = \mathbf{\Lambda}, \tag{3}$$

where $\mathbf{\Lambda} = \text{diag} [\lambda_1, \dots, \lambda_G]$. Now we set

$$\boldsymbol{\psi}(\mathbf{r}) = \mathbf{\Xi}^{-1}\boldsymbol{\phi}(\mathbf{r}) \tag{4}$$

and, reciprocally, $\boldsymbol{\phi}(\mathbf{r}) = \mathbf{\Xi}\boldsymbol{\psi}(\mathbf{r})$. After left multiplication by $\mathbf{\Xi}^{-1}$ Eq. 2 is transformed as follows

$$-\nabla_{\mathbf{r}}^2\boldsymbol{\psi}(\mathbf{r}) + \mathbf{\Lambda}\boldsymbol{\psi}(\mathbf{r}) = 0. \tag{5}$$

In terms of the components of $\boldsymbol{\psi}(\mathbf{r})$, $\psi_h(\mathbf{r})$ say, we have

$$-\nabla_{\mathbf{r}}^2\psi_h(\mathbf{r}) + \lambda_h\psi_h(\mathbf{r}) = 0 \quad (h = 1, \dots, G), \tag{6}$$

actually a set of G uncoupled equations. The usual procedure of the BEM direct technique is then applied to each equation.

When looking for the fundamental solution, i.e. the solution of the following non-homogeneous equation,

$$-\nabla_{\mathbf{r}}^2\tilde{\psi}_h(\mathbf{r}, \mathbf{r}') + \lambda_h\tilde{\psi}_h(\mathbf{r}, \mathbf{r}') + \delta(\mathbf{r} - \mathbf{r}') = 0 \quad (h = 1, \dots, G), \tag{7}$$

one must consider that the eigenvalues of the real matrix \mathbf{Q} are either real or distributed in couples of complex-conjugates. If $\lambda_h = \zeta_h + i\eta_h$ we take $\mu_h = \gamma_h + i\omega_h$, where

$$\gamma_h = \frac{1}{\sqrt{2}} \left(\sqrt{\zeta_h^2 + \eta_h^2} + \zeta_h \right)^{\frac{1}{2}}, \quad \omega_h = \frac{1}{\sqrt{2}} \left(\sqrt{\zeta_h^2 + \eta_h^2} - \zeta_h \right)^{\frac{1}{2}}, \tag{8}$$

so that $\mu_h^2 = \lambda_h$. Then, the fundamental h -th solution is

$$\tilde{\psi}_h(\mathbf{r}, \mathbf{r}') = \frac{e^{-(\gamma_h + i\omega_h)|\mathbf{r} - \mathbf{r}'|}}{4\pi|\mathbf{r} - \mathbf{r}'|}. \tag{9}$$

In particular, if λ_h is real and positive then $\gamma_h = \zeta_h > 0$, $\omega_h = 0$, so that the classical Green function of the diffusion equation in the infinite space, which is exponentially decreasing to zero as $R = |\mathbf{r} - \mathbf{r}'| \rightarrow \infty$, is recovered. An exponential decay also holds for a complex λ_h with $\zeta_h > 0$, $\eta_h \neq 0$, the most general case that occurs with the problems which are of interest here. An exception is presented by the case in which λ_h is real and negative, so that $\gamma_h = 0$, $\omega_h = \zeta_h$ and the asymptotic behaviour

of $\tilde{\psi}_h$ is only $O(1/R)$, but the Sommerfeld radiation condition is fulfilled, so that the uniqueness of the fundamental solution is still ensured.

Continuing with the direct BEM procedure, the usual machinery based on applying the Green's second identity to the function $\tilde{\psi}_h$ leads to the following, classical integral relation,

$$c(\mathbf{r}) \psi_h(\mathbf{r}) + \int_S \left[\frac{\partial \tilde{\psi}_h}{\partial n'_S}(\mathbf{r}, \mathbf{r}'_S) \psi_h(\mathbf{r}'_S) - \tilde{\psi}_h(\mathbf{r}, \mathbf{r}'_S) \frac{\partial \psi_h}{\partial n'_S}(\mathbf{r}'_S) \right] dS' = 0 \quad (h = 1, \dots, G), \tag{10}$$

where $S = \partial V$. The label S is also used as a suffix for the points on the boundary, while \mathbf{n}_S indicates the outward normal at such points. Moreover, $c(\mathbf{r})$ is the characteristic function of V and, in particular,

$$c(\mathbf{r}_S) = \int_V \delta(\mathbf{r}_S - \mathbf{r}') dV' = \frac{1}{4\pi} \Omega_S(\mathbf{r}_S), \tag{11}$$

Ω_S being the angle of aperture of the tangent cone at \mathbf{r}_S ($c(\mathbf{r}_S) = 1/2$ for a smooth point).

Let us now denote by ξ_{hg}^* the elements of the matrix Ξ^{-1} (we recall that the elements of Ξ were called ξ_{gh}) and consider the following sum:

$$\tilde{\phi}_{gg'}(\mathbf{r}, \mathbf{r}'_S) = \sum_{h=1}^G \xi_{gh} \tilde{\psi}_h(\mathbf{r}, \mathbf{r}'_S) \xi_{hg'}^* \tag{12}$$

or, in matrix form,

$$\tilde{\phi}(\mathbf{r}, \mathbf{r}'_S) = \Xi \tilde{\psi}(\mathbf{r}, \mathbf{r}'_S) \Xi^{-1}, \tag{13}$$

where $\tilde{\psi}(\mathbf{r}, \mathbf{r}'_S) = \text{diag}[\tilde{\psi}_1(\mathbf{r}, \mathbf{r}'_S), \dots, \tilde{\psi}_G(\mathbf{r}, \mathbf{r}'_S)]$. Eq. 4 and its reciprocal allow to write Eq. 10 also in matrix form, i.e., after left multiplication by Ξ ,

$$c(\mathbf{r}) \phi(\mathbf{r}) + \int_S \Xi \left(\frac{\partial \tilde{\psi}}{\partial n'_S}(\mathbf{r}, \mathbf{r}'_S) - \tilde{\psi}(\mathbf{r}, \mathbf{r}'_S) \frac{\partial}{\partial n'_S} \right) \Xi^{-1} \phi(\mathbf{r}'_S) dS' = 0 \tag{14}$$

or, using Eq. 13,

$$c(\mathbf{r}) \phi(\mathbf{r}) + \int_S \left(\frac{\partial \tilde{\phi}}{\partial n'_S}(\mathbf{r}, \mathbf{r}'_S) - \tilde{\phi}(\mathbf{r}, \mathbf{r}'_S) \frac{\partial}{\partial n'_S} \right) \phi(\mathbf{r}'_S) dS' = 0. \tag{15}$$

In terms of the components the above equation reads

$$c(\mathbf{r}) \phi_g(\mathbf{r}) + \sum_{g'=1}^G \int_S \left(\frac{\partial \tilde{\phi}_{gg'}}{\partial n'_S}(\mathbf{r}, \mathbf{r}'_S) \phi_{g'}(\mathbf{r}'_S) - \tilde{\phi}_{gg'}(\mathbf{r}, \mathbf{r}'_S) \frac{\partial \phi_{g'}}{\partial n'_S}(\mathbf{r}'_S) \right) dS' = 0 \tag{16}$$

