Solution of 3D multigroup, linearly anisotropic scattering, criticality problems by the A_N Boundary-Element Response-Matrix method☆

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Abstract

A short summary devoted to the origin and the development of the A_N method, as well as its relationship with the simplified spherical harmonics (SP_N), is given. Attempts have been made to derive the A_N partial differential equations and the related interface and boundary conditions as much as possible from first principles. The theory developed in previous works is extended to many energy groups and includes a rigorous treatment of the linearly anisotropic scattering. It is shown that also in this extended framework the A_N differential equations can be transformed into a set of boundary integral equations that can be given a partial current form. This allows for a natural application of the response matrix method, a technique that is particularly suitable for application to large multiregion systems. The calculation procedures have been implemented into a computer code (BERM-AN). Solutions of a 2D and 3D cartesian coordinates multigroup criticality problems, with different A_N approximations, are compared with those obtained by well assessed reference codes such as DORT, TORT and MCNP.

Keywords: Simplified spherical harmonics, Boundary Element Method, 3D multigroup criticality problems, Linearly anisotropic scattering

1. Introduction

The A_N method was proposed in a paper by Coppa and Ravetto (1982) with the purpose of obtaining accurate solutions of one-velocity problems in homogeneous, convex bodies surrounded by a vacuum or a perfectly absorbing medium. It was based on approximating the kernel of the integral transport equation by a sum of diffusion-type kernels, a long lasting idea of neutron physics (see e.g. Stewart and Zweifel (1958)), which was exploited in the above paper not only in order to replace the integral Peierls equation by an equation system analogous to the usual multigroup diffusion systems (with up-scattering), but also to work out void boundary conditions that could take into account the curvature and, possibly, the existence of singular points (edges and vertices) of the boundary surface. This resulted into a non-local boundary condition that is strictly connected with the boundary integral equation technique for solving the diffusion-like A_N equation themselves. A different derivation based on the even-parity of the S_N equations, is also sketched in the same paper. The A_N equations, which were first developed under the assumption of isotropic scattering, were then extended to the linearly anisotropic scattering, starting from the correspondingly extended integral transport equations (Coppa et al., 1983). It was also shown that, for a homogeneous finite body, the A_N solution converges to the exact transport solution as the order N tends to infinity. This result was completed by the proof that, under the above condition, the A_N method is equivalent to the odd-order spherical harmonics method

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P_{2N-1}, (Coppa et al., 1982). At the same time it was realized that, in order that the equivalence statement may hold, only the total cross section is required to be constant, while the absorption cross section may be arbitrarily varying over the system.

The necessity of giving a full account of the A_N theory and its connection with the boundary integral equation method became then evident and this task was accomplished in Ciolini et al. (2002) (see also Colombo et al. (1988)). In this paper (as well as in further papers) the problems for which the total cross section is constant are shortly called "constant sigma", or "Cσ" problems. The class of the Cσ problems, although very restricted, is highly privileged and, from a practical point of view, the solutions obtained by the A_N method for the non-Cσ problems were always found to be less accurate. All such previous studies were performed in a complete independence of the SP_N theory. The merging of the A_N and SP_{2N-1} methods came just with the last paper, where it was recognized that, at least in the case of the isotropic scattering, the A_N equations are a diagonalized form of the SP_{2N-1} equations. The proof is general and does not require any restriction as regards the space dependence of the cross sections (including the total cross section). As a consequence, for the Cσ problems with isotropic scattering not only the A_N, but also the SP_{2N-1} method is equivalent to the P_{2N-1} method (a direct equivalence proof can be also found in Ciolini et al. (2002)). On the contrary, for the general class of the non-Cσ problems a recourse to Gelbard's *ad hoc* assumptions (Gelbard, 1960, 1961, 1962) appears to be unavoidable.

However, although the asymptotic analysis by Larsen et al. (1993, 1996), Larsen (2011) and by Pomraning (1993) has now provided a firm basis for the SP_N theory, attempts to introduce procedures that are free from some of the severe limitations there involved, not only as regards the absorption cross section, but even as regards the assumption of a nearly uniform total cross section, have been pursued in the past (Spinrad and Altaç, 1990), and also at present (Coppa et al., 2011). Such attempts are, however, outside the domain of interest of this paper.

The present paper contains the recent developments of the A_N method. It has been preceded by a preliminary short publication (Giusti et al., 2010) in the $N = 2$ case and by another paper (Giusti and Montagnini, 2012) in which the boundary element-response matrix (BERM) technique is applied to the classical SP_3 equations. It should be observed that the genuine A_N equations can now be presented as a particular case of the "canonical SP_N" equations (Larsen et al., 1993, 1996) which have been derived in a form that allows for a scattering of an arbitrarily high order of anisotropy (thus, instead of A_N or A_N-SP_{2N-1}, as in past works, one could say "canonical SP_N"). However, owing to its strong relationship with the BEM approach, the A_N method has some specific features and a more appropriate name should be perhaps "A_N boundary-element response-matrix method". In the rest of the paper we shall use the name A_N, without further specifications, only for brevity.

Sect. 2 aims at extending previous works on the A_N method to many energy groups and a linearly anisotropic scattering, here dealt with in a completely rigorous way (the previous multigroup treatment in Giusti and Montagnini (2012) is only approximate, being based on the assumption of a balance between the (anisotropic) down and up scattering events, (Bell and Glasstone, 1970; Beckert and Grundmann, 2008)). The present rigorous treatment leads to a non negligible improvement of the accuracy (sect. 5). The continuity conditions accompanying the A_N partial differential equations are also discussed in this section. The A_N boundary integral equations (BIE's) are obtained, in their classical form, in sect. 3, while sect. 4 deals with the transformation of the previous boundary integral equations into a partial current form that is particularly suitable for the response matrix technique. This section deals also with the boundary conditions to be used in such a context and points out one important choice of the method, namely that only interface conditions are considered, the no-entry conditions being treated as interface conditions with a perfectly absorbing medium. Sect. 5 reports a 2D and 3D numerical example. Although the theory is general and includes therefore the problems in which an external source is present, the numerical applications have been worked out only for criticality problems. Conclusions are drawn in sect. 6.

2. The multigroup A_N differential equations for linearly anisotropic scattering and their interface conditions.

The derivation of the A_N differential equations as developed by Coppa and Ravetto (1982) and Ciolini et al. (2002) according to a discrete ordinate arguments is here extended to multigroup problems, in which the scattering is linearly anisotropic. As anticipated in the Introduction, the treatment of the scattering does not involve any simplifying assumptions.

The integrodifferential transport equation in plane geometry, with the assumption of a linearly anisotropic scattering and isotropic sources, is, for G energy groups, as follows

$$\mu \frac{\partial \varphi_g}{\partial x}(x,\mu) + \sigma_g(x)\,\varphi_g(x,\mu) = q_g(x,\mu) \quad (g = 1,\ldots,G), \tag{1}$$

with standard notations. Namely, $\varphi_g(x,\mu)$ is the g-group angular flux, $\sigma_g(x)$ the g-group macroscopic total cross section, while

$$q_g(x,\mu) = \sum_{g'=1}^{G} \int_{-1}^{1} \left[\frac{1}{2}\sigma_{0gg'}(x) + \frac{3}{2}\mu\mu'\sigma_{1gg'}(x)\right]\varphi_{g'}(x,\mu')\,\mathrm{d}\mu' + \frac{1}{2}s_g(x) \tag{2}$$

is the g-group angular emission density. Here, $\sigma_{0gg'}(x)$ and $\sigma_{1gg'}(x)$ denote the first two Legendre moments of the differential scattering cross section from group g' to group g and $s_g(x)$ the source, which includes the fission source and the (possibly existing) external source $s_g^{ext}(x)$, both terms being assumed to be isotropic:

$$s_g(x) = \frac{1}{k}\chi_g \sum_{g'=1}^{G} \nu\sigma_{fg'}(x) \int_{-1}^{1} \varphi_{g'}(x,\mu')\,\mathrm{d}\mu' + s_g^{ext}(x). \tag{3}$$

Moreover, χ_g denotes the fission-spectrum fraction, $\nu\sigma_{fg}(x)$ the fission cross section times the average number of secondaries and k the multiplication factor.

Let μ_α, w_α be the points and weights of the Gauss-Legendre quadrature formula of order $2N$ on the $[-1,1]$ interval. The discrete ordinate S_{2N} approximation of Eqs. (1) and (2) is as follows

$$\begin{aligned}
&\mu_\alpha \frac{\mathrm{d}\varphi_{+\alpha,g}}{\mathrm{d}x}(x) + \sigma_g(x)\,\varphi_{+\alpha,g}(x) = q_{+\alpha,g}(x)\\
&-\mu_\alpha \frac{\mathrm{d}\varphi_{-\alpha,g}}{\mathrm{d}x}(x) + \sigma_g(x)\,\varphi_{-\alpha,g}(x) = q_{-\alpha,g}(x) \quad (\alpha = 1,\ldots,N; g = 1,\ldots,G),
\end{aligned} \tag{4}$$

the sign $\pm$ in $\varphi_{\pm\alpha,g}$ being chosen according to the direction of the neutron ray with respect to the x-axis. The discrete form of the emission density, Eq. (2), in which the expression of the $s_g(x)$ source is also discretized, is

$$\begin{aligned}
q_{\pm\alpha,g}(x) = {}& \frac{1}{2}\sum_{g'=1}^{G}\sigma_{0gg'}(x)\sum_{\beta=1}^{N} w_\beta\left[\varphi_{+\beta,g'}(x) + \varphi_{-\beta,g'}(x)\right]\\
&\pm \frac{3}{2}\mu_\alpha\sum_{g'=1}^{G}\sigma_{1gg'}(x)\sum_{\beta=1}^{N} w_\beta\mu_\beta\left[\varphi_{+\beta,g'}(x) - \varphi_{-\beta,g'}(x)\right]\\
&+ \frac{1}{2}\frac{\chi_g}{k}\sum_{g'=1}^{G}\nu\sigma_{fg'}(x)\sum_{\beta=1}^{N} w_\beta\left[\varphi_{+\beta,g'}(x) + \varphi_{-\beta,g'}(x)\right] + \frac{1}{2}s_g^{ext}(x).
\end{aligned} \tag{5}$$

Summing and subtracting Eqs. (4) and setting

$$\phi_{\alpha,g}(x) = \varphi_{+\alpha,g}(x) + \varphi_{-\alpha,g}(x),\ j_{\alpha,g}(x) = \varphi_{+\alpha,g}(x) - \varphi_{-\alpha,g}(x), \tag{6}$$

the multigroup even-odd S_{2N} equations are obtained:

$$\begin{aligned}
\mu_\alpha \frac{\mathrm{d}j_{\alpha,g}}{\mathrm{d}x}(x) + \sigma_g(x)\,\phi_{\alpha,g}(x) = {}& \sum_{g'=1}^{G}\left[\sigma_{0gg'}(x) + \frac{\chi_g}{k}\nu\sigma_{fg'}(x)\right]\\
&\cdot \sum_{\beta=1}^{N} w_\beta\phi_{\beta,g'}(x) + s_g^{ext}(x)\\
\mu_\alpha \frac{\mathrm{d}\phi_{\alpha,g}}{\mathrm{d}x}(x) + \sigma_g(x)\,j_{\alpha,g}(x) = {}& 3\mu_\alpha\sum_{g'=1}^{G}\sigma_{1gg'}(x)\sum_{\beta=1}^{N} w_\beta\mu_\beta j_{\beta,g'}(x)\\
&(\alpha = 1,\ldots,N; g = 1,\ldots,G).
\end{aligned} \tag{7}$$

By introducing the further quantities $\Phi_g(x) = \sum_{\beta=1}^{N} w_\beta \phi_{\beta,g}(x)$ and $J_g(x) = \sum_{\beta=1}^{N} w_\beta \mu_\beta j_{\beta,g}(x)$, which are immediately recognized as the angle-integrated flux and current, respectively, the above equations can be written as follows

$$\mu_\alpha \frac{\mathrm{d}j_{\alpha,g}}{\mathrm{d}x}(x) + \sigma_g(x)\phi_{\alpha,g}(x) = \sum_{g'=1}^{G}\left[\sigma_{0gg'}(x) + \frac{\chi_g}{k}\nu\sigma_{fg'}(x)\right]\Phi_{g'}(x) + s_g^{ext}(x)$$

$$\mu_\alpha \frac{\mathrm{d}\phi_{\alpha,g}}{\mathrm{d}x}(x) + \sigma_g(x) j_{\alpha,g}(x) = 3\mu_\alpha \sum_{g'=1}^{G}\sigma_{1gg'}(x) J_{g'}(x) \quad (\alpha = 1,\ldots,N; g = 1,\ldots,G). \tag{8}$$

According to Gelbard's basic postulates of the simplified spherical harmonics method the scalar quantities $j_{\alpha,g}(x)$ are replaced by the vectors $\mathbf{j}_{\alpha,g}(\mathbf{r})$ and the d/dx derivative by the divergence operator, when applied to a vector, and by the gradient operator when applied to a scalar function of the space variable $\mathbf{r}$. Then, Eqs. (8) are replaced by the following ones

$$\mu_\alpha \nabla\cdot\mathbf{j}_{\alpha,g}(\mathbf{r}) + \sigma_g(\mathbf{r})\phi_{\alpha,g}(\mathbf{r}) = \sum_{g'=1}^{G}\left[\sigma_{0gg'}(\mathbf{r}) + \frac{\chi_g}{k}\nu\sigma_{fg'}(\mathbf{r})\right]\Phi_{g'}(\mathbf{r}) + s_g^{ext}(\mathbf{r})$$

$$\mu_\alpha \nabla\phi_{\alpha,g}(\mathbf{r}) + \sigma_g(\mathbf{r})\mathbf{j}_{\alpha,g}(\mathbf{r}) = 3\mu_\alpha \sum_{g'=1}^{G}\sigma_{1gg'}(\mathbf{r})\mathbf{J}_{g'}(\mathbf{r})$$

$$(\alpha = 1,\ldots,N; g = 1,\ldots,G), \tag{9}$$

where

$$\Phi_g(\mathbf{r}) = \sum_{\beta=1}^{N} w_\beta \phi_{\beta,g}(\mathbf{r}), \tag{10}$$

$$\mathbf{J}_g(\mathbf{r}) = \sum_{\beta=1}^{N} w_\beta \mu_\beta \mathbf{j}_{\beta,g}(\mathbf{r}). \tag{11}$$

From the second Eq. (9) we get

$$\mathbf{j}_{\alpha,g}(\mathbf{r}) = -\frac{1}{\sigma_g(\mathbf{r})}\left[\mu_\alpha \nabla\phi_{\alpha,g}(\mathbf{r}) - 3\mu_\alpha \sum_{g'=1}^{G}\sigma_{1gg'}(\mathbf{r})\mathbf{J}_{g'}(\mathbf{r})\right]. \tag{12}$$

Substitution into the first equation then yields

$$\begin{aligned}\nabla\cdot\left[\frac{\mu_\alpha^2}{\sigma_g(\mathbf{r})}\nabla\phi_{\alpha,g}(\mathbf{r})\right] - \sigma_g(\mathbf{r})\phi_{\alpha,g}(\mathbf{r}) + \sum_{g'=1}^{G}\left[\sigma_{0gg'}(\mathbf{r}) + \frac{\chi_g}{k}\nu\sigma_{fg'}(\mathbf{r})\right]\Phi_{g'}(\mathbf{r}) \\ - 3\nabla\cdot\left[\frac{\mu_\alpha^2}{\sigma_g(\mathbf{r})}\sum_{g'=1}^{G}\sigma_{1gg'}(\mathbf{r})\mathbf{J}_{g'}(\mathbf{r})\right] + s_g^{ext}(\mathbf{r}) = 0 \\ (\alpha = 1,\ldots,N; g = 1,\ldots,G).\end{aligned} \tag{13}$$

Using again Eq. (12) and taking account of Eq. (11), other than of the identity $\sum_{\beta=1}^{N} w_\beta \mu_\beta^2 = 1/3$, it is readily shown that

$$\mathbf{J}_g(\mathbf{r}) - \frac{1}{\sigma_g(\mathbf{r})}\sum_{g'=1}^{G}\sigma_{1gg'}(\mathbf{r})\mathbf{J}_{g'}(\mathbf{r}) = -\frac{1}{\sigma_g(\mathbf{r})}\sum_{\beta=1}^{N} w_\beta \mu_\beta^2 \nabla\phi_{\beta,g}(\mathbf{r}), \tag{14}$$

Eqs. (13) and (14), together with Eq. (10), are the multigroup A_N differential equations for a linearly anisotropic scattering.

