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# Solution of the one-velocity 2D and 3D source and criticality problems by the Boundary Element-Response Matrix (BERM) method in the $A_2$-$SP_3$

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**Summary.** — The paper illustrates some applications of a variant of the simplified spherical harmonics ($SP_N$) method, called $A_N$, in order to solve 2D and 3D source and criticality problems. The $A_N$ equations (here considered only for $N = 2$, which corresponds to the $SP_3$ approximation) are solved by means of a Boundary Element-Response Matrix technique.

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## 1. – Introduction

The purpose of this paper is to show some results obtained by the $A_N$ method, a variant of the odd-order simplified spherical harmonics ($SP_N$) method. The $A_N$ method is characterized, at least in the case of isotropic and linearly anisotropic scattering, by a set of partial differential equations of the diffusion type, holding for general $N$, which is simpler than the corresponding set of the $SP_N$ equations (actually, the $A_N$ equation system is equivalent to the simplified spherical harmonics system of order $2N-1$, whence the name $A_N$-$SP_{2N-1}$ that will be also used for the method). A short sketch of some main features of the $A_N$ method is given in sect. **2**. To achieve a deeper understanding of the subject the reader can refer, other than to the original papers illustrating the basic idea [1,2], to papers [3] and [4], in which the full equivalence of $A_N$ and $SP_{2N-1}$ method is shown, together with other relevant results of the theory. The application of the

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Boundary Element-Response Matrix technique (BERM) [5,6] to solve the $A_N$ diffusion-like equations (sect. **3**) is also rather novel. It turns out that the BERM method ensures both a remarkable accuracy and a good efficiency.

## 2. – The $A_N$-$SP_{2N-1}$

The $A_N$ method was initially proposed [1,2] as a method for the solution of the transport equation in simple geometrical configurations and was extended, later on, to the class of the diffusing systems in which the total cross-section is everywhere constant, in short "constant $\sigma$" systems [3,4]. What is here of a particular relevance is that $A_N$ is equivalent, even for general space-dependent cross-sections, to the odd-order simplified spherical harmonics, $SP_{2N-1}$, method. Namely, if the scattering is isotropic, a suitable diagonalization procedure allows to transform the one-velocity $SP_{2N-1}$ equations into the following $A_N$ differential system, which has the structure of a system of multigroup diffusion equations with up-scattering:

$$\nabla\cdot\left(\frac{\mu_\alpha^2}{\Sigma_t(\vec{r})}\nabla\varphi_\alpha(\vec{r})\right)-\Sigma_t(\vec{r})\,\varphi_\alpha(\vec{r})+\Sigma_s(\vec{r})\sum_{\beta=1}^{N}w_\beta\varphi_\beta(\vec{r})+Q(\vec{r})=0 \qquad (\alpha=1,\dots,N)\,. \tag{1}$$

Here, $\mu_i$ and $w_i$ for $i=1,\dots,N$ are the points and the weights of the $N$-th order Gauss-Legendre integration formula, respectively, and the other symbols are the usual ones. The "pseudo-fluxes" $\varphi_\alpha$ are simply related to the $SP_{2N-1}$ moments of the angular flux. In particular, the physical scalar flux $\phi_0(\vec{r})$ is

$$\phi_0(\vec{r})=\sum_{\alpha=1}^{N}w_\alpha\varphi_\alpha(\vec{r})\,, \tag{2}$$

while the physical current vector is

$$\vec{J}(\vec{r})=\vec{\phi_1}(\vec{r})=\sum_{\alpha=1}^{N}\left(\frac{\mu_\alpha^2}{\Sigma_t(\vec{r})}\nabla\varphi_\alpha(\vec{r})\right).$$