($g = 1, \dots, G$),

another classical relationship that allows to determine the fluxes, $\phi_g(\mathbf{r})$, at any point of the V cell, provided the boundary values of these fluxes and their normal derivatives are known. Taking, in particular, $\mathbf{r} = \mathbf{r}_S$, we arrive at the system of the boundary integral equations for such quantities. However, we shall not make a direct use of the ϕ_g 's (or their normal derivatives). Rather, we shall introduce the following linear combinations of them, namely (Maiani and Montagnini, 1999, 2004)

$$J_g^\pm(\mathbf{r}_S) = \frac{1}{4}\phi_g(\mathbf{r}_S) \mp \frac{1}{2}D_g \frac{\partial \phi_g}{\partial n_S}(\mathbf{r}_S), \quad (17)$$

together with the reciprocal relations

$$\phi_g(\mathbf{r}_S) = 2(J_g^+(\mathbf{r}_S) + J_g^-(\mathbf{r}_S)) \quad (18)$$

$$-D_g \frac{\partial \phi_g}{\partial n_S}(\mathbf{r}_S) = J_g^+(\mathbf{r}_S) - J_g^-(\mathbf{r}_S). \quad (19)$$

The quantities $J_g^\pm(\mathbf{r}_S)$ are known, respectively, as the *outgoing and ingoing partial current* (in the general language of mathematical physics they should rather be called outward and inward particle fluxes per unit area). We defer the reader to the Appendix for more details; here we only observe that $J_g(\mathbf{r}_S) = J_g^+(\mathbf{r}_S) - J_g^-(\mathbf{r}_S)$ represents the *net* current at \mathbf{r}_S and Eq. 19 is simply the Fick's law (Davison, 1958; Weinberg and Wigner, 1958; Bell and Glasstone, 1970; Stacey, 2007).

If expressions 18 and 19 are substituted into Eqs. 16 and the following new kernels

$$\tilde{J}_{gg'}^\pm(\mathbf{r}_S, \mathbf{r}'_S) = \frac{1}{4D_g} \tilde{\phi}_{gg'}(\mathbf{r}_S, \mathbf{r}'_S) \pm \frac{1}{2} \frac{\partial \tilde{\phi}_{gg'}}{\partial n'_S}(\mathbf{r}_S, \mathbf{r}'_S) \quad (20)$$

are introduced, we get a partial current form of the G -group boundary integral equations (Maiani and Montagnini, 1999, 2004):

$$\begin{aligned} \frac{1}{2}c(\mathbf{r}_S)J_g^+(\mathbf{r}_S) + \sum_{g'=1}^G \int_S \tilde{J}_{gg'}^+(\mathbf{r}_S, \mathbf{r}'_S) J_{g'}^+(\mathbf{r}'_S) dS' = -\frac{1}{2}c(\mathbf{r}_S)J_g^-(\mathbf{r}_S) \\ + \sum_{g'=1}^G \int_S \tilde{J}_{gg'}^-(\mathbf{r}_S, \mathbf{r}'_S) J_{g'}^-(\mathbf{r}'_S) dS' \quad (g = 1, \dots, G). \end{aligned} \quad (21)$$

Let the ingoing currents $J_g^-(\mathbf{r}_S)$ be known, so that the *r.h.s.* of the latter equations is also known. Then the response of the V cell in terms of the outgoing currents $J_g^+(\mathbf{r}_S)$ will be determined by solving the above boundary integral equations with the kernels $\tilde{J}_{gg'}^+(\mathbf{r}_S, \mathbf{r}'_S)$. Although perfectly equivalent to the classical setting of the BIE's, the present rearrangement facilitates the subsequent calculations. It is, in

fact, quite intuitive how to proceed for the second, or global, level of the calculation, in which the cells are connected all together. It is based on the following iteration steps, to be applied to each cell of the general system:

$$\begin{aligned} \frac{1}{2}c(\mathbf{r}_S)J_g^{+(t+1)}(\mathbf{r}_S) + \sum_{g'=1}^G \int_S \tilde{J}_{gg'}^+(\mathbf{r}_S, \mathbf{r}'_S) J_{g'}^{+(t+1)}(\mathbf{r}'_S) dS' = -\frac{1}{2}c(\mathbf{r}_S)J_g^{-(t)}(\mathbf{r}_S) \\ + \sum_{g'=1}^G \int_S \tilde{J}_{gg'}^-(\mathbf{r}_S, \mathbf{r}'_S) J_{g'}^{-(t)}(\mathbf{r}'_S) dS' \quad (g = 1, \dots, G). \end{aligned} \quad (22)$$

The eigenvalue k is updated at the end of each one of these steps.

4 Numerical solution of the cell problem

Let us continue with the cell problem. As regards the numerical solution of Eqs. 22 (we omit the superscript t , with the understanding that the *r.h.s.* is known from the outset), the classical procedure based on a distribution of source and evaluation points (with a local expansion) on the contour of even a two-dimensional cell domain was found to be computationally expensive (Maiani and Montagnini, 1999). We then adopted a *weak* or, better, a *moment* formulation, based on the expansion of the boundary partial currents on a set of orthogonal polynomials (Maiani and Montagnini, 2004). This approach was maintained in all subsequent works, including the problems with 3D cells (Cossa, Giusti, and Montagnini, 2010; Giusti and Montagnini, 2012; Giusti, Montagnini, and Ravetto, 2013). The motivation, as already pointed out in sect. 2, was that the reactor cores can be usually considered as made of cells with simple shape. A direct, elementary evaluation of the face-to-face boundary integrals is then possible and there is no need to adopt special techniques such as the multipoles algorithms (Gumerov and Duraiswami, 2004; Brunner, Junge, Rapp, Bebendorf, and Gaul, 2010; Mallardo and Aliabadi, 2012), which would be otherwise mandatory in other contexts.

Let (u, v) be the coordinates of a point \mathbf{r}_S on the face $S^{(s)}$ ($s = 1, \dots, s_M$, with $s_M = 6$) of the parallelepiped V and the functions $e_{sm}(t)$ be such that the products $W_{s,mn}(\mathbf{r}_S) = e_{sm}(u) e_{sn}(v)$ constitute an orthogonal set on this face. By completing the $W_{s,mn}(\mathbf{r}_S)$ functions by zero on the remaining faces, we expand the inward and outward partial currents in terms of these $W_{s,mn}$'s. It is highly expedient that each $e_{sm}(t)$ may belongs to a set of orthogonal functions, most easily a set of orthogonal polynomials (in our case normalized Legendre polynomials). Then we introduce the following truncated expansions

$$J_g^\pm(\mathbf{r}_S) = \sum_{s=1}^{s_M} \sum_{m=0}^{m_M} \sum_{n=0}^{n_M} J_{g,smn}^\pm W_{s,mn}(\mathbf{r}_S), \quad (23)$$

where

$$J_{g,smn}^{\pm} = \int_{S^{(s)}} J_g^{\pm}(u, v) e_{sm}(u) e_{sn}(v) du dv \quad (24)$$

and the analogous expansion for the kernels:

$$\tilde{J}_{gg'}^{\pm}(\mathbf{r}_S, \mathbf{r}'_S) = \sum_{s,s'=1}^{SM} \sum_{m,m'=0}^{m_M} \sum_{n,n'=0}^{n_M} \tilde{J}_{gg',ss',mm',nn'}^{\pm} W_{s,mn}(\mathbf{r}_S) W_{s',m'n'}(\mathbf{r}'_S), \quad (25)$$

where

$$\tilde{J}_{gg',ss',mm',nn'}^{\pm} = \int_{S^{(s)}} \int_{S^{(s')}} \tilde{J}_{gg'}^{\pm}(u, v, u', v') e_{sm}(u) e_{s'm'}(u') e_{sn}(v) e_{s'n'}(v') du du' dv dv'. \quad (26)$$