An equivalent second order form for the A_N equations is obtained by substituting $\mathbf{J}_g(\mathbf{r})$, as given by Eq. (14), into Eq. (13). Namely, introducing the GxG matrix $\mathbf{E}$ with elements

$$E_{gg'}(\mathbf{r}) = \delta_{gg'} - \frac{\sigma_{1gg'}(\mathbf{r})}{\sigma_g(\mathbf{r})} \tag{15}$$

and the inverse matrix $\mathbf{F} = \mathbf{E}^{-1}$, with elements $F_{gg'}(\mathbf{r})$, we get

$$\mathbf{J}_g(\mathbf{r}) = -\sum_{g'=1}^{G} \frac{F_{gg'}(\mathbf{r})}{\sigma_{g'}(\mathbf{r})} \sum_{\beta=1}^{N} w_\beta \mu_\beta^2 \nabla\phi_{\beta,g'}(\mathbf{r}). \tag{16}$$

This allows to write Eqs. (13) as follows

$$\nabla\cdot\left\{\frac{\mu_\alpha^2}{\sigma_g(\mathbf{r})}\left[\nabla\phi_{\alpha,g}(\mathbf{r}) + 3\sum_{g'=1}^{G}\sigma_{1gg'}(\mathbf{r})\sum_{\beta=1}^{N} w_\beta\mu_\beta^2 \sum_{g''=1}^{G}\frac{F_{g'g''}(\mathbf{r})}{\sigma_{g''}(\mathbf{r})}\nabla\phi_{\beta,g''}(\mathbf{r})\right]\right\}$$
$$-\sigma_g(\mathbf{r})\phi_{\alpha,g}(\mathbf{r}) + \sum_{g'=1}^{G}\left[\sigma_{0gg'}(\mathbf{r}) + \frac{\chi_g}{k}\nu\sigma_{fg'}\right]\sum_{\beta=1}^{N} w_\beta\phi_{\beta,g'}(\mathbf{r}) + s_g^{ext}(\mathbf{r}) = 0. \tag{17}$$

Setting

$$H_{gg''}(\mathbf{r}) = 3\sum_{g'=1}^{G}\sigma_{1gg'}\frac{F_{g'g''}(\mathbf{r})}{\sigma_{g''}(\mathbf{r})}, \tag{18}$$

then changing g'' into g' in the elements of the $\mathbf{H}$ matrix so calculated, we obtain

$$\nabla\cdot\left\{\frac{\mu_\alpha^2}{\sigma_g(\mathbf{r})}\left[\nabla\phi_{\alpha,g}(\mathbf{r}) + \sum_{g'=1}^{G}H_{gg'}(\mathbf{r})\sum_{\beta=1}^{N} w_\beta\mu_\beta^2\nabla\phi_{\beta,g'}(\mathbf{r})\right]\right\} - \sigma_g(\mathbf{r})\phi_{\alpha,g}(\mathbf{r})$$
$$+\sum_{g'=1}^{G}\left[\sigma_{0gg'}(\mathbf{r}) + \frac{\chi_g}{k}\nu\sigma_{fg'}(\mathbf{r})\right]\sum_{\beta=1}^{N} w_\beta\phi_{\beta,g'}(\mathbf{r}) + s_g^{ext}(\mathbf{r}) = 0 \tag{19}$$

and, finally,

$$\nabla\cdot\sum_{\beta=1}^{N}\sum_{g'=1}^{G} D_{\alpha\beta,gg'}(\mathbf{r})\nabla\phi_{\beta,g'}(\mathbf{r}) - \sum_{\beta=1}^{N}\sum_{g'=1}^{G}\Sigma_{\alpha\beta,gg'}(\mathbf{r})\phi_{\beta,g'}(\mathbf{r}) + s_g^{ext}(\mathbf{r}) = 0$$
$$(\alpha = 1,\ldots,N; g = 1,\ldots,G), \tag{20}$$

where the following notations have been used:

$$D_{\alpha\beta,gg'}(\mathbf{r}) = \frac{\mu_\alpha^2}{\sigma_g(\mathbf{r})}\left[\delta_{\alpha\beta}\delta_{gg'} + w_\beta\mu_\beta^2 H_{gg'}(\mathbf{r})\right] \tag{21}$$

$$\Sigma_{\alpha\beta,gg'}(\mathbf{r}) = \sigma_g(\mathbf{r})\delta_{\alpha\beta}\delta_{gg'} - w_\beta\left[\sigma_{0gg'}(\mathbf{r}) + \frac{\chi_g}{k}\nu\sigma_{fg'}(\mathbf{r})\right]. \tag{22}$$

(the multiplication factor k in $\Sigma_{\alpha\beta,gg'}$ is understood and, if an external source is present, is set equal to 1).

The compact notation of Eq.(21) allows to introduce the following vectors

$$\hat{\mathbf{J}}_{\alpha,g}(\mathbf{r}) = -\sum_{\beta=1}^{N}\sum_{g'=1}^{G} D_{\alpha\beta,gg'}(\mathbf{r})\,\nabla\phi_{\beta,g'}(\mathbf{r}), \tag{23}$$

which will be of much use in the rest of the paper.

If the system is made of Z homogeneous regions, V^i $(i = 1,\ldots,Z)$, the above coefficients are constant inside each region (so that they can be written $D^i_{\alpha\beta,gg'}$ etc.). Moreover, the indices α, g, β, g' can be unified, according to the scheme $\alpha, g \to \gamma, \beta, g' \to \gamma'$, so that the matrix with the elements $\phi_{\alpha,g}$ is rearranged (by columns) as a vector $[\phi_{1,1},\ldots,\phi_{1,G},\phi_{2,1},\ldots,\phi_{2,G},\ldots,\phi_{N,1},\ldots,\phi_{N,G}]$ or, shortly, a vector with components ϕ_γ with $\gamma = 1,\ldots,NG$. A similar reduction being made for the matrices of the coefficients and the source, the i-th region Eqs. (20) can be written as follows

$$-\sum_{\gamma'=1}^{NG} D^i_{\gamma\gamma'}\nabla^2\phi^i_{\gamma'}(\mathbf{r}) + \sum_{\gamma'=1}^{NG}\Sigma^i_{\gamma\gamma'}\phi^i_{\gamma'}(\mathbf{r}) = s^{ext}_\gamma(\mathbf{r}) \quad (\gamma = 1,\ldots,NG). \tag{24}$$

Eqs. (24) have the formal structure of a system of multigroup diffusion equations with upscattering, in which a tensorial definition of the leakage term has been introduced.

The diffusion-like features of these equations suggest to give the A_N moments some more appealing names. No matter if the single index or the double index notation has been chosen, we may call the ϕ_γ or $\phi_{\alpha,g}$ quantities "A_N fluxes" and the vectors $\hat{\mathbf{J}}_\gamma(\mathbf{r}_S) = \sum_{\gamma'=1}^{NG} D_{\gamma\gamma'}(\mathbf{r})\,\nabla\phi_{\gamma'}(\mathbf{r})$ (or $\hat{\mathbf{J}}_{\alpha,g}(\mathbf{r})$) as expressed by Eq. (23), "A_N current vectors".

It is to be noted that, even if these names derive from a formal similitude, the quantities ϕ_γ $(\phi_{\alpha,g})$ and $\hat{\mathbf{J}}_\gamma$ $(\hat{\mathbf{J}}_{\alpha,g})$ have a direct link with the corresponding basic physical quantities of the method. Namely, Eq. (10) shows that the Legendre-weighted sum of the $\phi_{\alpha,g}$'s gives the (A_N approximated) g-group physical flux $\Phi_g(\mathbf{r})$. As regards the $\hat{\mathbf{J}}_{\alpha,g}(\mathbf{r})$'s, using Eqs. (23) and the definition of $D_{\alpha\beta,gg'}$ it is seen that Eq. (19) coincides with the first of Eqs. (9), so that we can identify $\hat{\mathbf{J}}_{\alpha,g}(\mathbf{r})$ with $\mu_\alpha \mathbf{j}_{\alpha,g}(\mathbf{r})$. Thus, Eq. (11) can be written as follows

$$\mathbf{J}_g(\mathbf{r}) = \sum_{\alpha=1}^{N} w_\alpha \hat{\mathbf{J}}_{\alpha,g}(\mathbf{r}) \tag{25}$$

which means that the Legendre-weighted sum of the $\hat{\mathbf{J}}_{\alpha,g}(\mathbf{r})$'s gives the ($A_N$ approximated) g-group physical current vector $\mathbf{J}_g(\mathbf{r})$. Otherwise stated, the $\hat{\mathbf{J}}_{\alpha,g}(\mathbf{r})$ vectors can be seen as the components of $\mathbf{J}_g(\mathbf{r})$ in an expansion of the latter vectors in terms of the A_N moments. Owing to this relation we are allowed to suppress the hat and simply write $\mathbf{J}_{\alpha,g}(\mathbf{r})$.

Although the γ-indexed quantities allow the calculations to be, in general, quite handy, a better understanding of some aspects of the A_N theory is obtainable if a distinct rôle for the indexes α and g is maintained, as shown by the above argument concerning the α sums and, even more, the problem of continuity of the A_N fluxes and normal currents in presence of a discontinuity of the cross sections.

We take a step backwards. In plane geometry, the S_{2N} angular fluxes $\varphi_{\pm\alpha,g}(x)$, Eq. (4), are absolutely continuous (as integral functions (Royden, 1988; Titchmarsh, 1975)) and therefore continuous, as is, in general transport, the angular flux along the trajectory of the neutrons. As a consequence, the functions $\phi_{\alpha,g}(x)$ and $j_{\alpha,g}(x)$, Eqs. (6), are also continuous and this holds for the Legendre sums that define $\Phi_g(x)$ and $J_g(x)$, too. The three dimensional A_N equations, however, as well as the SP_N equations, cannot be derived from the transport equation in a direct way, if exception is made for the Cσ problems, in which an alternative derivation from the integral transport equation, independent of Gelbard's assumptions, is possible (Coppa and Ravetto (1982), Coppa et al. (1983) and Ciolini et al. (2002)). Therefore, physical intuition is not expected to give more than some heuristic help, when dealing with such properties as the continuity of the A_N (and the SP_N) moments at the interface, S say, between two regions, V^I and V^{II}, which have different total cross sections. However, in the vicinity of a smooth interface the behaviour of each $\phi_{\alpha,g}(\mathbf{r})$ should be essentially dependent on the normal coordinate to the surface, say x, and to a much lesser extent on the remaining local coordinates, say y and z, which are tangential to the surface. This nearly one-dimensional,

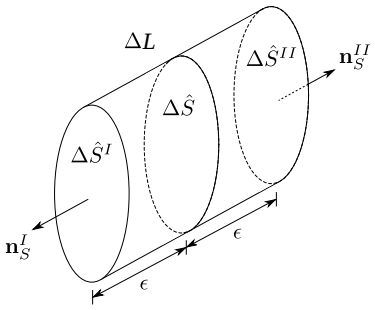

Figure 1: Geometrical setting for the interface conditions of the $\mathbf{J}_\alpha(\mathbf{r})$ vectors.

quasi-planar dependence on the space variables allows to assimilate the 3D A_N-fluxes $\phi_{\alpha,g}(\mathbf{r})$ to the 1D fluxes $\phi_{\alpha,g}(x)$ of the plane geometry case and extend therefore the continuity property of the latter functions to the general $\phi_{\alpha,g}(\mathbf{r})$ (similar arguments are encountered in the classical SP_N theory, see e.g. Pomraning (1993)). We conclude that the condition of continuity

$$\phi^I_{\alpha,g}(\mathbf{r}_S) = \phi^{II}_{\alpha,g}(\mathbf{r}_S) \quad (\alpha = 1,\ldots,N; g = 1,\ldots,G) \tag{26}$$

can be reasonably assumed to be valid for the A_N fluxes at a smooth point $\mathbf{r}_S$ of the interface between any two adjacent regions V^I, V^{II}.

On the contrary, the interface conditions for the $\mathbf{J}_{\alpha,g}(\mathbf{r})$ vectors, can be rigorously derived from the differential equations themselves. Let $\Delta\hat{S}$ be an arbitrary, smooth part of the interface, say $\hat{S}$, between V^I and V^{II} and let $\Delta\hat{S}^I$, $\Delta\hat{S}^{II}$ be two pieces of surface parallel to $\Delta\hat{S}$, at a distance ϵ from it and such that $\Delta\hat{S}^I$ is belonging to V^I and $\Delta\hat{S}^{II}$ to V^{II}. Considering the cylinder ΔV with bases $\Delta\hat{S}^I$ and $\Delta\hat{S}^{II}$, let ΔL be its lateral surface (Fig. 1). Finally, let $\mathbf{n}_S^I$ and $\mathbf{n}_S^{II}$ be the outward normal to $\Delta\hat{S}^I$, respectively $\Delta\hat{S}^{II}$; more generally, let $\mathbf{n}_S$ denote the outward normal at any point of the boundary $\partial(\Delta V)$ of ΔV, so that, in particular, $\mathbf{n}_S = \mathbf{n}_S^I$ if $\mathbf{r}_S \in \Delta\hat{S}^I$ and $\mathbf{n}_S = \mathbf{n}_S^{II}$ if $\mathbf{r}_S \in \Delta\hat{S}^{II}$. An integration of Eq. (20) over ΔV then gives

$$\int_{\Delta V} \nabla\cdot\mathbf{J}_{\alpha,g}(\mathbf{r})\,\mathrm{d}V + \int_{\Delta V} U_{\alpha,g}(\mathbf{r})\,\mathrm{d}V = 0 \quad (\alpha = 1,\ldots,N; g = 1,\ldots,G), \tag{27}$$

where

$$U_{\alpha,g}(\mathbf{r}) = \sum_{\beta=1}^{N}\sum_{g'=1}^{G} \Sigma_{\alpha\beta,gg'}(\mathbf{r})\,\phi_{\beta,g'}(\mathbf{r}) - s^{ext}_g(\mathbf{r}). \tag{28}$$

Assuming that the measure of ΔV is $O(\epsilon)$ (Fig. 1), the integral involving $U_{\alpha,g}$ is also $O(\epsilon)$, by virtue of the boundedness of $\Sigma_{\alpha\beta,gg'}(\mathbf{r})$, $\phi_{\beta,g'}(\mathbf{r})$ and $s^{ext}_g(\mathbf{r})$. The remaining integral gives, after an application of the divergence theorem and the introduction of the normal components of the $\mathbf{J}_{\alpha,g}$'s vectors,

$$\begin{aligned}\int_{\partial(\Delta V)} \mathbf{J}_{\alpha,g}(\mathbf{r}_S)\cdot\mathbf{n}_S\,\mathrm{d}S \;=\; &\int_{\Delta\hat{S}^{II}} J^{II}_{n_S,\alpha g}\left(\mathbf{r}_S + \epsilon\mathbf{n}_S^{II}\right)\mathrm{d}S \\ &+ \int_{\Delta\hat{S}^{I}} J^{I}_{n_S,\alpha g}\left(\mathbf{r}_S + \epsilon\mathbf{n}_S^{I}\right)\mathrm{d}S + O(\epsilon),\end{aligned} \tag{29}$$

where the $O(\epsilon)$ term is now referring to the contribution of the lateral surface, ΔL, of ΔV. Taking the limit as $\epsilon\to 0$ in both integrals of Eq. (27) we conclude, owing to the arbitrariness of $\Delta\hat{S}$ and therefore of $\Delta\hat{S}^I$ and $\Delta\hat{S}^{II}$,

$$J^{II}_{n_S,\alpha g}\left(\mathbf{r}_S + \epsilon\mathbf{n}_S^{II}\right) + J^{I}_{n_S,\alpha g}\left(\mathbf{r}_S + \epsilon\mathbf{n}_S^{I}\right) \to 0 \tag{30}$$

or also, since $\mathbf{n}_S^{II} = -\mathbf{n}_S^I = \mathbf{n}_S$ and using simpler notations

$$J^I_{n_S,\alpha g}(\mathbf{r}_S) = J^{II}_{n_S,\alpha g}(\mathbf{r}_S) \quad (\alpha = 1,\ldots,N; g = 1,\ldots,G), \tag{31}$$

an equation that establishes the continuity of the (net) normal A_N currents $J_{n_S,\alpha g}$ at the interface, thus completing, together with Eqs. (26), the set of the interface conditions to be used with the A_N differential equations.

Remark 1. The continuity of the normal A_N currents has been here directly derived from the A_N differential equations, thus ensuring, in full generality, the consistency of these interface conditions with the A_N equations themselves. As we have already observed, this is not true for the continuity conditions of the A_N fluxes, which need being supported by an argument of physical nature. It must be recalled, however, that for the more restricted class of the $C\sigma$ systems with isotropic scattering both relations of continuity, Eqs. (26) and (31), can be derived in a rigorous way as simple regularity properties of the A_N solutions (Ciolini et al., 2002). In Appendix C we give an extension of this proof to $C\sigma$ systems with a linearly anisotropic scattering. In such a proof we shall limit ourselves to show the interface continuity of the A_N fluxes, since the argument concerning the normal currents has been autonomously treated above.

We feel therefore ourselves legitimate to conclude that the classical continuity conditions, Eqs. (26) and (31), can be adopted for the A_N fluxes and normal currents at the interface between two adjacent regions.

Of the other types of conditions, the reflection conditions are obvious (one must simply impose the vanishing of the A_N normal currents). The void (no-entry) boundary conditions, however, deserve a special discussion, which will be developed in sect. 4.

Remark 2. The continuity of the physical g-group fluxes and normal currents, Φ_g and $J_{n_S,g}$, is an obvious consequence of Eqs. (10) and (25).

3. The classical version of the A_N boundary integral equations

Differently from the arguments of the previous section, the passage from the differential to the boundary integral form of the A_N equations can be more easily developed in an abstract way, without making reference to the physical meaning of the involved quantities. Accordingly, the single-index notation (as in Eqs. (24)) will be preferred.