A general formula is also obtained in the case of a linearly anisotropic scattering [7]. We report, in this case, only the equations holding for a homogeneous region

$$\frac{\mu_\alpha^2}{\Sigma_t}\Delta\phi_\alpha(\vec{r})-\Sigma_t\phi_\alpha(\vec{r})+\Sigma_s\left[1+3\frac{\mu_\alpha^2}{\Sigma_t}\bar{\mu_0}\left(\Sigma_t-\Sigma_s\right)\right]\sum_{\beta=1}^{N}w_\beta\varphi_\beta(\vec{r})+ \\ +\left(1-3\frac{\mu_\alpha^2}{\Sigma_t}\bar{\mu_0}\Sigma_s\right)Q(\vec{r})=0 \quad (\alpha=1,\dots,N)\,, \tag{3}$$

where $\bar{\mu_0}$ is the mean cosine of the scattering angle.

The $A_N$ diagonalized form of the $SP_{2N-1}$ equations allows to investigate the higher-order approximations very easily [4]. This is not devoid of interest, since, at least in the special case of the above "constant $\sigma$" systems, the accuracy of the $A_N$ method can be arbitrarily increased by letting $N$ go to infinity.

Of course, any multigroup diffusion problem solver can be applied to eqs. (1) or (3). Here below we sketch one such method, the Boundary Element-Response Matrix method, which, in this field, is now becoming a competitor of the finite-element methods.

## 3. – The Boundary Element-Response Matrix method

Considering the neutron diffusion equation in a homogeneous body $V$ with a boundary surface $S$,

$$D\Delta\phi\left(\vec{r}\right)-\Sigma_a\phi\left(\vec{r}\right)+Q\left(\vec{r}\right)=0,\quad \vec{r}\in V, \tag{4}$$

a classical procedure of the boundary element theory leads to the following boundary integral relationship:

$$\begin{aligned} c\left(\vec{r}\right)\phi\left(\vec{r}\right)+\int_S\left[D\frac{\partial\tilde{\phi}}{\partial n'_S}\left(\vec{r},\vec{r}'_S\right)\phi\left(\vec{r}'_S\right)-\tilde{\phi}\left(\vec{r},\vec{r}'_S\right)\frac{\partial\phi}{\partial n'_S}\left(\vec{r}'_S\right)\right]\mathrm{d}S\left(\vec{r}\right)&=\\ =\tilde{q}\left(\vec{r}\right)\quad\left(\alpha=1,\ldots,N\right),& \end{aligned} \tag{5}$$

where $\tilde{\phi}$ is the infinite medium Green function,

$$\tilde{\phi}\left(\vec{r},\vec{r}'\right)=\frac{\exp\left[-\left|\vec{r}-\vec{r}'\right|/L\right]}{4\pi D\left|\vec{r}-\vec{r}'\right|}$$

with $L=\sqrt{D/\Sigma_a}$ while $\tilde{q}(\vec{r})=\int_V\tilde{\phi}(\vec{r},\vec{r}')Q(\vec{r}')\mathrm{d}V'$ is a new source term and $c(\vec{r})=\int_V\delta(\vec{r}-\vec{r}')\mathrm{d}V'$, so that, by the properties of the $\delta$ function, $c(\vec{r})=1,0,\frac{1}{2}$ according to $\vec{r}$ is inside $V$, outside $V$ or is coincident with a smooth point $\vec{r}_S$ of the boundary $S$ (if $\vec{r}_S$ is an edge or corner point, then $c(\vec{r}_S)=\Omega_S/4\pi$, where $\Omega_S$ is the angle of aperture of the tangent cone at $\vec{r}_S$). If we just take $\vec{r}=\vec{r}_S$ in eq. (5), this equation becomes a relationship between $\phi(\vec{r}_S)$ and $\frac{\partial\phi(\vec{r}_S)}{\partial n_S}$.

If, for instance, $\frac{\partial\phi(\vec{r}_S)}{\partial n_S}$ is assigned on the boundary (which corresponds to a Neumann boundary condition for eq. (4)), then we get a boundary integral equation for the remaining quantity, the boundary flux $\phi(\vec{r}_S)$. Once the integral equation has been solved, substitution of $\phi(\vec{r}_S)$ and its normal derivative into eq. (5) allows to determine $\phi(\vec{r})$ for any $\vec{r}$ in the interior of $V$, thus obtaining the complete solution of the problem.