After the expansions have been introduced into Eqs. 22 (or, simply into Eqs. 21, since the iteration index has been understood), owing to the orthonormality the following linear system is obtained

$$\begin{aligned} \frac{1}{4} J_{g,smn}^{+} + \sum_{g'=1}^G \sum_{s'=1}^{SM} \sum_{m'=0}^{m_M} \sum_{n'=0}^{n_M} \tilde{J}_{gg',ss'mm'nn'}^{+} J_{g',s'm'n'}^{+} = \\ - \frac{1}{4} J_{g,smn}^{-} + \sum_{g'=1}^G \sum_{s'=1}^{SM} \sum_{m'=0}^{m_M} \sum_{n'=0}^{n_M} \tilde{J}_{gg',ss'mm'nn'}^{-} J_{g',s'm'n'}^{-}. \end{aligned} \quad (27)$$

Note that the moment approach overcomes (perhaps in a somewhat brute force way) the otherwise fine and elegant problems implied by the edges and vertices, since the points where $c(\mathbf{r}_S) \neq 1/2$ are a set of zero measure.

Eqs. 27 can be given a compact form, namely

$$\mathbf{M}^{+} \mathbf{J}^{+} = \mathbf{M}^{-} \mathbf{J}^{-}, \quad (28)$$

where the \mathbf{M}^{\pm} matrices have the elements

$$M_{gg',ss'mm'nn'}^{\pm} = \tilde{J}_{gg',ss'mm'nn'}^{\pm} \pm \frac{1}{4} \delta_{gg'} \delta_{ss'} \delta_{mm'} \delta_{nn'}$$

and the \mathbf{J}^{\pm} vectors have elements $J_{g,smn}^{\pm}$. After inversion of \mathbf{M}^{+} we obtain

$$\mathbf{J}^{+} = \tilde{\mathbf{R}} \mathbf{J}^{-}, \quad (29)$$

where $\tilde{\mathbf{R}} = (\mathbf{M}^{+})^{-1} \mathbf{M}^{-}$. It is to be noted that the elements of the matrices \mathbf{M}^{\pm} and therefore of $\tilde{\mathbf{R}}$ may be complex, due to the constants in the fundamental solution,

which are in general complex. However, \mathbf{J}^- must be real (owing to its physical meaning) and the imaginary part of $\tilde{\mathbf{R}}$ can be discarded. The real matrix \mathbf{R} so obtained then replaces the $\tilde{\mathbf{R}}$ matrix in Eq. 29 and we finally obtain

$$\mathbf{J}^+ = \mathbf{R}\mathbf{J}^- \tag{30}$$

The above equation expresses what is usually meant as a *response matrix* approach and justifies the name Boundary Element - Response Matrix (BERM) we have given to the technique here presented.

The evaluation of the elements of the matrices \mathbf{M}^\pm , although elementary, is very tedious, even for a cell with the shape of a rectangular prism. Let us first deal with the part of the calculation of the $\tilde{J}_{gg'}^\pm$ integrals that involves the fundamental solution $\tilde{\Psi}_h$ (the part involving the normal derivative will be considered afterwards).

Considering the interaction, so to say, of the faces 1 and 4 in Fig. 1, the pertinent integral, called $\tilde{I}F_{14,mm,m'n'}$, is as follows (Cossa, Giusti, and Montagnini, 2010)

$$\tilde{I}F_{14,mm,m'n'} = \int_{S(1)} dx dz \int_{S(4)} dy' dz' \tilde{\Psi}_h(x, z, y', z') e_{1m}(x) e_{1n}(z) e_{4m'}(y') e_{4n'}(z') \tag{31}$$

and, if the polynomials e_{sm} are expressed in terms of monomials, we are led to compute the following integrals

$$\tilde{I}F_{14,mnpq} = \int_0^a dx \int_0^c dz \int_0^b dy \int_0^c dz' \frac{e^{-\mu_h \sqrt{x^2+y^2+(z-z')^2}}}{\sqrt{x^2+y^2+(z-z')^2}} x^m y^n z^p z'^q \tag{32}$$

where $y^{m'}$ in the preceding integral has been replaced by y^n , $z^{n'}$ by z^p and $z^{n'}$ by z'^q ; the factor $1/4\pi$ in the fundamental solution is understood. Now we introduce the following integral, which corresponds to the z, z' integrations in Eq. 32:

$$H_{pq}(\rho) = \int_0^c \int_0^c \frac{e^{-\mu_h \sqrt{\rho^2+(z-z')^2}}}{\sqrt{\rho^2+(z-z')^2}} z^p z'^q dz dz' \tag{33}$$

where $\rho^2 = x^2 + y^2$. Setting $u = z - z'$ and performing another couple of changes of variables (for details see (Cossa, Giusti, and Montagnini, 2010)) $H_{pq}(\rho)$ can be given the following form

$$H_{pq}(\rho) = \int_0^c du \frac{e^{-\mu_h \sqrt{\rho^2+u^2}}}{\sqrt{\rho^2+u^2}} \int_0^c dz (z-u)^p z^q + \text{a similar term with } p \text{ and } q \text{ interchanged.} \tag{34}$$

By using the binomial formula, we get

$$H_{pq}(\rho) = \sum_{k=0}^p \frac{(-1)^{p-k}}{q+k+1} \binom{p}{k} \int_0^c \left(c^{q+k+1} u^{p-k} - u^{p+q+1} \right) \frac{e^{-\mu_h \sqrt{\rho^2+u^2}}}{\sqrt{\rho^2+u^2}} du$$

+ a similar term with p and q interchanged (35)

and, finally, recalling that $\rho^2 = x^2 + y^2$ and introducing this expression of the H_{pq} integrals into Eq.(32) we arrive at the following formula, where the fourfold integrals $\bar{I}F_{14,mnpq}$ are given as a sum of triple integrals:

$$\begin{aligned} \bar{I}F_{14,mnpq} &= \int_0^a \int_0^b x^m y^n H_{pq}(\sqrt{x^2+y^2}) dx dy \\ &= \sum_{k=0}^p \frac{(-1)^{p-k}}{q+k+1} \binom{p}{k} \left[c^{q+k+1} \hat{I}F_{14,mn,p-k} - \hat{I}F_{14,mn,p+q+1} \right] \end{aligned}$$

+ a similar sum with p and q interchanged, (36)

with

$$\hat{I}F_{14,mnr} = \int_0^a x^m dx \int_0^b y^n dy \int_0^c u^r \frac{e^{-\mu_h \sqrt{x^2+y^2+u^2}}}{\sqrt{x^2+y^2+u^2}} du. \tag{37}$$

If $n \geq 2$ the latter integrals obey a recurrence relationship that alleviates very much the calculational bargain.