Let V be a region of a general neutron diffusing system. It is assumed that V is convex and with a piecewise smooth boundary surface S. Let, moreover,

$$(\mathbf{u},\mathbf{v}) = \sum_{\gamma=1}^{\Gamma} \int_V u_\gamma(\mathbf{r})\, v_\gamma(\mathbf{r})\, \mathrm{d}V \tag{32}$$

be the scalar product of any two vectors $\mathbf{u}(\mathbf{r}) = [u_1(\mathbf{r}),\ldots,u_\Gamma(\mathbf{r})]^T$ and $\mathbf{v}(\mathbf{r}) = [v_1(\mathbf{r}),\ldots,v_\Gamma(\mathbf{r})]^T$ with $\Gamma = NG$ components. Let, finally, $L_{\gamma\gamma'}$ be the following $\Gamma x \Gamma$ matrix

$$L_{\gamma\gamma'} = -\nabla\cdot D_{\gamma\gamma'}\nabla + \Sigma_{\gamma\gamma'} \tag{33}$$

which allows to rewrite Eqs. (24) as follows

$$\sum_{\gamma'=1}^{\Gamma} L_{\gamma\gamma'}\phi_{\gamma'} = s^{ext}_\gamma \quad (\gamma = 1,\ldots,\Gamma) \tag{34}$$

or, in a self-evident compact form, $\mathbf{L}\boldsymbol{\phi} = \mathbf{s}^{ext}$. The weak form of the latter expression is $(\mathbf{L}\boldsymbol{\phi},\boldsymbol{\phi}^*) = (\mathbf{s}^{ext},\boldsymbol{\phi}^*)$ or, in terms of the components,

$$\sum_{\gamma=1}^{\Gamma}\int_V \sum_{\gamma'=1}^{\Gamma} L_{\gamma\gamma'}\phi_{\gamma'}\phi^*_\gamma\,\mathrm{d}V = \sum_{\gamma=1}^{\Gamma}\int_V s^{ext}_\gamma\phi^*_\gamma\,\mathrm{d}V, \tag{35}$$

where $\boldsymbol{\phi}^*$ is an arbitrary vector (sufficiently smooth as regards its space dependence). Let us now consider a single integral $\int_V L_{\gamma\gamma'}\phi_{\gamma'}\phi^*_\gamma \,\mathrm{d}V$. An application of the Green identity states that, if $f(\mathbf{r})$, $g(\mathbf{r})$, $k(\mathbf{r})$ are three functions that admit all the partial derivatives that are necessary, then

$$\int_V \left[(\nabla\cdot k\nabla f)\, g - f\,(\nabla\cdot k\nabla g)\right]\mathrm{d}V = \int_S \left[\left(k\frac{\partial f}{\partial n_S}\right)g - f\left(k\frac{\partial g}{\partial n_S}\right)\right]\mathrm{d}S. \tag{36}$$

Namely, since for any vector $\mathbf{v}(\mathbf{r}) = \left[v_x(\mathbf{r}), v_y(\mathbf{r}), v_z(\mathbf{r})\right]^T$ we have $\nabla\cdot(g\mathbf{v}) = g\nabla\cdot\mathbf{v} + \nabla g\cdot\mathbf{v}$, by setting $\mathbf{v} = k\nabla f$ we obtain

$$\nabla\cdot(gk\nabla f) = g\nabla\cdot(k\nabla f) + \nabla g\cdot(k\nabla f) = \left[\nabla\cdot(k\nabla f)\right]g + k\nabla f\cdot\nabla g \tag{37}$$

and, similarly,

$$\nabla\cdot(fk\nabla g) = \left[\nabla\cdot(k\nabla g)\right]f + k\nabla g\cdot\nabla f. \tag{38}$$

Thus

$$\begin{aligned}\int_V \left[(\nabla\cdot k\nabla f)\, g - (\nabla\cdot k\nabla g)\, f\right]\mathrm{d}V &= \int_V \left[\nabla\cdot(gk\nabla f) - \nabla\cdot(fk\nabla g)\right]\mathrm{d}V\\ &= \int_S \left[gk\nabla f\cdot\mathbf{n}_S - fk\nabla g\cdot\mathbf{n}_S\right]\mathrm{d}S\\ &= \int_S \left[gk\frac{\partial f}{\partial n_S} - fk\frac{\partial g}{\partial n_S}\right]\mathrm{d}S,\end{aligned} \tag{39}$$

where the divergence theorem has been applied to the vectors $\mathbf{v}_1 = gk\nabla f$ and $\mathbf{v}_2 = fk\nabla g$. Eq. (36) then follows.

Concerning the integral $\int_V L_{\gamma\gamma'}\phi_{\gamma'}\phi^*_\gamma \,\mathrm{d}V$ we get, by deleting the opposite terms involving $\Sigma_{\gamma\gamma'}$ and applying the above identity,

$$\begin{aligned}&\int_V \left(L_{\gamma\gamma'}\phi_{\gamma'}\right)\phi^*_\gamma \,\mathrm{d}V - \int_V \phi_{\gamma'}\left(L_{\gamma\gamma'}\phi^*_\gamma\right)\mathrm{d}V =\\ &\qquad - \int_V \left[\nabla\cdot\left(D_{\gamma\gamma'}\nabla\phi_{\gamma'}\right)\phi^*_\gamma - \phi_{\gamma'}\nabla\cdot\left(D_{\gamma\gamma'}\nabla\phi^*_\gamma\right)\right]\mathrm{d}V\\ &\qquad = -\int_S \left[\left(D_{\gamma\gamma'}\frac{\partial\phi_{\gamma'}}{\partial n_S}\right)\phi^*_\gamma - \phi_{\gamma'}\left(D_{\gamma\gamma'}\frac{\partial\phi^*_\gamma}{\partial n_S}\right)\right]\mathrm{d}S.\end{aligned} \tag{40}$$

Then, Eq. (35) can be written as follows

$$\begin{aligned}\int_V \sum_{\gamma,\gamma'=1}^{\Gamma}\phi_{\gamma'}L_{\gamma\gamma'}\phi^*_\gamma \,\mathrm{d}V - \int_S \sum_{\gamma,\gamma'=1}^{\Gamma}\Bigg[&\left(D_{\gamma\gamma'}\frac{\partial\phi_{\gamma'}}{\partial n_S}\right)\phi^*_\gamma\\ &-\phi_{\gamma'}\left(D_{\gamma\gamma'}\frac{\partial\phi^*_\gamma}{\partial n_S}\right)\Bigg]\mathrm{d}S = \int_V\sum_{\gamma=1}^{\Gamma} s^{ext}_\gamma\phi^*_\gamma \,\mathrm{d}V.\end{aligned} \tag{41}$$

It is convenient to introduce the (formal) adjoint of the matrix differential operator $\mathbf{L}$:

$$\mathbf{L}^* = -\nabla\cdot\mathbf{D}^*\nabla + \boldsymbol{\Sigma}^* \tag{42}$$

where $L^*_{\gamma\gamma'} = L_{\gamma'\gamma}$, $D^*_{\gamma\gamma'} = D_{\gamma'\gamma}$, $\Sigma^*_{\gamma\gamma'} = \Sigma_{\gamma'\gamma}$. Eq. (41) takes the following form

$$\begin{aligned}\int_V \sum_{\gamma'=1}^{\Gamma}\phi_{\gamma'}\sum_{\gamma=1}^{\Gamma}L^*_{\gamma'\gamma}\phi^*_\gamma \,\mathrm{d}V - \int_S \Bigg[&\sum_{\gamma=1}^{\Gamma}\phi^*_\gamma\left(\sum_{\gamma'=1}^{\Gamma}D_{\gamma\gamma'}\frac{\partial\phi_{\gamma'}}{\partial n_S}\right)\\ &-\sum_{\gamma'=1}^{\Gamma}\left(\sum_{\gamma=1}^{\Gamma}D^*_{\gamma'\gamma}\frac{\partial\phi^*_\gamma}{\partial n_S}\right)\phi_{\gamma'}\Bigg]\mathrm{d}S = \int_V\sum_{\gamma=1}^{\Gamma}s^{ext}_\gamma\phi^*_\gamma \,\mathrm{d}V.\end{aligned} \tag{43}$$

A procedure that has been used for diffusion and A_N problems in the case of a diagonal $\mathbf{D}$ (Colombo et al. (1988), Temesvari and Makai (1992), Ciolini et al. (2002)) will be now extended to a full $\mathbf{D}$ matrix.

Let us consider the following non-homogeneous differential systems

$$\mathbf{L}^* \tilde{\boldsymbol{\phi}}^{(\nu)} = \delta(\mathbf{r} - \mathbf{r}_0)\, \mathbf{e}^{(\nu)} \quad (\nu = 1, \ldots, \Gamma), \tag{44}$$

where $\mathbf{e}^{(1)} = [1, 0, \ldots, 0]^T$, $\mathbf{e}^{(2)} = [0, 1, \ldots, 0]^T$, ..., $\mathbf{e}^{(\Gamma)} = [0, 0, \ldots, 1]^T$ or, in terms of the components

$$\sum_{\gamma=1}^{\Gamma} L^*_{\gamma'\gamma} \tilde{\phi}^{(\nu)}_{\gamma} = \delta(\mathbf{r} - \mathbf{r}_0)\, \delta_{\gamma'\nu} \quad (\gamma', \nu = 1, \ldots, \Gamma) \tag{45}$$

and let $\tilde{\boldsymbol{\phi}}^{(\nu)}$ be a solution of the ν-th system. Namely, $\tilde{\boldsymbol{\phi}}^{(\nu)}$ is such that, for each ν, (*i*) the Γ-ple of functions $\tilde{\phi}^{(\nu)}_{\gamma}(\mathbf{r})$ satisfies the equations of the ν-th system (45), (*ii*) the vectors $\tilde{\boldsymbol{\phi}}^{(\nu)}(\mathbf{r}) = \left[\tilde{\phi}^{(\nu)}_1(\mathbf{r}), \tilde{\phi}^{(\nu)}_2(\mathbf{r}), \ldots, \tilde{\phi}^{(\nu)}_{\Gamma}(\mathbf{r})\right]^T$ are linearly independent (see Appendix A). It is also useful to have more complete notations for the $\tilde{\boldsymbol{\phi}}^{(\nu)}$ vectors and their $\tilde{\phi}^{(\nu)}_{\gamma}$ components, namely $\tilde{\boldsymbol{\phi}}^{(\nu)}(\mathbf{r}_0, \mathbf{r})$ and $\tilde{\phi}^{(\nu)}_{\gamma}(\mathbf{r}_0, \mathbf{r})$, respectively, in order to have an explicit indication of the point where the source is located. The functions ϕ^*_{γ} in Eq. (43) are then replaced by the functions $\tilde{\phi}^{(\nu)}_{\gamma}(\mathbf{r}_0, \mathbf{r})$, which will be given the name of fundamental solutions (or Green functions). Owing to Eq. (45), the first integral on the l.h.s. of Eq. (43) yields

$$\begin{aligned}
\int_V \sum_{\gamma'=1}^{\Gamma} \phi_{\gamma'} \sum_{\gamma=1}^{\Gamma} L^*_{\gamma'\gamma} \tilde{\phi}^{(\nu)}_{\gamma}\, \mathrm{d}V &= \int_V \sum_{\gamma'=1}^{\Gamma} \phi_{\gamma'} \delta_{\gamma'\nu} \delta(\mathbf{r} - \mathbf{r}_0)\, \mathrm{d}V \\
&= \int_V \phi_{\nu}(\mathbf{r})\, \delta(\mathbf{r} - \mathbf{r}_0)\, \mathrm{d}V \\
&= c(\mathbf{r}_0)\, \phi_{\nu}(\mathbf{r}_0) \quad (\nu = 1, \ldots, \Gamma),
\end{aligned} \tag{46}$$

where, by the properties of the delta function, $c(\mathbf{r}_0)$ is equal to 1, 0, 1/2 according to $\mathbf{r}_0$ is inside V, outside V or coincides with a smooth point of the boundary surface, S (if $\mathbf{r}_0$ is not a smooth point, i.e. it is a vertex, or is belonging to an edge, then $c(\mathbf{r}_0) = \Omega/4\pi$, Ω being the angle of aperture of the tangent cone at $\mathbf{r}_0$). With these positions and replacing the couple $\mathbf{r}_0$, $\mathbf{r}$ by $\mathbf{r}$, $\mathbf{r}'_S$ Eq. (43) takes the following form

$$\begin{aligned}
c(\mathbf{r})\, \phi_{\nu}(\mathbf{r}) - \int_S \Bigg\{ &\sum_{\gamma=1}^{\Gamma} \tilde{\phi}^{(\nu)}_{\gamma}(\mathbf{r}, \mathbf{r}'_S) \sum_{\gamma'=1}^{\Gamma} D_{\gamma\gamma'}(\mathbf{r}'_S) \frac{\partial \phi_{\gamma'}}{\partial n'_S}(\mathbf{r}'_S) \\
&- \sum_{\gamma'=1}^{\Gamma} \left[\sum_{\gamma=1}^{\Gamma} D^*_{\gamma'\gamma}(\mathbf{r}'_S) \frac{\partial \tilde{\phi}^{(\nu)}_{\gamma}}{\partial n'_S}(\mathbf{r}, \mathbf{r}'_S) \right] \phi_{\gamma'}(\mathbf{r}'_S) \Bigg\} \mathrm{d}S' \\
= \int_V &\sum_{\gamma=1}^{\Gamma} \tilde{\phi}^{(\nu)}_{\gamma}(\mathbf{r}, \mathbf{r}')\, s^{ext}_{\gamma}(\mathbf{r}')\, \mathrm{d}V' \quad (\nu = 1, \ldots, \Gamma).
\end{aligned} \tag{47}$$

Let us now consider the normal components of the vectors $\mathbf{J}_{\gamma}$ at a point of the boundary surface, $J_{n_S,\gamma}$:

$$J_{n_S,\gamma}(\mathbf{r}_S) = \mathbf{J}_{\gamma}(\mathbf{r}_S) \cdot \mathbf{n}_S = -\sum_{\gamma'=1}^{\Gamma} D_{\gamma\gamma'}(\mathbf{r}_S) \frac{\partial \phi_{\gamma'}}{\partial n_S}(\mathbf{r}_S). \tag{48}$$

and let, moreover,

$$\tilde{J}^{(\nu)}_{n_S,\gamma}(\mathbf{r}, \mathbf{r}'_S) = \sum_{\gamma'=1}^{\Gamma} D^*_{\gamma'\gamma}(\mathbf{r}'_S) \frac{\partial \tilde{\phi}^{(\nu)}_{\gamma'}}{\partial n'_S}(\mathbf{r}, \mathbf{r}'_S). \tag{49}$$

Eqs. (47) can be written as follows

$$c(\mathbf{r})\,\phi_\nu(\mathbf{r}) + \sum_{\gamma=1}^{\Gamma}\int_S \left[\tilde{\phi}_\gamma^{(\nu)}(\mathbf{r},\mathbf{r}'_S)\,J_{n'_S,\gamma}(\mathbf{r}'_S) + \tilde{J}_{n'_S,\gamma}^{(\nu)}(\mathbf{r},\mathbf{r}'_S)\,\phi_\gamma(\mathbf{r}'_S)\right]\mathrm{d}S' = \sum_{\gamma=1}^{\Gamma}\int_V \tilde{\phi}_\gamma^{(\nu)}(\mathbf{r}_S,\mathbf{r}')\,s_\gamma^{ext}(\mathbf{r}')\,\mathrm{d}V' \quad (\nu=1,\ldots,\Gamma), \tag{50}$$

a relation that allows to determine the $\phi_\nu(\mathbf{r})$ moments (i.e. the A_N fluxes) at any point $\mathbf{r}\in V$, provided the values of these moments and their normal derivatives (and therefore the $J_{n_S,\gamma}$'s) are known at the points of the boundary. Taking $\mathbf{r}=\mathbf{r}_S$, Eq. (50) becomes a system of boundary integral equations (BIE):

$$c(\mathbf{r}_S)\,\phi_\nu(\mathbf{r}_S) + \sum_{\gamma=1}^{\Gamma}\int_S \left[\tilde{\phi}_\gamma^{(\nu)}(\mathbf{r}_S,\mathbf{r}'_S)\,J_{n'_S,\gamma}(\mathbf{r}'_S) + \tilde{J}_{n'_S,\gamma}^{(\nu)}(\mathbf{r}_S,\mathbf{r}'_S)\,\phi_\gamma(\mathbf{r}'_S)\right]\mathrm{d}S' = \sum_{\gamma=1}^{\Gamma}\int_V \tilde{\phi}_\gamma^{(\nu)}(\mathbf{r}_S,\mathbf{r}')\,s_\gamma^{ext}(\mathbf{r}')\,\mathrm{d}V' \quad (\nu=1,\ldots,N). \tag{51}$$

We shall call these BIE's the classical form of the A_N boundary integral equations. If the functions $J_{n_S,\gamma}(\mathbf{r}_S)$ are assigned at the boundary, by solving this system the boundary values of the moments $\phi_\gamma(\mathbf{r}_S)$ are also obtained and the substitution of both the $\phi_\gamma(\mathbf{r}_S)$ and the $J_{n_S,\gamma}(\mathbf{r}_S)$ functions into Eq. (50) yields the moments $\phi_\nu(\mathbf{r})$ and therefore the physical flux $\Phi(\mathbf{r})$ at any $\mathbf{r}\in V$. Alternatively, if the $\phi_\gamma(\mathbf{r}_S)$ are assigned at the boundary (which corresponds to Dirichlet-type conditions, as opposed to the previous Neumann-type conditions) then Eqs. (51) are to be solved with respect to the $J_{n_S,\gamma}(\mathbf{r}_S)$ (as integral equations of the first kind) and the solution of the problem follows, as before. Now, solving the Γ partial differential systems in Eq. (45) with general, space dependent coefficients $D_{\gamma\gamma'}$ and $\Sigma_{\gamma\gamma'}$ would make the present method quite cumbersome or even completely unsuitable. A simplifying assumption is therefore necessary. Thus, we assume that the general neutron diffusing system is an array of homogeneous regions, an assumption that is fortunately fulfilled, sometimes also at different scales, by the architecture of most nuclear reactors. Eq. (45) can be rewritten as follows

$$-\sum_{\gamma=1}^{\Gamma} D^*_{\gamma'\gamma}\nabla^2_{\mathbf{r}}\tilde{\phi}_\gamma^{(\nu)}(\mathbf{r}_0,\mathbf{r}) + \sum_{\gamma=1}^{\Gamma}\Sigma^*_{\gamma'\gamma}\tilde{\phi}_\gamma^{(\nu)}(\mathbf{r}_0,\mathbf{r}) = \delta(\mathbf{r}-\mathbf{r}_0)\,\delta_{\gamma'\nu} \quad (\gamma'=1,\ldots,\Gamma), \tag{52}$$

with $\nu=1,\ldots,\Gamma$. The solutions of the above differential systems (where the physical parameters are referred to a specific region) are now sought on the whole $\mathbb{R}^3$ space, with a vanishing condition at infinity or, if necessary, a Sommerfeld radiation condition. The solution procedure is sketched in Appendix A, where it is shown that the kernels $\tilde{\phi}_\nu$ are linear combinations of diffusion-like Green functions.

Once the kernels $\tilde{\phi}_\gamma^{(\nu)}$ and $\tilde{J}_\gamma^{(\nu)}$ of the boundary integral equations describing a single region have been determined, one can tackle the problem of two (or more) interacting regions, each of which with its own cross sections. It will suffice to consider only two regions V^I and V^{II}, of which V^I is finite and convex and V^{II} is the complement of V^I with respect to $\mathbb{R}^3$. Let S be the interface between V^I and V^{II}. Eqs. (51) are then written for the two regions:

$$c^I(\mathbf{r}_S)\,\phi^I_\nu(\mathbf{r}_S) + \sum_{\gamma=1}^{\Gamma}\int_S \left[\tilde{\phi}_\gamma^{I(\nu)}(\mathbf{r}_S,\mathbf{r}'_S)\,J^I_{n^{I'}_S,\gamma}(\mathbf{r}'_S) + \tilde{J}_{n^{I'}_S,\gamma}^{I(\nu)}(\mathbf{r}_S,\mathbf{r}'_S)\,\phi^I_\gamma(\mathbf{r}'_S)\right]\mathrm{d}S' = \sum_{\gamma=1}^{\Gamma}\int_V \tilde{\phi}_\gamma^{I(\nu)}(\mathbf{r}_S,\mathbf{r}')\,s^I_\gamma(\mathbf{r}')\,\mathrm{d}V' \tag{53}$$

$$c^{II}(\mathbf{r}_S)\,\phi_\nu^{II}(\mathbf{r}_S) + \sum_{\gamma=1}^{\Gamma}\int_S \left[\tilde{\phi}_\gamma^{II(\nu)}(\mathbf{r}_S,\mathbf{r}'_S)\,J^{II}_{n_S^{II},\gamma}(\mathbf{r}'_S) + \tilde{J}^{II(\nu)}_{n_S^{II},\gamma}(\mathbf{r}_S,\mathbf{r}'_S)\,\phi_\gamma^{II}(\mathbf{r}'_S)\right]\mathrm{d}S'$$
$$= \sum_{\gamma=1}^{\Gamma}\int_V \tilde{\phi}_\gamma^{II(\nu)}(\mathbf{r}_S,\mathbf{r}')\,s_\gamma^{II}(\mathbf{r}')\,\mathrm{d}V' \quad (\nu=1,\ldots,\Gamma)\,, \tag{54}$$

with obvious notations. Elimination of $\phi_\nu^{II}(\mathbf{r}_S)$ and $J^{II}_{n_S^{II},\nu}(\mathbf{r}_S)$ by means of the interface conditions $\phi_\nu^{I}(\mathbf{r}_S) = \phi_\nu^{II}(\mathbf{r}_S)$ and $J^{I}_{n_S^{I},\nu}(\mathbf{r}_S) = -J^{II}_{n_S^{II},\nu}(\mathbf{r}_S)$, with $\mathbf{n}_S^{II} = -\mathbf{n}_S^{I}$ (see Eq. (26) and (30) or (31)), allows to obtain a system of two integral equations for the remaining unknowns $\phi_\nu^{I}(\mathbf{r}_S)$ and $J^{I}_{n_S^{I},\nu}(\mathbf{r}_S)$, which can be solved by a numerical method. The procedure can be immediately generalized to more regions.

4. The partial current boundary integral form of the $\mathbf{A}_N$ equations and their interface conditions

Let us consider the classical boundary integral equation system for a single homogeneous region V, Eqs. (51), and introduce the following kernels

$$\tilde{J}^{(\nu)\pm}_{n_S,\gamma}(\mathbf{r}_S,\mathbf{r}'_S) = \frac{1}{4}\tilde{\phi}^{(\nu)}_\gamma(\mathbf{r}_S,\mathbf{r}'_S) \mp \frac{1}{2}\tilde{J}^{(\nu)}_{n_S,\gamma}(\mathbf{r}_S,\mathbf{r}'_S)\,, \tag{55}$$

where, reciprocally,

$$\tilde{\phi}^{(\nu)}_\gamma(\mathbf{r}_S,\mathbf{r}'_S) = 2\left[\tilde{J}^{(\nu)+}_{n_S,\gamma}(\mathbf{r}_S,\mathbf{r}'_S) + \tilde{J}^{(\nu)-}_{n_S,\gamma}(\mathbf{r}_S,\mathbf{r}'_S)\right] \tag{56}$$

$$\tilde{J}^{(\nu)}_{n_S,\gamma}(\mathbf{r}_S,\mathbf{r}'_S) = \tilde{J}^{(\nu)-}_{n_S,\gamma}(\mathbf{r}_S,\mathbf{r}'_S) - \tilde{J}^{(\nu)+}_{n_S,\gamma}(\mathbf{r}_S,\mathbf{r}'_S)\,. \tag{57}$$

We proceed in a similar way with the unknowns $\phi_\gamma(\mathbf{r}_S)$ and $J_{n_S,\gamma}(\mathbf{r}_S)$ of Eqs. (51). Namely, we set

$$J^{\pm}_{n_S,\gamma}(\mathbf{r}_S) = \frac{1}{4}\phi_\gamma(\mathbf{r}_S) \pm \frac{1}{2}J_{n_S,\gamma}(\mathbf{r}_S) \tag{58}$$

and, reciprocally,

$$\phi_\gamma(\mathbf{r}_S) = 2\left[J^{+}_{n_S,\gamma}(\mathbf{r}_S) + J^{-}_{n_S,\gamma}(\mathbf{r}_S)\right] \tag{59}$$

$$J_{n_S,\gamma}(\mathbf{r}_S) = J^{+}_{n_S,\gamma}(\mathbf{r}_S) - J^{-}_{n_S,\gamma}(\mathbf{r}_S)\,. \tag{60}$$

Substitution into Eqs. (51) leads to the following BIE system in terms of the $J^{\pm}_{n_S,\gamma}(\mathbf{r}_S)$:

$$\frac{1}{2}c(\mathbf{r}_S)\,J^{+}_{n_S,\nu}(\mathbf{r}_S) + \sum_{\gamma=1}^{\Gamma}\int_S \tilde{J}^{(\nu)+}_{n'_S,\gamma}(\mathbf{r}_S,\mathbf{r}'_S)\,J^{+}_{n'_S,\gamma}(\mathbf{r}'_S)\,\mathrm{d}S'$$
$$= -\frac{1}{2}c(\mathbf{r}_S)\,J^{-}_{n_S,\nu}(\mathbf{r}_S) + \sum_{\gamma=1}^{\Gamma}\int_S \tilde{J}^{(\nu)-}_{n'_S,\gamma}(\mathbf{r}_S,\mathbf{r}'_S)\,J^{-}_{n'_S,\gamma}(\mathbf{r}'_S)\,\mathrm{d}S'$$
$$+ \frac{1}{4}\int_V \tilde{\phi}^{(\nu)}_\gamma(\mathbf{r}_S,\mathbf{r}')\,s_\gamma(\mathbf{r}')\,\mathrm{d}V' \quad (\nu=1,\ldots,\Gamma)\,. \tag{61}$$

The following iterative process is then applied:

$$\begin{aligned}\frac{1}{2}c\left(\mathbf{r}_S\right)\ {}^{(n+1)}J^{+}_{n_S,\nu}\left(\mathbf{r}_S\right)+\sum_{\gamma=1}^{\Gamma}\int_S \tilde{J}^{(\nu)+}_{n'_S,\gamma}\left(\mathbf{r}_S,\mathbf{r}'_S\right)\ {}^{(n+1)}J^{+}_{n'_S,\gamma}\left(\mathbf{r}'_S\right)\mathrm{d}S'\\ =-\frac{1}{2}c\left(\mathbf{r}_S\right)\ {}^{(n)}J^{-}_{n_S,\nu}\left(\mathbf{r}_S\right)\\ +\sum_{\gamma=1}^{\Gamma}\int_S \tilde{J}^{(\nu)-}_{n'_S,\gamma}\left(\mathbf{r}_S,\mathbf{r}'_S\right)\ {}^{(n)}J^{-}_{n'_S,\gamma}\left(\mathbf{r}'_S\right)\mathrm{d}S'\\ +\frac{1}{4}\int_V \tilde{\phi}^{(\nu)}_{\gamma}\left(\mathbf{r}_S,\mathbf{r}'\right)s^{ext}_{\gamma}\left(\mathbf{r}'\right)\mathrm{d}V'\quad(\nu=1,\ldots,\Gamma).\end{aligned}\tag{62}$$

The motivation of this process is transparent, provided we look at the $J^{\pm}_{n_S,\nu}$'s as if they were true partial currents: if the partial currents entering V, ${}^{(n)}J^{-}_{n_S,\nu}\left(\mathbf{r}_S\right)$'s are known, then the r.h.s. of Eqs. (62) is known and the integral equation system can be solved with respect to the outgoing partial currents ${}^{(n+1)}J^{+}_{n_S,\nu}\left(\mathbf{r}_S\right)$'s. The above intuitive approach needs, however, some more analysis.

We recall that, for a system constituted of only two regions V^I, V^{II}, as at the end of sect.3, the transport process is described, according to the classical A_N boundary integral version, by Eqs. (53) and (54), coupled via the interface conditions $\phi^I_\nu\left(\mathbf{r}_S\right)=\phi^{II}_\nu\left(\mathbf{r}_S\right)$ and $J^{I}_{n^I_S,\nu}\left(\mathbf{r}_S\right)=-J^{II}_{n^{II}_S,\nu}\left(\mathbf{r}_S\right)$, with $n^{II}_S=-n^I_S$. In the partial current version, the integral equation for the V^I region is

$$\begin{aligned}\frac{1}{2}c^I\left(\mathbf{r}_S\right)J^{I+}_{n_S,\nu}\left(\mathbf{r}_S\right)+\sum_{\gamma=1}^{\Gamma}\int_S \tilde{J}^{I(\nu)+}_{n'_S,\gamma}\left(\mathbf{r}_S,\mathbf{r}'_S\right)J^{I+}_{n'_S,\gamma}\left(\mathbf{r}'_S\right)\mathrm{d}S'\\ =-\frac{1}{2}c^I\left(\mathbf{r}_S\right)J^{I-}_{n_S,\nu}\left(\mathbf{r}_S\right)+\sum_{\gamma=1}^{\Gamma}\int_S \tilde{J}^{I(\nu)-}_{n'_S,\gamma}\left(\mathbf{r}_S,\mathbf{r}'_S\right)J^{I-}_{n'_S,\gamma}\left(\mathbf{r}'_S\right)\mathrm{d}S'\\ +\frac{1}{4}\int_V \tilde{\phi}^{I(\nu)}_{\gamma}\left(\mathbf{r}_S,\mathbf{r}'\right)s^{I,ext}_{\gamma}\left(\mathbf{r}'\right)\mathrm{d}V'\quad(\nu=1,\ldots,\Gamma).\end{aligned}\tag{63}$$

while a similar equation holds for the V^{II} region. As it concerns the interface conditions that are appropriate for the partial currents we have, according to Eqs. (58) the following (abstract) definition

$$J^{I\pm}_{n^I_S,\nu}\left(\mathbf{r}_S\right)=\frac{1}{4}\phi^I_\nu\left(\mathbf{r}_S\right)\pm\frac{1}{2}J^{I}_{n^I_S,\nu}\left(\mathbf{r}_S\right)\quad(\mathbf{r}_S\in S)\tag{64}$$

while a similar relation is written, with $\mathbf{n}^I_S$ replaced by $\mathbf{n}^{II}_S=-\mathbf{n}^I_S$, if the point $\mathbf{r}_S$ is seen as a limit point of V^{II}. However, we can retain the unit vector $\mathbf{n}^I_S$, provided the $\pm$ signs are replaced by $\mp$. Thus, if the continuity of the ϕ_ν's and the $J_{n_S,\nu}$'s is also taken into account, we have

$$\begin{aligned}J^{II\pm}_{n^I_S,\nu}\left(\mathbf{r}_S\right)&=\frac{1}{4}\phi^{II}_\nu\left(\mathbf{r}_S\right)\mp\frac{1}{2}J^{II}_{n^I_S,\nu}\left(\mathbf{r}_S\right)\\ &=\frac{1}{4}\phi^{I}_\nu\left(\mathbf{r}_S\right)\mp\frac{1}{2}J^{I}_{n^I_S,\nu}\left(\mathbf{r}_S\right)\end{aligned}\tag{65}$$

which amounts to say, by comparison with Eqs. (64) and putting $\mathbf{n}^I_S=\mathbf{n}_S$,

$$J^{II\pm}_{n_S,\nu}\left(\mathbf{r}_S\right)=J^{I\mp}_{n_S,\nu}\left(\mathbf{r}_S\right)\tag{66}$$

as may be expected from an intuitive point of view.

It is to be remarked that Eqs. (66) have been derived from the continuity relations for ϕ_ν and $J_{n_S,\nu}$ at the S interface by means of algebraic manipulations. No physical meaning has been given to the new quantities $J^{\pm}_{n_S,\nu}$. The only consequence to be drawn is, however, an important one, namely that, since there is an obvious one-to-one mapping

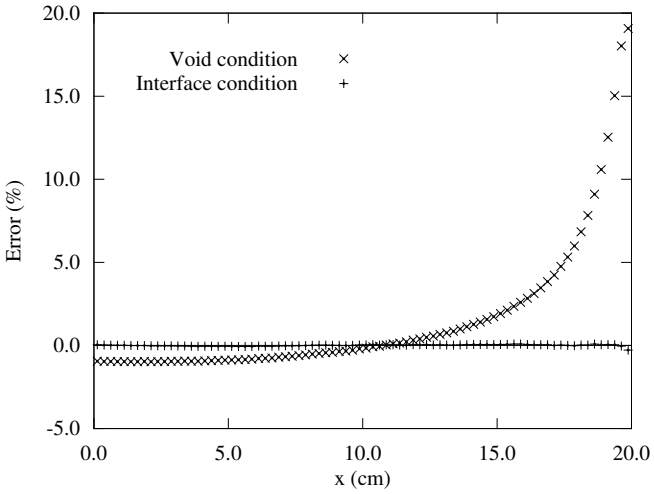

Figure 2: The error with respect to the MCNP reference calculation of the flux, $\Phi(x)$, in the multiplying layer, as calculated with the A_N method for $N = 8$, by using both the interface conditions with a purely absorbing medium and Marshak-like void conditions.

connecting the ϕ_ν, $J_{ns,\nu}$ and the $J^{\pm}_{ns,\nu}$ variables, Eqs. (66) are equivalent to Eqs. (26) and (31), so that if the solution of a problem satisfies a set of continuity conditions, it must satisfy the other set as well. The classical and the partial current A_N approaches are therefore completely equivalent as regards both the BIE system by which they are expressed and the interface conditions that are connecting the nearby regions. Even for a general, multiregion system, Eqs. (66) represent the interface conditions to be used within the partial current framework, in particular when applying the iterative solution procedure. Moreover (and this is the other main point of the method) only the interface conditions are considered and, as anticipated in the Introduction, even the void conditions are replaced by interface conditions with a supplementary, purely absorbing medium. The expedience of this procedure has been the subject of discussions since the early days of reactor physics and we would not insist any more on the argument. In order to appreciate the accuracy of our own application we limit ourselves to show a simple example, namely the following two-region, one-velocity criticality problem. A multiplying layer, $0 \leq x \leq a$, where $a = 20.0$ cm, with cross sections $\sigma = 1.5$ cm^{-1}, $\sigma_0 = 1.35$ cm^{-1}, $\sigma_1 = 0.3375$ cm^{-1} and with $\nu\sigma_f = 0.18$ cm^{-1}, is considered. A reflection condition holds at $x = 0$, while at $x = a$ the multiplying layer is followed by a purely absorbing layer, with the same total cross section and the same thickness of 20.0 cm, which ensures in practice the vanishing of the flux at its right boundary. This two-region problem has been solved in the A_N approximation and also, after removal of the absorbing layer, by using the simple Marshak-like approximation $J^-_{n,\nu}(a) = 0$ for $\nu = 1, \ldots, N$, with N ranging from 2 to 8. Fig. 2 shows the physical flux $\Phi(x)$ for $0 \leq x \leq a$, as obtained by the two-region calculation, and that obtained by eliminating the absorbing layer and applying the Marshak-like void conditions at $x = a$. A suitable one-group MCNP calculation with the same cross sections is used as reference. While the full two-region calculation shows an excellent agreement with MCNP, the use of the Mashak-like conditions shows a considerable error when approaching the boundary. Since the fluxes in Fig. 2 are average values on the computational intervals (0.25 cm), in order to get a better comparison we have reported in Table 1 the value of the multiplication constant, k, and that of the net physical current at $x = a$ (which obviously coincides with the outgoing partial current in the MCNP and Marshak cases).