Namely, since the expression $\left(y/\sqrt{x^2+y^2+u^2} \right) \exp\left(-\mu_h \sqrt{x^2+y^2+u^2}\right)$ can be written as $(-1/\mu_h) \partial/\partial y \left(\exp\left(-\mu_h \sqrt{x^2+y^2+u^2}\right) \right)$, an integration by parts with respect to the y variable and a further integration by parts with respect to the u variable (for details see again Cossa, Giusti, and Montagnini (2010)) allows to get the desired recurrence

$$\begin{aligned} \hat{I}F_{14,mnr} &= \frac{1}{r+1} \left[-b^{n-1} U_{m,r+2}(0, a, 0, c, b, \mu_h) \right. \\ &\quad \left. + c^{r+1} U_{mn}(0, a, 0, b, c, \mu_h) + (n-1) \hat{I}F_{14,m,n-2,r+2} \right], \end{aligned} \tag{38}$$

with

$$U_{pq}(x_1, x_2, u_1, u_2, d, \mu_h) = \int_{x_1}^{x_2} x^p dx \int_{u_1}^{u_2} u^q \frac{e^{-\mu_h \sqrt{d^2+x^2+u^2}}}{\sqrt{d^2+x^2+u^2}} du, \tag{39}$$

where the latter integrals can also be evaluated by a similar recurrence relationship. The initial integrals $\hat{I}F_{14}$, such as $\hat{I}F_{14,m1s}$ or $\hat{I}F_{14,m0s}$, as well as the low-index integrals U_{pq} are amenable to one-dimensional integrals, which are readily evaluated

by a Gauss-Legendre numerical integration, with only one exception, concerning $\hat{I}F_{14,00s}$, for which a double integration is required. But, even in this case, a passage to polar coordinates $\rho = \sqrt{x^2 + y^2}$, $\theta = \arccos(y/\rho)$ allows to smooth the inherent singularity and still achieve an accurate numerical result (Cossa, Giusti, and Montagnini, 2010).

The integrals $\bar{I}J_{14,mm,m'n'}$, involving the normal derivative of $\tilde{\Psi}_h$ and therefore related to the current (just as the previous integrals $\bar{I}F_{14}$ were related to the fluxes), turn out to be as follows (Cossa, Giusti, and Montagnini, 2010):

$$\bar{I}J_{14,mnpq} = \int_0^a x^{m+1} dx \int_0^b y^n dy \int_0^c z^p dz \int_0^c z'^q dz' \cdot K \left(\sqrt{x^2 + y^2 + (z - z')^2} \right), \quad (40)$$

where

$$K(t) = \left(\mu_h + \frac{1}{t} \right) \frac{e^{-\mu_h t}}{t^2}. \quad (41)$$

Since

$$\frac{\partial}{\partial x} \left(\frac{e^{-\mu_h \sqrt{x^2 + y^2 + (z - z')^2}}}{\sqrt{x^2 + y^2 + (z - z')^2}} \right) = -xK \left(\sqrt{x^2 + y^2 + (z - z')^2} \right) \quad (42)$$

the same procedure as from Eqs. 33 to 38 allows to get a recurrence relation also for the $\bar{I}J_{14}$ integrals:

$$\begin{aligned} \bar{I}J_{14,mnpq} = & \sum_{k=0}^p \frac{(-1)^{p-k}}{q+k+1} \binom{p}{k} \left(c^{q+k+1} \hat{I}J_{14,mm,p-k} - \hat{I}J_{14,mm,p+q+1} \right) \\ & + \text{a similar sum with } p \text{ and } q \text{ interchanged,} \end{aligned} \quad (43)$$

in which the triple integrals $\hat{I}J_{14,mnr}$, i.e.

$$\hat{I}J_{14,mnr} = \int_0^a x^{m+1} dx \int_0^b y^n dy \int_0^c u^r du K \left(\sqrt{x^2 + y^2 + u^2} \right) \quad (44)$$

can be expressed in terms of the U_{pq} integrals and the previously calculated flux integrals $\hat{I}F_{14,mnr}$.

Similar calculations are performed for all the other couples of faces of the V cell. The symmetry of the cell (for instance, in the case V is a prism with a square base) can also be exploited, in particular by means of the circulant properties of the \mathbf{M}^\pm matrices.

By this way, our "all boundary" program is completed. No subdivision of the V cell into subcells appears to be necessary, at least for the problems that are considered

in the reactor field. The interior fluxes never come into play, with the exception of the average fluxes over the whole cell volume, which are required in order to evaluate the local reactor power and are elementarily derived from the balance condition between the absorption-production events inside the cell and the currents at its boundary. If the case, however, further analytical calculations, analogous to the above concerning the surface integrals, allow to determine the fluxes $\phi_g(\mathbf{r})$ inside V , both pointwise or by means of a polynomial in the xyz variables.

It is to be noted, finally, that the cases of V cells with the shape of a hexagonal or a triangular base can be treated essentially in the same way as the above.

5 The second level of the calculation

We now give some details about the second level of the calculation. If the reactor is divided into N homogeneous cells we can write

$$\mathbf{J}^+ = \mathbf{Z}(k)\mathbf{J}^-, \quad (45)$$

where the dependence on the eigenvalue k is now explicitly mentioned and the vectors \mathbf{J}^+ and \mathbf{J}^- are made of N blocks, which correspond to the outward and inward partial currents from each cell. The matrix $\mathbf{Z}(k)$ is therefore a block ($N \times N$) diagonal matrix where each block corresponds to a cell response matrix \mathbf{R} . Defining a suitable coupling matrix $\mathbf{\Pi}$ it is possible to write the partial currents entering each cell in terms of the partial currents leaving the neighbouring ones:

$$\mathbf{J}^- = \mathbf{\Pi}\mathbf{J}^+. \quad (46)$$

A few words are needed concerning the boundary conditions. The global physical system is always assumed to be surrounded by the vacuum or, equivalently, by a purely absorbing material of an infinite extent. Thus the typical condition to be imposed at the boundary is that the inward partial currents of the exposed faces of the peripheral cells are all vanishing.

Combining now equations 45 and 46, we get

$$\mathbf{J}^+ = \mathbf{Z}(k)\mathbf{\Pi}\mathbf{J}^+ = \mathbf{\Theta}(k)\mathbf{J}^+. \quad (47)$$

This homogeneous system admits a non trivial solution only for specific values of the multiplication constant k . The following procedure can be devised in order to determine, in particular, the minimum value of k , which corresponds to the multiplication constant. Let us consider the following auxiliary eigenvalue problem

$$\alpha\mathbf{J}^+ = \mathbf{\Theta}(k)\mathbf{J}^+. \quad (48)$$

We must look for the value of k that gives an α -eigenvalue equal to unity (Maiani and Montagnini, 1999, 2004). This means that the J^+ 's must be invariant under the transformation given by Eq. 48. Thus, an iterative procedure (actually the classical power method) can be exploited to determine the α -eigenvalue for a fixed value of k :

$${}^{(n+1)}\mathbf{J}^+ = \Theta(k) {}^{(n)}\mathbf{J}^+ \quad (49)$$

$${}^{(n+1)}\alpha = \left\{ \frac{\langle {}^{(n+1)}\mathbf{J}^+, {}^{(n+1)}\mathbf{J}^+ \rangle}{\langle {}^{(n)}\mathbf{J}^+, {}^{(n)}\mathbf{J}^+ \rangle} \right\}^{\frac{1}{2}}, \quad (50)$$

where Eq. 49 is iterated until a suitable convergence on the estimated value of ${}^{(n+1)}\alpha$ is achieved. As $\alpha(k)$ turns out to be a monotonic function of k (Maiani and Montagnini, 1999), the new value of k can be estimated e.g. by means of the Newton's chord method. The process is stopped when a suitable convergence on the value of the multiplication constant k is obtained.