The introduction of the absorbing medium implies that the calculations must include an additional region, which should be in principle of an infinite extent, since it is the complement of the system with respect to $\mathbb{R}^3$. However, it is sufficient, practically, to add an absorbing shell with a thickness of a few mean free paths, at the outer boundary of which the flux is expected to be small enough so as to allow the Marshak conditions to be applied without any harm for the accuracy of the calculation. Sometimes the reflector itself can be a reasonable substitute of the outer shell.

Table 1: Multiplication constant, k, and net current, J, at the free boundary of the multiplying layer obtained both with Marshak-like void conditions (VC) and interface conditions (IC) with a fully absorbing medium, are compared with reference values obtained by the MCNP calculation.

MCNP (ref.)				A_2	A_3	A_4	A_5	A_6	A_7	A_8
k	1.18681[a]	Δk (pcm)	VC	26	29	30	30	30	30	30
			IC	0	1	2	2	2	2	2
J	0.17537[b]	ΔJ (%)	VC	-1.69	-1.91	-2.00	-2.02	-2.02	-2.05	-2.06
			IC	0.25	0.18	0.15	0.14	0.13	0.13	0.12

[a] With an estimated standard deviation of 0.00004.
[b] With an estimated relative error of 0.04%.

5. Numerical applications

The present paper has been focused on the aspects that are specific of the A_N method. A key point of the numerical procedure, namely the actual solution of the A_N partial current BIE's holding for each homogeneous region, V^i, in which the general system is subdivided has not insofar been considered. However, this argument has been thoroughly discussed, for criticality problems in the diffusion approximation, in Cossa et al. (2010) (see also Giusti and Montagnini (2012), in which the procedure has been extended to SP_3). Here we limit ourselves to a very short sketch. The $J^{\pm}_{n_S,\nu}(\mathbf{r}_S)$ partial currents are expanded into Legendre polynomials (in the space variables) on each face of any V^i region of the system (a prism with a rectangular base) and a similar Legendre expansion is performed for the kernels, so that the integral equations are transformed into an algebraic linear system for the coefficients of the partial current expansions. As the kernels are sums of many diffusion-like kernels (the fundamental functions) what is to be done is to evaluate the Legendre expansions of the latter kernels with respect to the $\mathbf{r}_S$, $\mathbf{r}'_S$ variables, which implies, considering the different faces of V^i, to calculate many fourfold integrals, a heavy task which is alleviated, however, by the use of suitable recursion formulas (for details the reader is deferred to Cossa et al. (2010)). The procedure ends with the evaluation of the response matrix, which gives the Legendre moments of the outcoming partial currents as induced by the incoming ones. This concludes the first level (or "cell level") part of the calculation. The second level (or "general system level") relies on the application of the classical response matrix approach and is also discussed in the above paper. For the criticality problems, actually the only ones that have been considered in that paper, as well as in the present one, the multiplication factor, k, is updated at any step of such a second level.

The numerical examples in this paper are all referring to the *xyz* geometry, too. The solution method, developed according to the iteration process based on the interface partial currents and the response matrix technique, has been implemented into a computer code called BERM-AN. All the calculations for the numerical examples reported in this section have been performed on a Linux based PC with an Intel® i7-860 CPU and 8 Gb of RAM. The executable BERM-AN file has been obtained compiling the Fortran source files, which implement the method described in this paper, with the Intel® Fortran Compiler, version 11.1. Moreover, in order to better exploit the multithread characteristics of the CPU, many Fortran routines take advantage of the easy parallelization offered by the OpenMP™Fortran compiler directives.

With this method, according to Cossa et al. (2010), a multi-node critical problem is reduced to the solution of a homogeneous linear system in terms of the outward nodal partial currents that are here collectively symbolized with the vector $\mathbf{J}^+$. The following iterative scheme (actually the classical power method) is adopted:

$$^{(n+1)}\mathbf{J}^+ = \mathbf{\Theta}(k)\,{}^{(n)}\mathbf{J}^+. \tag{67}$$

For a fixed value of k, Eq. (67) is iterated until the parameter

$$^{(n+1)}\alpha(k) = \sqrt{\frac{\langle {}^{(n+1)}\mathbf{J}^+, {}^{(n+1)}\mathbf{J}^+\rangle}{\langle {}^{(n)}\mathbf{J}^+, {}^{(n)}\mathbf{J}^+\rangle}} \tag{68}$$

differs from that evaluated at the previous iteration by less than a specified value, ϵ_α. Since $\alpha(k)$ turns out to be a monotonic function of k, once its value at the n-th iteration is known, a new value for the $(n+1)$-th iteration is estimated

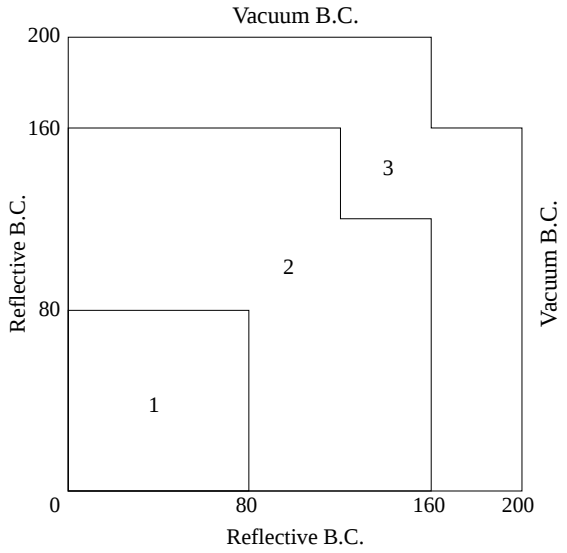

Figure 3: The geometry of the 2D, one energy group benchmark problem proposed by Hebért (dimensions are in cm).

Table 2: Cross section for the 2D, one energy group benchmark problem proposed by Hebért.

Mixture	Σ (cm^{-1})	Σ_{s0} (cm^{-1})	Σ_{s1}(cm^{-1})	$\nu\Sigma_f$ (cm^{-1})
1	0.025	0.013	0.0	0.0155
2	0.025	0.024	0.006	0.0
3	0.075	0.0	0.0	0.0

by the Newton's chord method. The calculation is stopped when the new value of k differs from the previous one by less than a specified value, ϵ_k.

For comparison purposes the numerical examples here presented have also been solved by means of the well known discrete ordinates codes DORT and TORT (Rhoades and Simpson, 1997), in the 2D and 3D cases, respectively. A rather high angular quadrature (S_{16}) has always been used. In the first example, a further comparison with the Monte Carlo code MCNP, version 5 (X-5 Monte Carlo Team, 2003), was also performed.

Finally, it has to be noted that the computing times reported for each numerical example are to be compared with caution, since for DORT and TORT only a sequential version of the executable file was available.

5.1. Example 1: A 2D, one energy group, benchmark problem

This problem, although not representative of a real situation, is designed in order to magnify the transport and anisotropic effects (Hébert, 2010). Three regions are characterizing the problem. A square homogeneous core (160×160 cm^2) is surrounded by a reflector. In its turn, the reflector is surrounded by a perfectly absorbing medium, on the external surface of which a vacuum boundary condition is finally applied (a Marshak condition will suffice), see Fig. 3. Differently from DORT, which is a 2D computational code, BERM-AN and MCNP are 3D codes and the geometry of the problem had to be modified. For BERM-AN, a finite height along the z-axis has been considered and boundary reflective conditions applied on the surfaces orthogonal to this axis. For MCNP the geometry was instead considered as infinite along the z-axis direction.

Table 2 shows the cross sections of the three different materials of this problem.

A suitable one-group cross section library has been produced in order to provide MCNP with the same cross sections reported in Table 2. In particular the linearly anisotropic Legendre representation of the scattering, $f(\mu)$, has been converted into a histogram probability density function (PDF) with 1000 steps of equal area. It has been shown

Table 3: The multiplication constant k for the 2D, one energy group with linearly anisotropic scattering benchmark problem.

Code	N	L	k	Δk (pcm)	CPU time (s)
MCNP (ref.)			0.99233[a]	–	4210.0
DORT S_{16}[b]			0.99226	-7	19.7
BERM-AN[c]	2	3	0.99115	-118	1.4
	2	4	0.99115	-118	2.8
	3	3	0.99216	-17	2.6
	3	4	0.99217	-16	4.9
	4	3	0.99237	4	4.1
	4	4	0.99237	4	8.2
	5	3	0.99245	12	6.2
	5	4	0.99245	12	12.9
	6	3	0.99249	16	8.5
	6	4	0.99249	16	17.2
	7	3	0.99251	18	11.4
	7	4	0.99252	19	25.1
	8	3	0.99253	20	15.3
	8	4	0.99253	20	34.1

[a] With an estimated standard deviation of 0.00003.
[b] With meshes of 2.0×2.0 cm^2.
[c] With a computational cell size of 10.0×10.0×10.0 cm^3.

that, by this approach, MCNP can match analytical solutions within statistics. To estimate the reference value of the multiplication constant k a total number of 2500 active cycles, each one of 250000 particles, has been used for the MCNP calculation. The MCNP multiplication constant k so calculated has been taken as reference.

In the case of the DORT calculation a spatial mesh of 2.0×2.0 cm^2 was deemed adequate, since it produced a multiplication constant, k, that was stable, at the pcm level, in comparison to that obtained with finer meshes. To terminate the calculation, a convergence criterion of 10^{-5} for the eigenvalue and of 10^{-4} for the fission source and the pointwise flux was adopted.

Finally, for the BERM-AN calculations the iteration over α and k were stopped when an accuracy ϵ_α and ϵ_k of 10^{-7} and 10^{-6}, respectively, was achieved. If not differently stated, the above convergence criteria for both DORT and BERM-AN have been used for all the other problems reported hereafter.

The multiplication constant k was calculated by BERM-AN, for N from 2 to 8, by expanding the partial currents on each nodal face into Legendre polynomials up to the L-th order, with $L=3$ and 4. Results are compared in Table 3 with the values obtained by MCNP and DORT.

The agreement between DORT and MCNP is very good (they differ by only 7 pcm), which is not surprising, if account is taken of the high order of angular quadrature used. As it concerns the results of BERM-AN, it appears that an increase of the order of the Legendre expansion from $L=3$ to $L=4$ yields at the most a difference of 1 pcm on k. Moreover, limiting the calculation at $L=3$ allows a reduction of the computing time between 30 and 45%. The error of the BERM-AN results towards the MCNP reference value of k is -118 pcm for $N=2$ and reaches a minimum (4 pcm) for $N=4$. A further increase of the order N, however, produces an increase, although moderate, of the error (up to 20 pcm for $N=8$). In some way, this is a kind of numerical confirmation of the fact that, being the A_N (as well as the SP_N) equations intrinsically approximate, there exists an optimal order N (which is unfortunately problem dependent and not known *a priori*) that produces the best solution in terms of accuracy (see also McClarren (2011)).

Finally, it is worth note that the values obtained with the present method in the A_2 and A_3 approximations match almost exactly (within 1 pcm) those obtained by Hebért in the SP_3 and SP_5 approximations, using a Raviart-Thomas finite element method with a polynomial basis of second degree (Hébert, 2010). Indeed an expected result, thanks again to the essential equivalence A_N-SP_{2N-1}.

This problem has been solved also by means of the BERM-SP3 code (Giusti and Montagnini, 2012). Owing to the fact that it is a one-speed problem, the anisotropic scattering is treated correctly by the latter code, too. Thus the numerical results coincide which those obtained by the present BERM-AN calculation for $N=2$ and have not been reported.

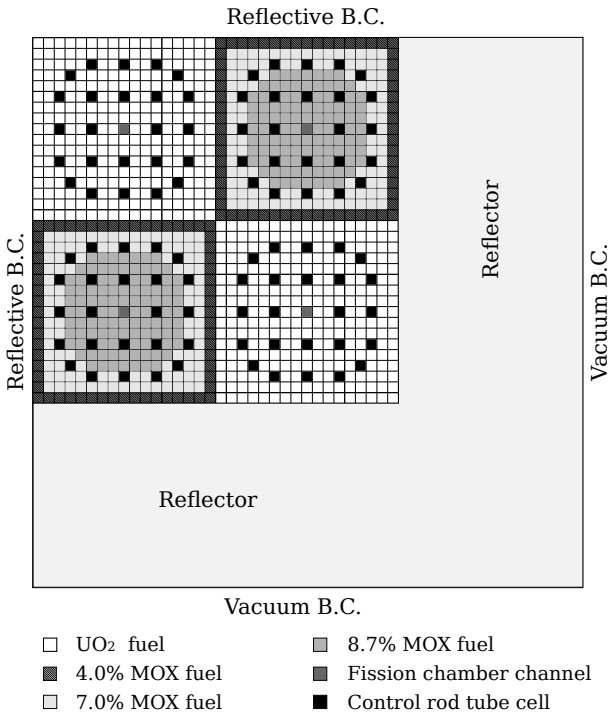

Figure 4: Horizontal cross section of the 3D reactor core loaded with mixed-oxide fuel assemblies.

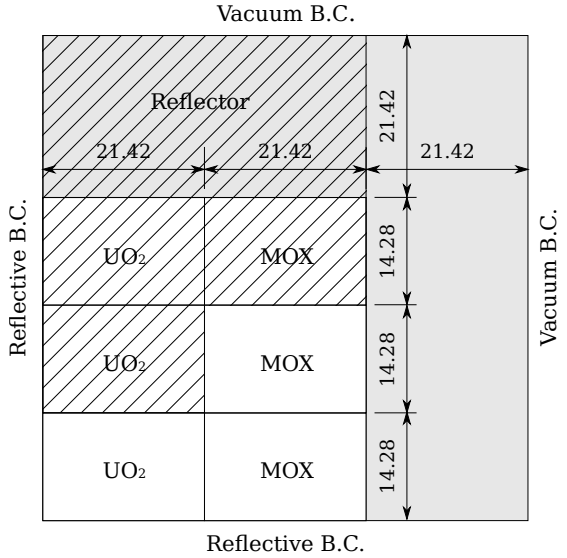

Figure 5: Vertical cross section of the 3D reactor core loaded with mixed-oxide fuel assemblies (dimensions are in cm). In the studied configuration the control rods are inserted 2/3 of the way into the inner UO_2 fuel assembly and 1/3 of the way into the two MOX fuel assemblies (hatched region).

Table 4: The multiplication constant k for a 3D reactor core loaded with mixed-oxide fuel assemblies.

Code	N	L	k	Δk (pcm)	CPU time (m)
TORT S_{16}[a] (ref.)			1.04566	–	1944
BERM-AN[b]	2	3	1.04417	-149	56
	2	4	1.04420	-146	73
	3	3	1.04444	-122	120
	3	4	1.04448	-118	161
	4	3	1.04452	-114	221
	4	4	1.04455	-111	300
BERM-SP3[b]		3	1.04893	327	56
		4	1.04896	330	80

[a] With mesh size of 0.315×0.315×0.595 cm^3.
[b] With a computational cell size of 1.26×1.26×7.14 cm^3.

5.2. *Example 2: A 3D reactor core loaded with mixed-oxide fuel assemblies*

The reference geometry of this example is that of a well known 3D benchmark problem (Smith et al., 2005). As shown in Fig. 4, it represents a small reactor core surrounded by a water reflector and made of 16 fuel assemblies (a quarter core symmetry is present) half of which are loaded with mixed-oxide fuel rods. Each fuel assembly is a 17×17 array of square pin cells with side of 1.26 cm. A vacuum boundary condition is applied on the external surface of the reflector. Moreover, in order to reduce the computational burden, a (non-realistic) axial symmetry is also assumed. Fig. 5 shows the vertical section of 1/8 of the core and the boundary conditions that have to be applied. The position of the control rods is that referred in the benchmark specification as *Rodded B configuration*, i.e. they are inserted by 2/3 of the way into the inner UO_2 assembly and by 1/3 of the way into both MOX assemblies, as indicated by the hatched region in Fig. 5.