To accelerate the convergence of the above procedure a multi-step approach was chosen: in the first step only the first moment of the partial current Legendre expansion is considered; once the convergence is achieved the procedure is then repeated considering the first two moments of the Legendre expansions and so on up to the maximum number of moments used (e.g. five). It was found that such an approach was able to cut down the computational time by a factor 20 with respect to a direct use, from the beginning of the calculation, of the maximum number of the available Legendre moments.

Finally, once the convergence over the multiplication constant k has been achieved, in order to obtain also an accurate eigenvector \mathbf{J}^+ it is necessary to perform some extra iterations according to Eq. 49, written now in the form $\hat{\Theta}\mathbf{J}^+ = 0$, where $\hat{\Theta} = \mathbf{I} - \Theta(k)$. To this purpose, instead of the power method, which may result quite lengthy, an algorithm based on a Krylov subspace projection method like the Generalized Minimal RESidual algorithm (GMRES) (Saad and Schultz, 1986) has been adopted.

Remark. The parameter k is usually introduced as the multiplication ratio of the neutrons, i.e. as the ratio between the total number of neutrons of the $(n+1)$ -th generation and the total number of those of the n -th generation. If e.g. $k > 1$ the neutron population would grow up and to get a (formally) stationary solution the factor $1/k$ is just put beforehand the fission cross sections $\Sigma_{f,g}$. k plays therefore the rôle of an eigenvalue (we are considering, more precisely, the fundamental eigenvalue, the other eigenvalues being associated to the higher order harmonics of the neutron distribution). The true steady state of the reactor is obtained when $k = 1$, which requires an adjustment of the physical constants, typically by moving

the control rods (this implies further calculations that are outside the purpose of this paper).

6 The neutron transport equation

The linear Boltzmann equation (or transport equation), here again written already in an energy discretized form, is as follows:

$$\begin{aligned} \boldsymbol{\Omega} \cdot \nabla_{\mathbf{r}} \phi_g(\mathbf{r}, \boldsymbol{\Omega}) + \Sigma_{t,g}(\mathbf{r}) \phi_g(\mathbf{r}, \boldsymbol{\Omega}) - \sum_{g'=1}^G \int \left[\Sigma_{s,gg'}(\mathbf{r}, \boldsymbol{\Omega}, \boldsymbol{\Omega}') \right. \\ \left. + \frac{\chi_g}{4\pi k} \nu_{g'} \Sigma_{f,g'}(\mathbf{r}) \right] \phi_{g'}(\mathbf{r}, \boldsymbol{\Omega}') d\boldsymbol{\Omega}' = 0 \quad (g = 1, \dots, G), \end{aligned} \quad (51)$$

where $\Sigma_{s,gg'}(\mathbf{r}, \boldsymbol{\Omega}, \boldsymbol{\Omega}')$ is the differential scattering cross section, which describes the change of the direction of motion of a neutron from $\boldsymbol{\Omega}'$ to $\boldsymbol{\Omega}$, due to a scattering collision, and the other symbols are already known. The capital improvement obtained by solving this equation, as compared with the much less accurate diffusion approach, is due to the intervention, in the definition of the ϕ_g fluxes, of the supplementary angular variable $\boldsymbol{\Omega}$, representing the direction of the particle beams in which the neutron field can be subdivided, indeed an important deepening of the description of the physical process.

The variable $\boldsymbol{\Omega}$ can be discretized or, in a more elegant form, the *angular fluxes* $\phi_g(\mathbf{r}, \boldsymbol{\Omega})$ can be expanded in terms of spherical harmonics $Y_{lm}(\boldsymbol{\Omega})$ (or $Y_{lm}(\theta, \varphi)$, with the usual notation), as well as the kernels $\Sigma_{s,gg'}(\mathbf{r}, \boldsymbol{\Omega}, \boldsymbol{\Omega}')$.

For plane-parallel problems (\mathbf{r} is then simply replaced by z , say) the spherical harmonics reduce to Legendre polynomials and it is not difficult to show that the system so obtained has the form of a system of (ordinary) linear differential equations of the first order or also, after suitable manipulations, of the second order.

In the general 3D case, even for a moderate value of the order N of the approximation, the differential spherical harmonics equation system turns out to be overwhelming. A successful, although rude, idea in order to simplify the matter is to ignore the dependence on the azimuthal angle φ . Then it is again possible to arrive at a system of 3D diffusion equations (Gelbard, 1960; Larsen, Morel, and McGhee, 1996; McClarren, 2011), to which BEM can still be applied (Chiba, 2011; Giusti and Montagnini, 2012; Giusti, Montagnini, and Ravetto, 2013). Some further details are given in the Appendix, together with a few topics of neutron transport.

The examples in the next section illustrate the improvement obtainable by the above simplified spherical harmonics method with respect to the diffusion method.

7 Numerical examples

The first numerical example is a transport version prepared by Hébert (Hébert, 2010) of the classical IAEA 3D benchmark problem of the Argonne Code Center ANL-7416 (1977) (see Fig. 2). As stated by the author, the original cross section data have been converted in order to allow transport-like calculations consistent with the diffusion theory results. The IAEA 3D benchmark concerns a full 3D simplified version of a typical LWR core, where nine assemblies have fully inserted control rods while four assemblies have partially inserted control rods. The active part of the reactor core is made of 17 layers, 20 cm high. The four control rods partially inserted are dipped from the top of the active core by 80 cm. Finally, a reflector layer, 20 cm high, is present at the top and the bottom of the reactor core. A vacuum boundary condition is adopted on the external surface of the lateral and axial reflector. The values of the multiplication constant obtained with the diffusion and SP3 (Simplified spherical harmonics with order $N=3$) approximations through the Boundary Element - Response Matrix (BERM) method are compared in Tab. 1 with the reference value obtained by a suitable two energy group MCNP Monte Carlo calculation (Pelowitz D.B. (Ed.), 2013).

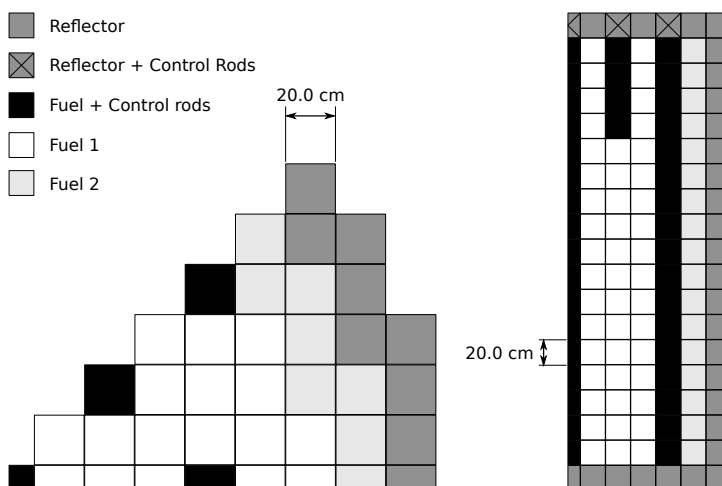


Figure 2: Geometrical configuration and material composition of the IAEA 3D benchmark problem.

The second example, which is much more demanding, is derived from a benchmark problem (Smith, Lewis, and Na, 2005) concerning the calculation of a 3D reactor core made of 16 fuel assemblies (quarter core simmetry), half of which contain

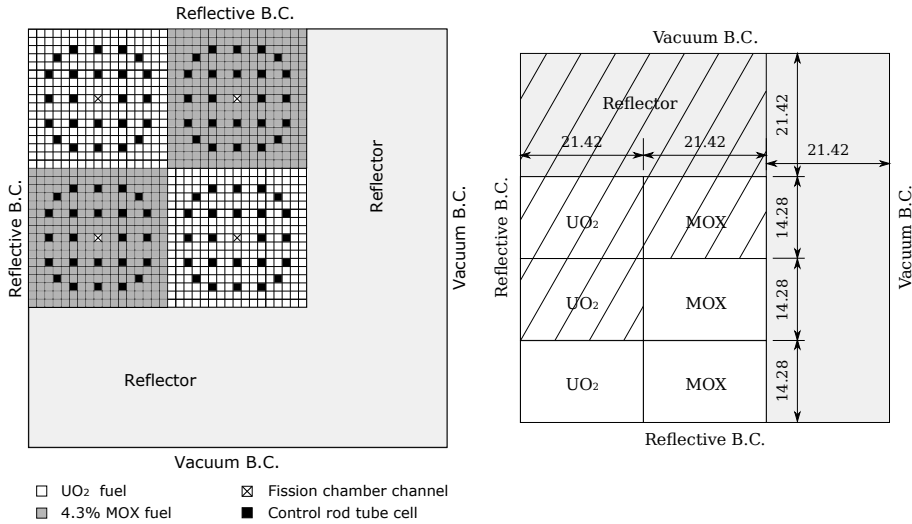


Figure 3: Horizontal (left) and vertical (right) sections of the 3D MOX reactor core (dimensions are in cm). In the present configuration the control rods are crossing the upper reflector and inserted by 2/3 of the way into the inner UO₂ fuel assembly and 1/3 of the way into the two MOX fuel assemblies (hatched region).

mixed-oxide (MOX) fuel rods, and completely surrounded by a water reflector (see Fig. 3). In the present case the number of mixed oxide mixtures has been reduced from three to one. Each fuel assembly is made of 17x17 square pin cells the side length of which is 1.26 cm. In this application, each pin cell has been spatially homogenized weighting the cross section over the volumes, with a preliminary estimate of the neutron flux within each cell. The sets of cross sections so obtained are reported in Giusti and Montagnini (2012, Appendix B). There are control rods inserted 2/3 of the way into the inner UO₂ assembly and 1/3 of the way into both MOX assemblies, as indicated by the hatched region in Fig. 3. Finally, a vacuum boundary condition is applied on the external surface of the reflector and, in order to reduce the computational burden, an axial symmetry is also assumed.

In order to define the reference multiplication constant, again a suitable MCNP Monte Carlo calculation was run making use of the same sets of cross sections used by the deterministic code.

Tab. 2 compares the reference value of the multiplication constant with those obtained by two BERM calculations in the SP3 and SP7 transport approximations (i.e. Simplified Spherical Harmonics with order $N=3$ and $N=7$, respectively). No

Table 1: The multiplication constant k for the transport version of the IAEA 3D benchmark.

Code	k	Δk (pcm)
MCNP6 ^a (ref.)	1.02955	–
BERM-diffusion	1.02907	-48
BERM-SP3	1.02956	1

^awith an estimated standard deviation of ± 0.00002 .

Table 2: The multiplication constant k for the 3D MOX reactor core.

Code	k	Δk (pcm)
MCNP6 ^a (ref.)	1.05932	–
BERM-SP3	1.05755	-177
BERM-SP7	1.05838	-94

^awith an estimated standard deviation of ± 0.00004 .

results obtained with the diffusion approximation are shown for this example because, due to the too small size of the computational cells, they turned out to be rather inaccurate, as expected.

8 Conclusion

The paper presents a review of some applications of BEM to neutron diffusion and transport. The lack of space has forced the authors to give particular emphasis to their own methodology. Some efforts have been made, however, to add some general rudiments about diffusion and the P_N and SP_N methods (see the Appendix). The global problem i.e. the calculation of the neutron population in a multiregion reactor core, which is made by an array of a large number of fuel cells, is divided into two steps, or levels. The first level deals with a single cell, assumed to be physically homogeneous and with a rather simple shape, the second level considers the interactions of all the cells and is directed to obtain the local and global distribution of the neutron flux and the value of the multiplication constant, k .

A main part of the paper is dedicated to the solution of the first level problem in the framework of diffusion theory, actually the simplest approach. The adopted BEM procedure in order to evaluate the cell response to an inward flux of neutrons from the neighbouring cells is a rather classical one, except for the presentation

of the boundary integral equations in terms of inward-outward partial currents. A great advantage is taken from the simple geometry of each cell, which allows to apply a moment approach, with an almost completely analytical evaluation of the fourfold boundary integrals that express the interactions between any two faces. The second level of calculation is then started. It involves very large matrices in order to connect the cells, but efficient acceleration procedures, based on increasing progressively the degree of the involved boundary polynomials (the lowest order calculations being used as precalculations of the highest) and the use of the GMRES algorithm have alleviated very much the calculational bargain.

The method based on diffusion theory has been then extended in order to comply with the Simplified Spherical Harmonics procedure.

The numerical results show that the present BERM method is very accurate and represents a good alternative to the usual Finite Element methods.

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Appendix A: An introduction to some topics of neutron transport

The linear integrodifferential neutron transport equations (Eq. 51 in the text) is here rewritten under some simplifying assumptions that do not imply any essential restriction. Only one energy group is considered ($G = 1$) and the scattering is assumed to be isotropic ($\Sigma_s(\mathbf{r}, \boldsymbol{\Omega}, \boldsymbol{\Omega}') = (1/4\pi)\Sigma_s(\mathbf{r})$). Setting $\Sigma_{sf}(\mathbf{r}) = \Sigma_s(\mathbf{r}) + (\chi/k)v\Sigma_f(\mathbf{r})$, Eq. 51 becomes

$$\boldsymbol{\Omega} \cdot \nabla_{\mathbf{r}}\phi(\mathbf{r}, \boldsymbol{\Omega}) + \Sigma_t(\mathbf{r})\phi(\mathbf{r}, \boldsymbol{\Omega}) = \frac{1}{4\pi}\Sigma_{sf}(\mathbf{r}) \int_{4\pi} \phi(\mathbf{r}, \boldsymbol{\Omega}') d\Omega', \tag{52}$$

which can also be written as follows

$$\nabla_{\mathbf{r}} \cdot (\phi(\mathbf{r}, \boldsymbol{\Omega})\boldsymbol{\Omega}) + \Sigma_t(\mathbf{r})\phi(\mathbf{r}, \boldsymbol{\Omega}) = \frac{1}{4\pi}\Sigma_{sf}(\mathbf{r}) \int_{4\pi} \phi(\mathbf{r}, \boldsymbol{\Omega}') d\Omega'. \tag{53}$$

Two simple relations are of fundamental importance. The first is that the integral of the angular flux over the $\boldsymbol{\Omega}$ directions is the ordinary flux, here denoted by $\Phi(\mathbf{r})$:

$$\Phi(\mathbf{r}) = \int_{4\pi} \phi(\mathbf{r}, \boldsymbol{\Omega}) d\Omega. \tag{54}$$