Although the original benchmark was devised in order to test deterministic transport methods and codes on realistic problems without any spatial homogenization, we have preferred, considering the approximate nature of A_N, to deal with homogenized pin cells. Thus, new sets of neutron cross sections with eight energy groups and linearly anisotropic scattering have been specially produced for all the types of pin cells of the problem by means of suitable calculations performed with the SCALE6 code (ORNL, 2009). The complete sets of cross sections for this modified benchmark problem are reported in Appendix C. These cross sections have been adopted by all the computational codes here used.

Unfortunately, for the present example, values of the average cosine of the scattering angle, $\bar{\mu}$, larger than 1/3 prevented the exact implementation into a histogram probability density function (PDF) of the linearly anisotropic Legendre representation of the scattering function, $f(\mu) = (1 + 3\bar{\mu}\mu)/2$ (here μ is the cosine of the scattering angle). As previously reported (Brown and Barnett, 2006), if $\bar{\mu} > 1/3$, the Legendre representation of the scattering can be converted into a histogram PDF only making some approximation to avoid the negative values of $f(\mu)$ that cannot be handled by a stochastic code as MCNP. We were therefore compelled to make use of a different code in order to perform the comparison and our choice was to use TORT.

Thus, the reference results have been obtained with the TORT code, using a S_{16} angular quadrature and a spatial mesh size of 0.315×0.315×0.595 cm^3. The size of the computational cells in the case of the BERM-AN calculations was coincident, on the xy plane, with the pin cell dimensions while along the z-axis a height of 1.42 cm was considered. Other than with BERM-AN, this problem had also been solved with the code BERM-SP3 (Giusti and Montagnini, 2012) using the same spatial discretization adopted for BERM-AN.

The values of the multiplication constant, k, obtained with BERM-AN, in the N approximation order from 2 to 4 (the maximum approximation order was limited, in this case, by the memory available on the computer) and with BERM-SP3, in both cases for L=3 and 4, are compared in Table 4 with the reference value obtained with TORT. Also in this case, for a fixed value of the approximation, N, the value of k for L=3 does not differ for more than a few pcm from the value obtained with L=4, while the reduction of the computing time for L=3 amounts to about 25%. The discrepancy between the BERM-AN values of k and that of reference ranges from -149 pcm (for N=2 and L=3) to -111 pcm (for N=4 and L=4). It is interesting to note that the absolute value of the discrepancy between the

Table 5: 3D reactor core loaded with mixed-oxide fuel assemblies: axially-integrated fission power in the homogenized fuel cells along the two main diagonals of the 4 fuel assemblies. Reference values obtained by TORT, normalized with respect to the average fission power over the whole reactor core, are compared with those obtained by BERM-AN, for N=2, and BERM-SP3. For the latter codes only the relative error with respect to the TORT value is shown.

	UO_2 diagonal			MOX diagonal	
TORT S_{16}	BERM-A2	BERM-SP3	TORT S_{16}	BERM-A2	BERM-SP3
0.47903	0.82%	-2.01%	2.06741	0.19%	1.22%
0.47518	0.04%	-2.65%	1.56299	0.54%	1.98%
0.46208	-0.25%	-2.89%	1.35895	0.29%	1.66%
0.45684	-0.47%	-2.93%	1.65839	-0.06%	0.96%
0.51709	-0.69%	-2.94%	1.65262	-0.01%	0.78%
0.56839	-0.69%	-2.82%	1.63121	0.10%	0.78%
0.63440	-0.84%	-2.71%	1.64288	0.03%	0.55%
0.65150	-0.97%	-2.72%	1.68301	-0.15%	0.26%
0.70799	-0.96%	-2.41%	1.75747	-0.34%	-0.19%
0.80903	-0.63%	-1.66%	1.53980	-0.22%	-0.39%
0.79865	-0.01%	-0.79%	1.69792	-0.10%	-0.47%
0.68044	0.12%	-0.49%	1.64675	-0.22%	-0.69%
0.68525	0.25%	-0.30%	1.64675	-0.22%	-0.69%
0.82723	0.42%	-0.24%	1.69792	-0.10%	-0.47%
0.92358	0.26%	-0.57%	1.53980	-0.22%	-0.39%
0.92309	0.20%	-0.96%	1.75747	-0.34%	-0.19%
0.73255	0.21%	-1.04%	1.68302	-0.15%	0.26%
0.62911	0.22%	-1.02%	1.64289	0.03%	0.55%
0.47954	0.42%	-0.84%	1.63122	0.10%	0.78%
0.41441	0.46%	-0.74%	1.65263	-0.01%	0.78%
0.30087	0.45%	-0.69%	1.65840	-0.06%	0.96%
0.21300	0.47%	-0.68%	1.35895	0.29%	1.66%
0.20789	0.36%	-0.97%	1.56300	0.54%	1.98%
0.26832	0.22%	-1.52%	2.06741	0.19%	1.22%

BERM-SP3 value of k and the reference is quite remarkable, namely 330 pcm (L=4), i.e. more than twice than the discrepancy shown by the value of k calculated by BERM-AN for N=2. This is most probably not a consequence of the different theoretical formalism of A_2 with respect to SP_3, but of the simplified treatment of the anisotropic scattering implemented into BERM-SP3, where, according to Bell and Glasstone (1970), an approximate balance, for each energy group, between the in-scattered and out-scattered neutrons is assumed. Such an approximation, however, is not made by the method described in the present paper and implemented into the BERM-AN code, where the treatment of the linearly anisotropic scattering is rigorous.

Finally, Table 5 compares the axially-integrated fission power obtained by TORT for the homogenized fuel cells along the two main diagonals of the four fuel assemblies with those calculated by BERM-AN, for N=2, and BERM-SP3. Here again, the BERM-AN results for $N = 2$ show a better agreement with respect to the reference values than the BERM-SP3 results. In particular the largest discrepancy is of -0.97% and 0.54% for the UO_2 and MOX diagonal, respectively, in case of BERM-AN while of -2.94% and 1.98% in case of BERM-SP3.

6. Conclusions

A 3D (xyz) multigroup boundary element-response matrix transport code (BERM-AN), which includes a full treatment of the linearly anisotropic scattering, is presented. The A_N approximation method on which this code is based is essentially a variant of the simplified spherical harmonics method (SP_N) and, as such, belongs to the class of the canonical SP_N methods (Larsen, 2011). However, the A_N method was originated in a way that is completely independent of SP_N (Coppa and Ravetto, 1982) and despite the essential equivalence of the two methods, some details suggest that A_N still retains its own individuality. One of these, which emerged quite early (Coppa and Ravetto, 1982), is concerning a non-local no-entry condition for the $A_1 \equiv P_1$ first moment (the scalar flux) at the boundary of an isolated, homogeneous body, V say. This condition, after being extended to all the A_N moments, can be equivalently replaced (Ciolini et al., 2002) by more intuitive conditions, in the style of the classical flux and net current continuity of neutron diffusion, at the interface with a purely absorbing medium that occupies the complement of V with respect to all space. This approach, the validity of which has been extended, in the case of isotropic scattering, to all the systems

for which the total cross section is constant (Cσ systems) (Ciolini et al., 2002), holds also in the case of linearly anisotropic scattering (Coppa et al., 1983; Ciolini et al., 2002) and is here generalized to multigroup problems. Two remarks are in order. For general (non-Cσ) systems the A_N equations have been obtained on the basis of Gelbard's approximate assumptions and the interface continuity conditions for the A_N currents have been consistently derived from the A_N equations themselves. The interface continuity conditions for the A_N fluxes are based instead on a physical plausibility argument (as it is for the classical SP_N approach) and a formal assessment of their validity can only be found in the asymptotic results by Brantley and Larsen (2000) and Larsen (2011). However, for the Cσ systems, a proof of the A_N flux continuity at an interface where the first order anisotropic scattering moment, σ_1, may have a jump, is still possible, independently of the Gelbard's assumptions. Thus we have considered that the A_N flux interface conditions were also reasonably well assessed and decided, even for a general non-Cσ system, to replace the usual no-entry conditions by interface conditions with an absorbing extra region surrounding the original system. The increased heaviness of the computations has been shown to be quite acceptable. Of course, any finite element method could be applied to solve a problem of this kind, but the above analysis of the interface conditions gives indeed a strong suggestion to fully exploit the boundary element method. This suggestion was also followed in previous papers and, with a greater generality, in the present one. Taking advantage of the fact that the system of the classical boundary integral equations into which the A_N partial differential equations are transformed can be given a partial current form, an iterative process involving the A_N partial currents is set down. A moment projection method (see Cossa et al. (2010), Giusti and Montagnini (2012) other than the literature therein) is used to numerically solve the boundary integral equations and determine the response matrix of each region of the system. A coupling matrix is then introduced in order to perform the final calculations at the level of the whole system, to evaluate (in the case of criticality problems) the multiplication constant and the overall flux distribution. The numerical examples presented in sect.5 illustrate the high accuracy of the present method as well as its good computational efficiency.

Appendix A.

The source point $\mathbf{r}_0$ in Eq. (52) will be taken as the origin of the reference system and the functions $\tilde{\phi}_\gamma^{(\nu)}(\mathbf{r})$ simply denoted by $\tilde{\phi}_\gamma^{(\nu)}(r)$, with $r = |\mathbf{r}|$, owing to their radial symmetry. It will suffice to consider a single system, for instance that for $\nu = 1$, so that we have

$$-\sum_{\gamma=1}^{\Gamma} D^*_{\gamma'\gamma} \nabla_r^2 \tilde{\phi}_\gamma^{(1)}(r) + \sum_{\gamma=1}^{\Gamma} \Sigma^*_{\gamma'\gamma} \tilde{\phi}_\gamma^{(1)}(r) = \delta(r)\,\delta_{\gamma' 1}, \quad (\gamma' = 1, \ldots, \Gamma)\,. \tag{A.1}$$

Let us first seek for solutions holding on the interval $\epsilon \le r < \infty$, with $\epsilon > 0$, i.e. excluding the points belonging to a small sphere of radius ϵ centred at the point source. Then the right hand side of Eq. (A.1) vanishes and this equation is replaced by the corresponding homogeneous equation

$$-\sum_{\gamma=1}^{\Gamma} D^*_{\gamma'\gamma} \nabla_r^2 \tilde{\phi}_\gamma^{(1)}(r) + \sum_{\gamma=1}^{\Gamma} \Sigma^*_{\gamma'\gamma} \tilde{\phi}_\gamma^{(1)}(r) = 0, \quad (\gamma' = 1, \ldots, \Gamma)\,. \tag{A.2}$$

A sum of solutions of the type $\xi_\gamma e^{-\kappa r}/4\pi r$ appears to be plausible, with κ real or complex (the factor $1/4\pi$ is for convenience). Substituting into Eq. (A.2) and observing that $\nabla^2_{\mathbf{r}}\left(e^{-\kappa r}/4\pi r\right) = \kappa^2\left(e^{-\kappa r}/4\pi r\right)$ the following linear system for the ξ_γ's is obtained

$$\sum_{\gamma=1}^{\Gamma} \left(-\kappa^2 D^*_{\gamma'\gamma} + \Sigma^*_{\gamma'\gamma}\right)\xi_\gamma = 0 \quad (\gamma' = 1, \ldots, \Gamma)\,. \tag{A.3}$$

In a compact matrix form we can write

$$\left(-\kappa^2 \mathbf{D}^* + \mathbf{\Sigma}^*\right)\boldsymbol{\xi} = 0 \tag{A.4}$$

or even, upon inversion of the $\mathbf{D}^*$ matrix,

$$\mathbf{Q}\boldsymbol{\xi} = \kappa^2 \boldsymbol{\xi} \tag{A.5}$$

where $\mathbf{Q} = \mathbf{D}^{*-1}\mathbf{\Sigma}^*$. Let κ_h^2, $\boldsymbol{\xi}^{(h)} = [\xi_1, \ldots, \xi_\Gamma]^T$ be the eigenvalues, respectively the eigenvectors (the latters being assumed to be linearly independent and normalized according to the usual l^2 norm) of this eigenvalue problem. The solutions $\tilde{\phi}_\gamma(r)$, which are therefore also linearly independent, can be written as follows

$$\tilde{\phi}_\gamma(r) = \sum_{h=1}^{\Gamma} g_h \xi_\gamma^{(h)} \frac{e^{-\kappa_h r}}{4\pi r} \quad (\gamma = 1, \ldots, \Gamma) \tag{A.6}$$

where the g_h coefficients are still to be determined. To do so, the net currents at $r = \epsilon$ are first evaluated

$$\tilde{J}_{n,\gamma'}(\epsilon) = -\sum_{\gamma=1}^{\Gamma} D_{\gamma'\gamma}^* \left(\frac{\mathrm{d}\tilde{\phi}_\gamma}{\mathrm{d}r}\right)_{r=\epsilon} = \sum_{\gamma=1}^{\Gamma} D_{\gamma'\gamma}^* \sum_{h=1}^{\Gamma} g_h \xi_\gamma^{(h)} \frac{e^{-\kappa_h \epsilon}}{4\pi\epsilon^2}(1 + \kappa_h \epsilon). \tag{A.7}$$

Integration of Eq. (A.1) over the volume of the small sphere surrounding the source, followed by an application of the divergence theorem, shows that

$$4\pi\epsilon^2 \tilde{J}_{n,\gamma'}(\epsilon) + O(\epsilon) = \delta_{\gamma' 1} \tag{A.8}$$

where it has been observed that the integrals involving $\Sigma_{\gamma'\gamma}^* \tilde{\phi}_\gamma$ are $O(\epsilon)$. Taking the limit as $\epsilon \to 0$ and using Eq. (A.7) yields

$$\sum_{\gamma=1}^{\Gamma} D_{\gamma'\gamma}^* \sum_{h=1}^{\Gamma} g_h \xi_\gamma^{(h)} = \delta_{\gamma' 1} \tag{A.9}$$

or, restoring a general ν and setting $A_{\gamma' h} = \sum_{\gamma=1}^{\Gamma} D_{\gamma'\gamma}^* \xi_\gamma^{(h)}$,

$$\sum_{h=1}^{\Gamma} A_{\gamma' h} g_h^{(\nu)} = \delta_{\gamma'\nu} \quad (\gamma' = 1, \ldots, \Gamma). \tag{A.10}$$

Thus, the solution of these non-homogeneous linear systems for each $\nu = 1, \ldots, \Gamma$ gives the coefficients $g_h^{(\nu)}$ and completes the evaluation of the fundamental functions $\tilde{\phi}_\gamma^{(\nu)}$:

$$\tilde{\phi}_\gamma^{(\nu)}(\mathbf{r}_0, \mathbf{r}) = \sum_{h=1}^{\Gamma} g_h^{(\nu)} \xi_\gamma^{(h)} \frac{e^{-\kappa_h |\mathbf{r} - \mathbf{r}_0|}}{4\pi |\mathbf{r} - \mathbf{r}_0|} \quad (\gamma = 1, \ldots, \Gamma; \nu = 1, \ldots, \Gamma) \tag{A.11}$$

where the point source has been again placed at an arbitrary point $\mathbf{r}_0$. A warning is necessary as regards the eigenvalues of Eq. (A.5), i.e. the "decay constants" κ_h. If the scattering is isotropic, it has been proved (Ciolini et al., 2002) that the parameters κ_h are all distinct and positive. More complicate problems (anisotropic scattering and multigroup problems, other than, of course, the problems referring to multiplying systems) may involve complex eigenvalues, a circumstance that is considered in Cossa et al. (2010) and Saracco et al. (2012); the $\mathbf{Q}$ matrix of the first paper corresponds essentially to minus the $\mathbf{Q}$ matrix now introduced and the κ^2 eigenvalue is now replacing $-B^2$. The following conclusions are drawn: (*i*) if $\kappa_h^2 > 0$, then one must simply take for κ_h the positive root of κ_h^2, (*ii*) if $\kappa_h^2 < 0$, then $\kappa_h = i\beta_h$, where β_h is the positive root of $-\kappa_h^2$, (*iii*) if κ_h^2 is complex, setting $-\kappa_h^2 = \zeta_h + i\eta_h$ one has $\kappa_h = \gamma_h + i\beta_h$, where $\beta_h = \left(1/\sqrt{2}\right)\left(\sqrt{\zeta_h^2 + \eta_h^2} + \zeta_h\right)^{1/2}$, $\gamma_h = \left(1/\sqrt{2}\right)\left(\sqrt{\zeta_h^2 + \eta_h^2} - \zeta_h\right)^{1/2}$. In the first and third case the fundamental solutions are exponentially decaying as $\rho = |\mathbf{r} - \mathbf{r}_0|$ tends to infinity, while in the second case the asymptotic behaviour is only $O(1/\rho)$. However, the Sommerfeld radiation condition, i.e.

$$\lim_{\rho \to \infty} \rho \left(\frac{\mathrm{d}}{\mathrm{d}\rho} + i\beta_h\right) \frac{e^{-i\beta_h \rho}}{4\pi\rho} = 0 \tag{A.12}$$

is fulfilled and the uniqueness of the corresponding fundamental solution still ensured. The determination of the fundamental solutions is therefore completed.

Appendix B.