The second is concerning the so-called *current vector*, namely,

$$\mathbf{J}(\mathbf{r}) = \int_{4\pi} \phi(\mathbf{r}, \boldsymbol{\Omega})\boldsymbol{\Omega} d\Omega. \tag{55}$$

The meaning of the latter quantity is immediate, if we look for e.g. the z -component

$$J_z(\mathbf{r}) = \int_{4\pi} \phi(\mathbf{r}, \boldsymbol{\Omega}) \Omega_z d\Omega = \int_0^{2\pi} d\varphi \int_0^\pi \phi(\mathbf{r}, \theta, \varphi) \cos \theta \sin \theta d\theta, \quad (56)$$

which represents the net number of the particles crossing a plane orthogonal to the z -axis per unit area (in the reactor language, the *net normal current*). If we integrate only over the $\boldsymbol{\Omega}$'s for which $\boldsymbol{\Omega} \cdot \mathbf{k} = \cos \theta > 0$, where \mathbf{k} is the unit vector specifying the direction of the z -axis, we obtain the partial current $J_z^+(\mathbf{r})$, already encountered in Sect. 3. Now let us try to work only with the quantities $\Phi(\mathbf{r})$ and $\mathbf{J}(\mathbf{r})$, with the purpose of avoiding, as much as possible, the use of the highly refined angular flux. A first result is obtained by integrating Eq. 53 over the $\boldsymbol{\Omega}$ directions. By virtue of Eq. 54 and Eq. 55 we get

$$\nabla_{\mathbf{r}} \cdot \mathbf{J}(\mathbf{r}) + [\Sigma_t(\mathbf{r}) - \Sigma_{sf}(\mathbf{r})] \Phi(\mathbf{r}) = 0, \quad (57)$$

actually the equation of continuity.

Another equation can be obtained, but only at the price of an important approximation on the gradient term, namely that the angular flux is practically isotropic: $\phi(\mathbf{r}, \boldsymbol{\Omega}) \simeq (1/4\pi) \Phi(\mathbf{r})$. By multiplying Eq. 52 by $\boldsymbol{\Omega}$ and again integrating on the directions (for simplicity we consider the single Ω_z component) we have, using Eq. 56,

$$\begin{aligned} \frac{1}{4\pi} \left(\frac{\partial}{\partial x} \Phi(\mathbf{r}) \int_{4\pi} \Omega_x \Omega_z d\Omega + \frac{\partial}{\partial y} \Phi(\mathbf{r}) \int_{4\pi} \Omega_y \Omega_z d\Omega + \frac{\partial}{\partial z} \Phi(\mathbf{r}) \int_{4\pi} \Omega_z^2 d\Omega \right) \\ + \Sigma_t(\mathbf{r}) J_z(\mathbf{r}) = \frac{1}{4\pi} \Sigma_{sf}(\mathbf{r}) \Phi(\mathbf{r}) \int_{4\pi} \Omega_z d\Omega. \end{aligned} \quad (58)$$

Obviously, $\int_{4\pi} \Omega_z d\Omega = 0$ and $\int_{4\pi} \Omega_z^2 d\Omega = \int_{4\pi} \cos^2 \theta \sin \theta d\theta d\varphi = (4\pi/3)$, while the integrals involving the products $\Omega_x \Omega_z$ and $\Omega_y \Omega_z$ are all vanishing. Then we remain with $(1/3) \partial \Phi / \partial z + \Sigma_t J_z(\mathbf{r}) = 0$, i.e.

$$J_z(\mathbf{r}) = -\frac{1}{3\Sigma_t} \frac{\partial}{\partial z} \Phi(\mathbf{r}) \quad (59)$$

and, considering all the components,

$$\mathbf{J}(\mathbf{r}) = -\frac{1}{3\Sigma_t} \nabla_{\mathbf{r}} \Phi(\mathbf{r}), \quad (60)$$

which is the Fick's law. Note that we have obtained also a prescription for the value of the diffusion coefficient, i.e. $D = (1/3\Sigma_t)$. Substitution of Eq. 60 into Eq. 57

leads to the diffusion equation, in which the neutron source is represented by the fission term included in $\Sigma_{sf}\Phi$

$$\nabla_{\mathbf{r}} \cdot D\nabla_{\mathbf{r}}\Phi(\mathbf{r}) - [\Sigma_t(\mathbf{r}) - \Sigma_{sf}(\mathbf{r})]\Phi(\mathbf{r}) = 0. \tag{61}$$

It can be seen that the last results can be obtained, in a more systematic way, by expanding $\phi(\mathbf{r}, \mathbf{\Omega})$ in spherical harmonics (see for instance Weinberg and Wigner (1958)) truncated after the second term. The expansion can be performed, however, up to an order N as high as we want, thus leading, in the limit, to exact solution of the transport equation. The problem is that the system of differential equations so obtained becomes rapidly so cumbersome as to be almost intractable, although a considerable progress has been made since the early days (Fletcher, 1983; Capilla, Talavera, Ginestar, and Verdú, 2012).

For plane-parallel problems, however, the situation is different. The \mathbf{r} variable is then replaced by the z -variable (say) and the angular flux is only dependent on z and the angle θ the unit vector $\mathbf{\Omega}$ makes with the z -axis or, equivalently, on $\mu = \cos \theta = \Omega_z$. The transport equation takes the following form:

$$\mu \frac{\partial}{\partial z} \phi(z, \mu) + \Sigma_t(z) \phi(z, \mu) = \frac{1}{2} \Sigma_{sf}(z) \int_{-1}^1 \phi(z, \mu') d\mu', \tag{62}$$

where the unknowns $\phi(z, \mu)$ now represents, more precisely, the original angular flux integrated on the azimuthal angle ϕ , which simply results in a multiplying factor 2π .

$\phi(z, \mu)$ can now be expanded in a much less demanding series of Legendre polynomials:

$$\phi(z, \mu) = \sum_{l=0}^{\infty} \frac{2l+1}{2} \phi_l(z) P_l(\mu), \tag{63}$$

with

$$\phi_l(z) = \int_{-1}^1 \phi(z, \mu) P_l(\mu) d\mu. \tag{64}$$

In particular,

$$\phi_0(z) = \int_{-1}^1 \phi(z, \mu) P_0(\mu) d\mu = \int_{-1}^1 \phi(z, \mu) d\mu = \Phi(z) \tag{65}$$

$$\begin{aligned} \phi_1(z) &= \int_{-1}^1 \phi(z, \mu) P_1(\mu) d\mu = \int_{-1}^1 \phi(z, \mu) \mu d\mu \\ &= \int_{-1}^1 \phi(z, \mu) \Omega_z d\mu = J_z(z) \equiv J(z), \end{aligned} \tag{66}$$

as expected (the suffix z in J_z has been suppressed). We now substitute the expansion in Eq. 62 and, making use of the recurrence formula for the Legendre polynomials, we replace the $\mu P_l(\mu)$ factor occurring in the term containing the derivative $d\phi_l/dz$ by a linear combination of $P_{l+1}(\mu)$ and $P_{l-1}(\mu)$:

$$\mu P_l(\mu) = \frac{l+1}{2l+1} P_{l+1}(\mu) + \frac{l}{2l+1} P_{l-1}(\mu). \tag{67}$$

The whole equation is then multiplied by $P_n(\mu)$ and integrated on $[-1, 1]$. Using the orthogonality of the polynomials, the following infinite system of first order linear differential equation is obtained:

$$\frac{n}{2n+1} \frac{d}{dz} \phi_{n-1} + \frac{n+1}{2n+1} \frac{d}{dz} \phi_{n+1} + \Sigma_t(z) \phi_n = \Sigma_{sf}(z) \phi_0 \delta_{0n} \quad (n = 0, 1, 2, \dots) \tag{68}$$

where δ_{0n} is the Kronecker delta.