Let the $\mathbb{R}^3$ space be occupied by a medium the total cross section of which, σ, is everywhere constant, while the space dependence of the other cross sections is arbitrary, with the only condition that the neutron scattering vanishes identically outside a large sphere S_0. Let, moreover, S_1 be another sphere that contains S_0 in its interior. The trajectory-integrated monokinetic transport equation to be considered is as follows

$$\psi(\mathbf{r},\mathbf{\Omega}) = \int_0^{R_1(\mathbf{r},\mathbf{\Omega})} \left[\sigma_s(\mathbf{r}-R\mathbf{\Omega},\mathbf{\Omega}\cdot\mathbf{\Omega}')\,\psi(\mathbf{r}-R\mathbf{\Omega},\mathbf{\Omega}')\,\mathrm{d}\Omega' + \frac{1}{4\pi}s(\mathbf{r}-R\mathbf{\Omega})\right] e^{-\sigma R}\,\mathrm{d}R, \tag{B.1}$$

where $\psi(\mathbf{r},\mathbf{\Omega})$ is the angular flux along, σ the total cross section (spatially constant), $\mathbf{\Omega}$, $\sigma_s(\mathbf{r},\mathbf{\Omega}\cdot\mathbf{\Omega}')$ the scattering differential cross section, $s(\mathbf{r})$ the neutron source, also vanishing outside S_0 and assumed to be isotropic, while $R_1(\mathbf{r},\mathbf{\Omega})$ is such that $\mathbf{r}-R_1(\mathbf{r},\mathbf{\Omega})\,\mathbf{\Omega}$ denotes the point where the line $\mathbf{r}-R\mathbf{\Omega}$ intersects the sphere S_1 (and where the ingoing angular flux is obviously equal to zero). If the scattering is linearly anisotropic we may write

$$\sigma_s(\mathbf{r},\mathbf{\Omega}\cdot\mathbf{\Omega}') = \frac{1}{4\pi}\left[\sigma_0(\mathbf{r}) + 3\sigma_1(\mathbf{r})\,\mathbf{\Omega}\cdot\mathbf{\Omega}'\right], \tag{B.2}$$

where σ_0, σ_1 have the same meaning as in sect.2 (for a one-group setting). After introducing expression (B.2) into Eq. (B.1) and setting, as customary,

$$\Phi(\mathbf{r}) = \int_{4\pi}\psi(\mathbf{r},\mathbf{\Omega})\,\mathrm{d}\Omega \tag{B.3}$$

$$\mathbf{J}(\mathbf{r}) = \int_{4\pi}\psi(\mathbf{r},\mathbf{\Omega})\,\mathbf{\Omega}\,\mathrm{d}\Omega \tag{B.4}$$

for the scalar flux and the current vector, we can perform the integration on Ω' and obtain

$$\psi(\mathbf{r},\mathbf{\Omega}) = \frac{1}{4\pi}\int_0^{R_1(\mathbf{r},\mathbf{\Omega})} \left[\sigma_0(\mathbf{r}-R\mathbf{\Omega})\,\Phi(\mathbf{r}-R\mathbf{\Omega}) + 3\sigma_1(\mathbf{r}-R\mathbf{\Omega})\,\mathbf{\Omega}\cdot\mathbf{J}(\mathbf{r}-R\mathbf{\Omega}) + s(\mathbf{r},\mathbf{\Omega})\right] e^{-\sigma R}\,\mathrm{d}R. \tag{B.5}$$

By integrating both sides of this equation on $\mathbf{\Omega}$ and putting $\mathbf{r}-R\mathbf{\Omega} = \mathbf{r}'$ we can replace, according to the usual procedure, the $\mathrm{d}R\,\mathrm{d}\Omega$ integral by a volume integral over V_1 (it is also convenient to separate the integrals involving σ_0 and σ_1), while $\psi(\mathbf{r},\mathbf{\Omega})$ reduces to $\Phi(\mathbf{r})$:

$$\Phi(\mathbf{r}) = \int_{V_1}\left[\sigma_0(\mathbf{r}')\,\Phi(\mathbf{r}') + s(\mathbf{r}')\right]\frac{e^{-\sigma|\mathbf{r}-\mathbf{r}'|}}{4\pi|\mathbf{r}-\mathbf{r}'|^2}\,\mathrm{d}V' + 3\int_{V_1}\sigma_1(\mathbf{r}')\,\mathbf{J}(\mathbf{r}')\cdot\frac{\mathbf{r}-\mathbf{r}'}{|\mathbf{r}-\mathbf{r}'|}\frac{e^{-\sigma|\mathbf{r}-\mathbf{r}'|}}{4\pi|\mathbf{r}-\mathbf{r}'|^2}\,\mathrm{d}V'. \tag{B.6}$$

Proceeding as in Davison and Sykes (1957), Ch. XVII, we observe that

$$(\mathbf{r}-\mathbf{r}')\frac{e^{-\sigma|\mathbf{r}-\mathbf{r}'|}}{4\pi|\mathbf{r}-\mathbf{r}'|^3} = \nabla_{\mathbf{r}'}\int_{|\mathbf{r}-\mathbf{r}'|}^{\infty} e^{-\sigma s}\frac{\mathrm{d}s}{s^2} = \nabla_{\mathbf{r}'}\left[\frac{1}{|\mathbf{r}-\mathbf{r}'|}E_2(\sigma|\mathbf{r}-\mathbf{r}'|)\right], \tag{B.7}$$

where $E_2(x) = \int_1^\infty e^{-xt}t^{-2}\,\mathrm{d}t = \int_0^1 e^{-x/\mu}\,\mathrm{d}\mu$ is the exponential integral of order two. Then, Eq. (B.6) can be written as follows

$$\Phi(\mathbf{r}) = \int_{V_1}\left[\sigma_0(\mathbf{r}')\,\Phi(\mathbf{r}') + s(\mathbf{r}')\right]\frac{e^{-\sigma|\mathbf{r}-\mathbf{r}'|}}{4\pi|\mathbf{r}-\mathbf{r}'|^2}\,\mathrm{d}V' + 3\int_{V_1}\sigma_1(\mathbf{r}')\,\mathbf{J}(\mathbf{r}')\cdot\nabla_{\mathbf{r}'}\left[\frac{1}{4\pi|\mathbf{r}-\mathbf{r}'|}E_2(\sigma|\mathbf{r}-\mathbf{r}'|)\right]\mathrm{d}V' \tag{B.8}$$

or, by Gauss's theorem,

$$\Phi(\mathbf{r}) = \int_{V_1} [\sigma_0(\mathbf{r}')\Phi(\mathbf{r}') + s(\mathbf{r}')] \frac{e^{-\sigma|\mathbf{r}-\mathbf{r}'|}}{4\pi|\mathbf{r}-\mathbf{r}'|^2} \, dV' - 3\int_{V_1} \frac{1}{4\pi|\mathbf{r}-\mathbf{r}'|} E_2(\sigma|\mathbf{r}-\mathbf{r}'|) \nabla_{\mathbf{r}'} \cdot [\sigma_1(\mathbf{r}')\mathbf{J}(\mathbf{r}')] \, dV' + 3\int_{S_1} \frac{1}{4\pi|\mathbf{r}-\mathbf{r}'_S|} E_2(\sigma|\mathbf{r}-\mathbf{r}'_S|) \sigma_1(\mathbf{r}'_S)\mathbf{J}(\mathbf{r}'_S) \cdot \mathbf{n}'_S \, dS'. \tag{B.9}$$

The surface integral (in which $\mathbf{n}'_S$ denotes the outer normal) is clearly equal to zero, since $\sigma_1 = 0$ on S_1.

Now we introduce the following A_N quadrature formulas, namely

$$\frac{e^{-\sigma r}}{4\pi r^2} = \frac{\sigma}{4\pi r}\int_0^1 e^{-\sigma r/\mu}\frac{d\mu}{\mu^2} \simeq \sum_{\alpha=1}^{N} w_\alpha \frac{\sigma e^{-\sigma r/\mu_\alpha}}{4\pi r \mu_\alpha^2} \tag{B.10}$$

$$\frac{1}{4\pi r}E_2(\sigma r) = \frac{1}{4\pi r}\int_0^1 e^{-\sigma r/\mu}\, d\mu \simeq \sum_{\alpha=1}^{N} w_\alpha \frac{e^{-\sigma r/\mu_\alpha}}{4\pi r}, \tag{B.11}$$

where μ_α and w_α are the points and weights of the $2N$ Gauss quadrature formula. Setting

$$\phi_\alpha(\mathbf{r}) = \int_{V_1} \frac{\sigma e^{-\sigma|\mathbf{r}-\mathbf{r}'|/\mu_\alpha}}{4\pi\mu_\alpha^2|\mathbf{r}-\mathbf{r}'|} \left\{\sigma_0(\mathbf{r}')\Phi(\mathbf{r}') + s(\mathbf{r}') - 3\frac{\mu_\alpha^2}{\sigma}\nabla_{\mathbf{r}'} \cdot [\sigma_1(\mathbf{r}')\mathbf{J}(\mathbf{r}')]\right\} dV' \quad (\alpha = 1, \ldots, N) \tag{B.12}$$

we see that

$$\Phi(\mathbf{r}) = \sum_{\alpha=1}^{N} w_\alpha \phi_\alpha(\mathbf{r}) \tag{B.13}$$

and, applying the operator $\left(\mu_\alpha^2/\sigma\right)\nabla_{\mathbf{r}}^2$ to both sides of Eqs. (B.12) and observing that the function

$$\tilde{\Phi}_\alpha(\mathbf{r}, \mathbf{r}') = \frac{\sigma e^{-\sigma|\mathbf{r}-\mathbf{r}'|/\mu_\alpha}}{4\pi\mu_\alpha^2|\mathbf{r}-\mathbf{r}'|} \tag{B.14}$$

is the Green function of the diffusion equation for an infinite medium with the point source at $\mathbf{r}'$, i.e.

$$\frac{\mu_\alpha^2}{\sigma}\nabla_{\mathbf{r}}^2\tilde{\phi}_\alpha - \sigma\tilde{\phi}_\alpha + \delta(\mathbf{r}-\mathbf{r}') = 0, \tag{B.15}$$

it is readily seen that Eqs. (B.12) can be replaced by the following differential equations

$$\frac{\mu_\alpha^2}{\sigma}\nabla_{\mathbf{r}}^2\phi_\alpha(\mathbf{r}) - \sigma\phi_\alpha(\mathbf{r}) + \sigma_0(\mathbf{r})\Phi(\mathbf{r}) + s(\mathbf{r}) - 3\frac{\mu_\alpha^2}{\sigma}\nabla_{\mathbf{r}} \cdot [\sigma_1(\mathbf{r})\mathbf{J}(\mathbf{r})] = 0 \quad (\alpha = 1, \ldots, N) \tag{B.16}$$

which coincide, on account of Eq. (B.13) with the A_N differential equations with linearly anisotropic scattering, see Eqs. (13) in the text, for the monokinetic case with constant total cross section. Note that s source is here comprising both the fission and the external source. The ϕ_α functions can therefore be identified with the A_N fluxes considered in the paper.

Coming back to Eqs. (B.12) let us arrange them as follows

$$\phi_\alpha(\mathbf{r}) = \phi_\alpha^{(1)}(\mathbf{r}) + \phi_\alpha^{(2)}(\mathbf{r}) \tag{B.17}$$

where

$$\phi_\alpha^{(1)}(\mathbf{r}) = \int_{V_1} \frac{\sigma e^{-\sigma|\mathbf{r}-\mathbf{r}'|/\mu_\alpha}}{4\pi\mu_\alpha^2|\mathbf{r}-\mathbf{r}'|}\left[\sigma_0(\mathbf{r}')\,\Phi(\mathbf{r}') + s(\mathbf{r}')\right] dV' \tag{B.18}$$

$$\phi_\alpha^{(2)}(\mathbf{r}) = -3\int_{V_1} \frac{e^{-\sigma|\mathbf{r}-\mathbf{r}'|/\mu_\alpha}}{4\pi|\mathbf{r}-\mathbf{r}'|}\nabla_{\mathbf{r}'}\cdot\left[\sigma_1(\mathbf{r}')\,\mathbf{J}(\mathbf{r}')\right] dV'. \tag{B.19}$$

A theorem of potential theory states that, since the kernel of Eq. (B.18) is $O(1/|\mathbf{r}-\mathbf{r}'|)$, if the function on which it applies (the sum in square brackets) is piecewise continuous, or even summable, on V_1 (which should be easily admitted) then $\phi_\alpha^{(1)}(\mathbf{r})$ is everywhere continuous, together with its partial derivatives of the first order ((Miranda (1955, Ch. II), Sternberg and Smith (1961, Ch. V, sect.2), Kellogg (1967, Ch. VI, sect.3)).

It remains to investigate Eqs. (B.19), in particular for the important case in which V_1 contains two regions, V^I and V^{II} say, such that $\sigma_1(\mathbf{r})$, albeit continuous inside each one of them, takes different values, $\sigma_1^I(\mathbf{r}_S)$ and $\sigma_1^{II}(\mathbf{r}_S)$ say, when approaching the interface between the two. By applying the same argument as in sect. 2, concerning the continuity at the interface of the A_N currents, we have (see again Fig. (1); notations are the same as the ones used there):

$$\begin{aligned}\int_{\Delta V}\nabla_{\mathbf{r}}\cdot\left[\sigma_1(\mathbf{r})\,\mathbf{J}(\mathbf{r})\right] dV = &\int_{\Delta\hat{S}^{II}}\sigma_1\left(\mathbf{r}_S+\epsilon\mathbf{n}_S^{II}\right)\mathbf{J}\left(\mathbf{r}_S+\epsilon\mathbf{n}_S^{II}\right)\cdot\mathbf{n}_S^{II}\,dS\\ &+\int_{\Delta\hat{S}^{I}}\sigma_1\left(\mathbf{r}_S+\epsilon\mathbf{n}_S^{I}\right)\mathbf{J}\left(\mathbf{r}_S+\epsilon\mathbf{n}_S^{I}\right)\cdot\mathbf{n}_S^{I}\,dS + O(\epsilon)\end{aligned} \tag{B.20}$$

so that the volume integral on the l.h.s. is equal, in the limit, to

$$\int_{\Delta\hat{S}}\left[\sigma_1^I(\mathbf{r}_S)-\sigma_1^{II}(\mathbf{r}_S)\right]J_{n_S}(\mathbf{r}_S)\,dS \tag{B.21}$$

(the continuity of J_{n_S} has also been used, Remark 2 of sect. 2) and can be seen as a volume integral containing a δ-function source laid on $\Delta\hat{S}$, the part of the interface that is contained in ΔV:

$$\int_{\Delta V}\left[\sigma_1^I(\mathbf{r}_S+t\mathbf{n}_S)-\sigma_1^{II}(\mathbf{r}_S+t\mathbf{n}_S)\right]J_{n_S}(\mathbf{r}_S+t\mathbf{n}_S)\,\delta(\mathbf{r}_S+t\mathbf{n}_S)\,dS\,dt. \tag{B.22}$$

In the language of potential theory, the source is expressed by a simple layer surface distribution on $\Delta\hat{S}$ with the charge density

$$\left[\sigma_1^I(\mathbf{r}_S)-\sigma_1^{II}(\mathbf{r}_S)\right]J_{n_S}(\mathbf{r}_S). \tag{B.23}$$

The contribution of the discontinuity surface of $\sigma_1(\mathbf{r})$ to the term $\phi_\alpha^{(2)}$ is therefore, in general,

$$-3\int_S \frac{e^{-\sigma|\mathbf{r}-\mathbf{r}'_S|/\mu_\alpha}}{4\pi|\mathbf{r}-\mathbf{r}'_S|}\left[\sigma_1^I(\mathbf{r}'_S)-\sigma_1^{II}(\mathbf{r}'_S)\right]J_{n_S}(\mathbf{r}'_S)\,dS' \tag{B.24}$$

and known theorems (Miranda (1955, Ch. II), Sternberg and Smith (1961, Ch. V, sect.4 and 6)) state that this contribution is continuous across the interface. We conclude that, even for a (finite) number of discontinuity surfaces of $\sigma_1(\mathbf{r})$, the term $\phi_\alpha^{(2)}(\mathbf{r})$ is continuous and therefore any $\phi_\alpha(\mathbf{r})$ ($\alpha = 1,\ldots,N$) is continuous at such discontinuity surfaces.

Appendix C.

The following table shows the eight energy group sets of cross sections, with linearly anisotropic scattering, used for the eight materials of the example reported in sect. 5.2. These sets have been employed for all the simulations with the BERM-AN, BERM-SP3 and TORT codes.

Mixture 1: homogenized UO_2 fuel cell.								
	Group							
	1	2	3	4	5	6	7	8
Σ_t	2.27699E-01	4.37750E-01	8.48733E-01	1.05439E+00	1.03541E+00	1.05303E+00	1.24254E+00	2.02577E+00
$\nu\Sigma_f$	1.18219E-02	6.20591E-04	9.08511E-04	8.22277E-03	9.88891E-03	1.76651E-02	4.87739E-02	1.36604E-01
χ	5.98360E-01	3.50904E-01	5.07305E-02	5.50000E-06	-	-	-	-
Σ_{s0}								
1	1.37585E-01	7.01417E-02	1.51514E-02	4.79079E-05	6.01237E-07	3.97058E-08	1.07384E-08	7.46715E-13
2	-	3.22109E-01	1.13994E-01	4.30913E-04	5.47422E-06	3.66589E-07	1.78996E-07	2.39359E-08
3	-	-	7.38882E-01	1.04247E-01	1.29494E-03	8.67181E-05	4.26854E-05	1.33791E-05
4	-	-	-	8.58783E-01	1.52764E-01	9.99125E-03	4.91805E-03	1.55289E-03
5	-	-	-	-	6.99407E-01	1.89715E-01	8.86912E-02	2.37434E-02
6	-	-	-	-	8.08106E-04	5.56896E-01	3.92621E-01	8.35331E-02
7	-	-	-	-	-	2.16496E-03	8.17938E-01	3.79548E-01
8	-	-	-	-	-	5.84950E-21	2.36009E-02	1.88684E+00
Σ_{s1}								
1	7.13917E-02	2.66555E-02	2.83042E-03	2.35612E-06	1.39797E-07	2.32277E-08	8.86583E-09	-
2	-	1.28387E-01	4.90500E-02	2.12813E-05	6.34947E-07	1.05614E-07	8.86847E-08	1.91086E-08
3	-	-	3.51967E-01	4.52757E-02	8.61703E-05	4.03807E-06	2.44987E-06	1.72696E-06
4	-	-	-	4.43503E-01	6.99653E-02	1.75674E-03	5.23953E-04	9.06730E-05
5	-	-	-	-	3.84973E-01	9.91290E-02	2.50231E-02	1.96935E-03
6	-	-	-	-	3.98603E-04	2.91823E-01	1.63351E-01	4.94307E-03
7	-	-	-	-	-	1.04627E-03	3.89107E-01	4.70663E-02
8	-	-	-	-	-	-3.37653E-21	5.53017E-03	3.82463E-01
Mixture 2: homogenized MOX 4.0% fuel cell.								
	Group							
	1	2	3	4	5	6	7	8
Σ_t	2.26710E-01	4.37766E-01	8.49347E-01	1.06286E+00	1.04976E+00	1.14035E+00	1.55596E+00	2.23436E+00
$\nu\Sigma_f$	1.32385E-02	1.77845E-03	1.83466E-03	1.79311E-02	3.38421E-02	3.58921E-02	4.63058E-01	4.28672E-01
χ	5.98360E-01	3.50904E-01	5.07305E-02	5.50000E-06	-	-	-	-
Σ_{s0}								
1	1.37891E-01	6.87607E-02	1.48734E-02	4.69897E-05	5.89706E-07	3.88883E-08	1.04247E-08	8.18127E-13
2	-	3.21988E-01	1.13781E-01	4.30321E-04	5.46668E-06	3.66085E-07	1.78736E-07	2.38658E-08
3	-	-	7.39230E-01	1.04130E-01	1.29351E-03	8.66220E-05	4.26380E-05	1.33641E-05
4	-	-	-	8.62980E-01	1.51216E-01	9.89371E-03	4.87002E-03	1.53773E-03
5	-	-	-	-	6.99756E-01	1.91377E-01	8.94809E-02	2.39498E-02
6	-	-	-	-	9.20879E-04	5.69768E-01	4.01803E-01	8.55020E-02
7	-	-	-	-	-	3.55271E-03	8.98590E-01	3.70567E-01
8	-	-	-	-	-	7.34781E-21	2.98049E-02	1.94259E+00
Σ_{s1}								
1	7.17290E-02	2.60752E-02	2.76721E-03	2.31520E-06	1.37735E-07	2.28260E-08	8.61153E-09	-
2	-	1.28550E-01	4.89637E-02	2.12485E-05	6.34473E-07	1.05540E-07	8.86087E-08	1.90539E-08
3	-	-	3.52157E-01	4.52107E-02	8.60573E-05	4.03423E-06	2.44804E-06	1.72577E-06
4	-	-	-	4.45630E-01	6.91123E-02	1.73518E-03	5.17653E-04	8.97307E-05
5	-	-	-	-	3.85933E-01	1.00105E-01	2.52676E-02	1.98820E-03
6	-	-	-	-	4.54630E-04	3.02211E-01	1.66938E-01	5.05147E-03
7	-	-	-	-	-	1.73559E-03	4.44180E-01	4.27903E-02
8	-	-	-	-	-	-4.23830E-21	7.65897E-03	4.12690E-01
Mixture 3: homogenized MOX 7.0% fuel cell.								
	Group							
	1	2	3	4	5	6	7	8
Σ_t	2.26747E-01	4.37890E-01	8.49880E-01	1.07129E+00	1.06172E+00	1.18230E+00	1.68098E+00	2.40261E+00
$\nu\Sigma_f$	1.43938E-02	2.92197E-03	3.12912E-03	2.86879E-02	5.21130E-02	5.94414E-02	6.17905E-01	6.38335E-01
χ	5.98360E-01	3.50904E-01	5.07305E-02	5.50000E-06	-	-	-	-
Σ_{s0}								
1	1.37937E-01	6.84879E-02	1.48081E-02	4.69377E-05	5.89176E-07	3.88503E-08	1.04078E-08	8.23408E-13
2	-	3.21830E-01	1.13687E-01	4.30067E-04	5.46346E-06	3.65869E-07	1.78625E-07	2.38364E-08
3	-	-	7.39418E-01	1.03895E-01	1.29063E-03	8.64297E-05	4.25434E-05	1.33342E-05
4	-	-	-	8.66880E-01	1.49699E-01	9.79772E-03	4.82276E-03	1.52281E-03
5	-	-	-	-	7.01026E-01	1.92287E-01	8.99250E-02	2.40719E-02
6	-	-	-	-	9.68941E-04	5.76810E-01	4.05630E-01	8.64164E-02
7	-	-	-	-	-	3.94087E-03	9.30226E-01	3.76151E-01
8	-	-	-	-	-	8.10988E-21	3.35768E-02	2.00165E+00
Σ_{s1}								
1	7.17830E-02	2.60453E-02	2.76336E-03	2.31152E-06	1.37653E-07	2.28091E-08	8.59807E-09	-
2	-	1.28654E-01	4.89257E-02	2.12346E-05	6.34260E-07	1.05506E-07	8.85757E-08	1.90310E-08
3	-	-	3.52307E-01	4.50870E-02	8.58383E-05	4.02637E-06	2.44409E-06	1.72317E-06
4	-	-	-	4.47840E-01	6.82613E-02	1.71372E-03	5.11380E-04	8.87970E-05
5	-	-	-	-	3.87177E-01	1.00616E-01	2.53988E-02	2.00016E-03
6	-	-	-	-	4.78247E-04	3.07720E-01	1.68508E-01	5.09670E-03
7	-	-	-	-	-	1.94199E-03	4.66863E-01	4.26360E-02
8	-	-	-	-	-	-4.67640E-21	8.99100E-03	4.35117E-01

Mixture 4: homogenized MOX 8.7% fuel cell.

	Group							
	1	2	3	4	5	6	7	8
Σ_f	2.26775E-01	4.37938E-01	8.50151E-01	1.07557E+00	1.06760E+00	1.20288E+00	1.73427E+00	2.48416E+00
$\nu\Sigma_f$	1.50477E-02	3.57084E-03	3.86167E-03	3.43218E-02	6.12760E-02	7.21971E-02	6.81908E-01	7.32525E-01
χ	5.98360E-01	3.50904E-01	5.07305E-02	5.50000E-06	-	-	-	-
Σ_{s0}								
1	1.37951E-01	6.83492E-02	1.47742E-02	4.69207E-05	5.89034E-07	3.88399E-08	1.04028E-08	8.25273E-13
2	-	3.21719E-01	1.13632E-01	4.29923E-04	5.46165E-06	3.65746E-07	1.78562E-07	2.38203E-08
3	-	-	7.39494E-01	1.03762E-01	1.28901E-03	8.63206E-05	4.24901E-05	1.33173E-05
4	-	-	-	8.68788E-01	1.48970E-01	9.75150E-03	4.80002E-03	1.51563E-03
5	-	-	-	-	7.01720E-01	1.92688E-01	9.01247E-02	2.41280E-02
6	-	-	-	-	9.91485E-04	5.80306E-01	4.07442E-01	8.68605E-02
7	-	-	-	-	-	4.07013E-03	9.43254E-01	3.80301E-01
8	-	-	-	-	-	8.37196E-21	3.51106E-02	2.03399E+00
Σ_{s1}								
1	7.18070E-02	2.60367E-02	2.76204E-03	2.30997E-06	1.37635E-07	2.28048E-08	8.59413E-09	-
2	-	1.28707E-01	4.89050E-02	2.12268E-05	6.34137E-07	1.05486E-07	8.85557E-08	1.90184E-08
3	-	-	3.52390E-01	4.50173E-02	8.57150E-05	4.02193E-06	2.44186E-06	1.72169E-06
4	-	-	-	4.48943E-01	6.78533E-02	1.70344E-03	5.08377E-04	8.83497E-05
5	-	-	-	-	3.87837E-01	1.00840E-01	2.54568E-02	2.00589E-03
6	-	-	-	-	4.89323E-04	3.10445E-01	1.69264E-01	5.11823E-03
7	-	-	-	-	-	2.01528E-03	4.76493E-01	4.29020E-02
8	-	-	-	-	-	-4.82703E-21	9.54580E-03	4.45713E-01

Mixture 5: fission chamber guide tube cell.

	Group							
	1	2	3	4	5	6	7	8
Σ_f	7.52979E-02	1.61294E-01	3.46805E-01	4.12538E-01	4.17652E-01	4.36580E-01	5.21727E-01	8.62641E-01
Σ_{s0}								
1	4.28923E-02	2.63531E-02	5.87679E-03	2.23650E-05	2.83486E-07	1.86967E-08	5.08076E-09	7.88327E-13
2	-	1.08748E-01	5.22870E-02	2.09601E-04	2.66343E-06	1.78361E-07	8.71286E-08	1.18727E-08
3	-	-	2.89902E-01	5.59028E-02	7.00608E-04	4.69172E-05	2.30942E-05	7.24469E-06
4	-	-	-	3.26006E-01	7.73602E-02	5.10285E-03	2.51179E-03	7.93117E-04
5	-	-	-	-	2.76209E-01	8.73557E-02	4.15094E-02	1.10906E-02
6	-	-	-	-	2.85263E-04	2.15108E-01	1.79138E-01	3.88628E-02
7	-	-	-	-	-	6.71995E-04	3.22892E-01	1.91956E-01
8	-	-	-	-	-	-	7.84316E-03	8.37815E-01
Σ_{s1}								
1	2.28023E-02	1.28927E-02	1.31751E-03	1.07367E-06	6.59030E-08	1.09206E-08	4.19047E-09	-
2	-	5.21333E-02	2.47856E-02	1.03755E-05	3.06708E-07	5.09933E-08	4.28537E-08	9.46310E-09
3	-	-	1.62533E-01	2.51534E-02	4.71277E-05	2.15319E-06	1.28726E-06	9.05400E-07
4	-	-	-	1.97613E-01	3.69473E-02	9.21570E-04	2.74247E-04	4.67327E-05
5	-	-	-	-	1.73599E-01	4.70403E-02	1.17511E-02	9.18660E-04
6	-	-	-	-	1.76790E-04	1.32623E-01	7.71420E-02	2.30380E-03
7	-	-	-	-	-	3.85853E-04	1.72240E-01	2.74342E-02
8	-	-	-	-	-	-	1.72522E-03	1.68001E-01

Mixture 6: control rod guide tube cell.

	Group							
	1	2	3	4	5	6	7	8
Σ_f	2.18662E-01	4.94064E-01	1.13054E+00	1.38038E+00	1.39800E+00	1.46332E+00	1.76008E+00	2.95009E+00
Σ_{s0}								
1	1.17021E-01	8.22984E-02	1.87518E-02	7.65941E-05	9.72551E-07	6.40489E-08	1.70885E-08	8.49734E-13
2	-	3.10561E-01	1.82703E-01	7.36525E-04	9.35920E-06	6.26757E-07	3.06104E-07	4.15634E-08
3	-	-	9.30529E-01	1.96974E-01	2.47162E-03	1.65515E-04	8.14718E-05	2.55580E-05
4	-	-	-	1.07757E+00	2.71661E-01	1.79446E-02	8.83292E-03	2.78905E-03
5	-	-	-	-	9.02164E-01	3.06030E-01	1.45784E-01	3.89507E-02
6	-	-	-	-	8.02797E-04	6.88672E-01	6.26596E-01	1.36410E-01
7	-	-	-	-	-	2.06845E-03	1.06577E+00	6.71118E-01
8	-	-	-	-	-	-	2.69064E-02	2.86548E+00
Σ_{s1}								
1	6.69913E-02	4.39677E-02	4.47490E-03	3.69693E-06	2.27939E-07	3.76707E-08	1.41236E-08	-
2	-	1.61884E-01	8.71617E-02	3.64473E-05	1.07947E-06	1.79490E-07	1.50777E-07	3.31300E-08
3	-	-	5.69170E-01	8.88007E-02	1.66235E-04	7.59540E-06	4.54100E-06	3.19411E-06
4	-	-	-	6.94270E-01	1.30044E-01	3.24058E-03	9.64357E-04	1.64333E-04
5	-	-	-	-	6.08943E-01	1.65435E-01	4.12707E-02	3.22630E-03
6	-	-	-	-	6.20153E-04	4.64410E-01	2.71343E-01	8.08650E-03
7	-	-	-	-	-	1.36969E-03	6.01770E-01	9.75193E-02
8	-	-	-	-	-	-	6.04653E-03	5.87293E-01

Mixture 7: H_2O moderator.

	Group							
	1	2	3	4	5	6	7	8
Σ_f	2.22346E-01	5.12692E-01	1.20902E+00	1.49316E+00	1.51036E+00	1.57803E+00	1.95595E+00	3.22986E+00
Σ_{s0}								
1	1.13811E-01	8.77528E-02	2.01845E-02	8.51099E-05	1.08150E-06	7.12849E-08	1.90113E-08	-
2	-	3.10405E-01	2.01460E-01	8.13984E-04	1.03436E-05	6.92672E-07	3.38292E-07	4.59312E-08
3	-	-	9.87667E-01	2.18275E-01	2.74030E-03	1.83508E-04	9.03289E-05	2.83368E-05
4	-	-	-	1.15897E+00	3.01031E-01	1.98957E-02	9.79331E-03	3.09231E-03
5	-	-	-	-	9.65398E-01	3.38676E-01	1.61489E-01	4.31229E-02
6	-	-	-	-	7.91944E-04	7.30332E-01	6.92395E-01	1.50933E-01
7	-	-	-	-	-	1.34328E-03	1.06218E+00	8.84935E-01
8	-	-	-	-	-	-	2.64629E-02	3.18390E+00
Σ_{s1}								
1	6.78860E-02	4.89080E-02	4.97040E-03	4.11047E-06	2.53323E-07	4.19307E-08	1.57199E-08	-
2	-	1.68959E-01	9.64070E-02	4.02820E-05	1.19305E-06	1.98377E-07	1.66636E-07	3.66093E-08
3	-	-	6.27467E-01	9.85220E-02	1.84334E-04	8.41863E-06	5.03187E-06	3.53930E-06
4	-	-	-	7.66353E-01	1.44354E-01	3.59563E-03	1.06995E-03	1.82247E-04
5	-	-	-	-	6.71757E-01	1.83510E-01	4.57363E-02	3.56773E-03
6	-	-	-	-	6.78763E-04	5.11977E-01	3.00691E-01	8.95283E-03
7	-	-	-	-	-	9.46170E-04	6.24490E-01	1.46731E-01
8	-	-	-	-	-	-	5.52627E-03	6.43940E-01

Mixture 8: control rod cell.								
	Group							
	1	2	3	4	5	6	7	8
Σ_t	2.21681E-01	3.75613E-01	6.98894E-01	1.26353E+00	2.97057E+00	4.35932E+00	5.22241E+00	7.10888E+00
Σ_{s0}								
1	1.54506E-01	5.47389E-02	6.29418E-03	2.37435E-05	3.01028E-07	1.99257E-08	5.55017E-09	6.63457E-13
2	-	2.93209E-01	7.44156E-02	2.06382E-04	2.62254E-06	1.75622E-07	8.58424E-08	1.14373E-08
3	-	-	5.94807E-01	4.16609E-02	4.73849E-04	3.17320E-05	1.56196E-05	4.88589E-06
4	-	-	-	7.20029E-01	4.60201E-02	2.93580E-03	1.44510E-03	4.56266E-04
5	-	-	-	-	7.11075E-01	1.40561E-01	6.43271E-02	1.77440E-02
6	-	-	-	-	8.73733E-04	5.79805E-01	4.01890E-01	8.37136E-02
7	-	-	-	-	-	3.36493E-03	9.11563E-01	3.72228E-01
8	-	-	-	-	-	-	3.49089E-02	2.14339E+00
Σ_{s1}								
1	5.28960E-02	6.09550E-03	1.40573E-03	1.13492E-06	6.91170E-08	1.15279E-08	4.57080E-09	-
2	-	8.65707E-02	1.73294E-02	1.01907E-05	3.03866E-07	5.05420E-08	4.25403E-08	9.13010E-09
3	-	-	1.85306E-01	1.44084E-02	3.02693E-05	1.52866E-06	9.65417E-07	6.89160E-07
4	-	-	-	2.85136E-01	1.66946E-02	4.33100E-04	1.31681E-04	2.57321E-05
5	-	-	-	-	3.55183E-01	6.71210E-02	1.76018E-02	1.54465E-03
6	-	-	-	-	5.58200E-04	3.12405E-01	1.59318E-01	4.90437E-03
7	-	-	-	-	-	1.83127E-03	4.52033E-01	4.12650E-02
8	-	-	-	-	-	-	9.22873E-03	4.66303E-01

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