To solve this system it is obviously necessary to replace the infinite series, Eq. 63, by a finite sum, retaining only the terms up to $l = N$, say, which corresponds to the so called P_N approximation. The derivative $d\phi_{N+1}/dz$ in Eq. 68 is also set equal to zero and the infinite recurrence implied in the system is therefore stopped. The first two levels of approximation are here of interest.

P₁ approximation. For $N = 1$ we have

$$\phi(z, \mu) = \frac{1}{2} \phi_0(z) + \frac{3}{2} \phi_1(z) \mu \tag{69}$$

and the differential equations are

$$\frac{d}{dz} \phi_1(z) + \Sigma_t(z) \phi_0(z) = \Sigma_{sf}(z) \phi_0(z) \tag{70}$$

$$\frac{1}{3} \frac{d}{dz} \phi_0(z) + \Sigma_t(z) \phi_1(z) = 0, \tag{71}$$

while ϕ_2 and $d\phi_2/dz$ are suppressed. By substitution, one obtains the one-dimensional diffusion equation

$$\frac{d}{dz} \left(D(z) \frac{d}{dz} \Phi(z) \right) + [\Sigma_t(z) - \Sigma_{sf}(z)] \Phi(z) = 0, \tag{72}$$

with $D = 1/3\Sigma_t$. Another result follows from a direct application of Eq. 69 to Eq. 56. We have, with obvious, slightly modified symbols,

$$\begin{aligned} J^+ &= \int_0^1 \phi(z, \mu) \mu \, d\mu = \int_0^1 \left[\frac{1}{2} \phi_0(z) + \frac{3}{2} \phi_1(z) \mu \right] \mu \, d\mu \\ &= \frac{1}{4} \phi_0(z) + \frac{1}{2} \phi_1(z) = \frac{1}{4} \Phi(z) - \frac{D}{2} \frac{d}{dz} \Phi(z) \end{aligned} \tag{73}$$

($\phi_1 = J$ is derived from Eq. 71), a result that has been used in Sect. 3 for the partial currents.

P₃ approximation. The differential equations are:

$$\begin{aligned} \frac{d\phi_1}{dz} + (\Sigma_t - \Sigma_{sf}) \phi_0 &= 0 \\ \frac{1}{3} \frac{d\phi_0}{dz} + \frac{2}{3} \frac{d\phi_2}{dz} + \Sigma_t \phi_1 &= 0 \\ \frac{2}{5} \frac{d\phi_1}{dz} + \frac{3}{5} \frac{d\phi_3}{dz} + \Sigma_t \phi_2 &= 0 \\ \frac{3}{7} \frac{d\phi_2}{dz} + \Sigma_t \phi_3 &= 0. \end{aligned} \tag{74}$$

Next, we set $\tilde{\phi}_0 = \phi_0 + 2\phi_2$, $\tilde{\phi}_2 = \phi_2$, while the remaining unknowns ϕ_1 and ϕ_3 remain as they stand. The equations become

$$\begin{aligned} \frac{d\phi_1}{dz} + (\Sigma_t - \Sigma_{sf}) \tilde{\phi}_0 &= 2(\Sigma_t - \Sigma_{sf}) \tilde{\phi}_2 \\ \frac{1}{3} \frac{d\tilde{\phi}_0}{dz} + \Sigma_t \phi_1 &= 0 \\ \frac{2}{5} \frac{d\phi_1}{dz} + \frac{3}{5} \frac{d\phi_3}{dz} + \Sigma_t \tilde{\phi}_2 &= 0 \\ \frac{3}{7} \frac{d\tilde{\phi}_2}{dz} + \Sigma_t \phi_3 &= 0. \end{aligned} \tag{75}$$

From the second and fourth equations we get

$$\phi_1 = -\frac{1}{3\Sigma_t} \frac{d\tilde{\phi}_0}{dz} \tag{76}$$

$$\phi_3 = -\frac{3}{7\Sigma_t} \frac{d\tilde{\phi}_2}{dz}. \tag{77}$$

Substituting into the first and third equations we readily obtain a couple of diffusion-like differential equations in terms of $\tilde{\phi}_0$ and $\tilde{\phi}_2$ only:

$$\begin{aligned} \frac{d}{dz} \left(\frac{1}{3\Sigma_t} \frac{d\tilde{\phi}_0}{dz} \right) - (\Sigma_t - \Sigma_{sf}) \tilde{\phi}_0 + 2(\Sigma_t - \Sigma_{sf}) \tilde{\phi}_2 &= 0 \\ \frac{d}{dz} \left(\frac{9}{35\Sigma_t} \frac{d\tilde{\phi}_2}{dz} \right) - \frac{1}{5} (9\Sigma_t - 4\Sigma_{sf}) \tilde{\phi}_2 + \frac{2}{5} (\Sigma_t - \Sigma_{sf}) \tilde{\phi}_0 &= 0. \end{aligned} \tag{78}$$

The Simplified Spherical Harmonics method (SP_N) consists in using, even for the 2D and 3D problems, the same structure of the P_N equations as for the one-dimensional case, as given by Eqs. 74 to 78, and introducing the following device

(we take for simplicity $N = 3$): the unknowns $\phi_1(z)$ and $\phi_3(z)$ are first transformed into vectors, $\phi_1(\mathbf{r})$ and $\phi_3(\mathbf{r})$, say, (see Eqs. 76 and 77, which have the form of the Fick's law), then the d/dz derivative is replaced by a divergence, if applied to vectors, and by a gradient, if applied to scalars (i.e. to $\tilde{\phi}_0(\mathbf{r})$ and $\tilde{\phi}_2(\mathbf{r})$). It is then easy to extend the above one-dimensional procedure and arrive to the following, diffusion-like, SP_3 equations

$$\nabla \cdot (\tilde{D}_0 \nabla \tilde{\phi}_0) - (\Sigma_t - \Sigma_{sf}) \tilde{\phi}_0 + 2(\Sigma_t - \Sigma_{sf}) \tilde{\phi}_2 = 0 \quad (79)$$

$$\nabla \cdot (\tilde{D}_2 \nabla \tilde{\phi}_2) - \frac{1}{5}(9\Sigma_t - 4\Sigma_{sf}) \tilde{\phi}_2 + \frac{2}{5}(\Sigma_t - \Sigma_{sf}) \tilde{\phi}_0 = 0, \quad (80)$$

with $\tilde{D}_0 = 1/3\Sigma_t$, $\tilde{D}_2 = 9/35\Sigma_t$. This audacious trick, due to Gelbard (1960), got a great success. As a method half-way between diffusion and transport, is going to become the up-to-date technique for the calculation of reactor cores or large regions of them. However, SP_N is intrinsically approximate and, differently from P_N , the error of the SP_N solution does not tend to zero as $N \rightarrow \infty$.