The boundary integral equation can be also given in a partial current form. If the partial currents

$$J^{\pm}\left(\vec{r}_S\right)=\frac{1}{4}\phi\left(\vec{r}_S\right)\mp\frac{D}{2}\frac{\partial\phi}{\partial n_S}\left(\vec{r}_S\right)$$

and the corresponding kernels

$$\tilde{J}^{\pm}\left(\vec{r}_S,\vec{r}'_S\right)=\frac{1}{4}\tilde{\phi}\left(\vec{r}_S,\vec{r}'_S\right)\pm\frac{D}{2}\frac{\partial\tilde{\phi}}{\partial n'_S}\left(\vec{r}_S,\vec{r}'_S\right)$$

are introduced, the integral equation reads

$$\begin{aligned}(6)\qquad & \frac{1}{2}c\,(\vec{r}_S)\,J^+\,(\vec{r}_S) + \int_S \tilde{J}^+\,(\vec{r}_S,\vec{r}\,'_S)\,J^+\,(\vec{r}\,'_S)\,\mathrm{d}S' = \\ & -\frac{1}{2}c\,(\vec{r}_S)\,J^-\,(\vec{r}_S) + \int_S \tilde{J}^-\,(\vec{r}_S,\vec{r}\,'_S)\,J^-\,(\vec{r}\,'_S)\,\mathrm{d}S' + \frac{1}{4}\tilde{q}\,(\vec{r}_S)\,.\end{aligned}$$

Let the partial current entering $V$, $J^-(\vec{r}_S)$, be known, as well as the volume source. Then the above equation yields the outward partial current, $J^+(\vec{r}_S)$, *i.e.* the response of the region $V$ to the injected current. Equation (6) can be solved by means of either a collocation method or a projection (or "weak") procedure. According to the latter, in the simple case of a 2D square region $V$, the partial currents $J^\pm$ are approximated, along each side, by, *e.g.*, a truncated Legendre polynomials expansion. After performing a number of integrals involving the kernels $\tilde{J}^\pm$ and the Legendre polynomials, eq. (6) is transformed into an algebraic linear system such as

$$M^+J^+ = M^-J^- + h,$$

where

$$J^+ = RJ^- + z$$

and $R = [M^+]^{-1} \cdot M^-$ is the response matrix of $V$ and $z = [M^+]^{-1} \cdot h$ a vector, which represents the source term.

The extension of the above theory to a multigroup system of diffusion equations is not difficult. A remark is in order as regards the void condition. It has been proven in [3] (see also [1]) that the usual Mark or Marshak void conditions can be advantageously replaced by an interface condition with a perfectly absorbing outer medium (a layer of a few mean free paths, with the same total cross-section as the region facing the void and the $J^- = 0$ condition at its end will suffice). This kind of interface condition has been used throughout all the examples here below.

## 4. – Application to multiregion systems

A reactor is usually represented as an array of cells, often coinciding with the homogenized fuel assemblies, or parts of them. The above boundary element method is applied to each cell and the corresponding response matrix is calculated and stored. Then a Response Matrix procedure [8] is applied, in order to connect the inward and outward currents of the cells and arrive, finally, at the flux distribution over the whole system.

In the case of reactor criticality problems the source term is suppressed and the response matrix of the cells containing a multiplying material involves the eigenvalue parameter $k$. As $k$ is a quantity referring to the global system, it is updated at the level of an outer iteration cycle. When performing the "cell level" of the calculation $k$ is kept constant, with the value determined at the previous "reactor level" outer iteration step.

Of course nothing prevents from applying the above Boundary Element-Response Matrix procedure, which was initially intended as a diffusion problem solver [5, 6] (a 3D $xyz$ version is in progress), also to the $A_2$-$SP_3$ problems. Here below we present some one-group $A_2$-$SP_3$ examples, solved by the projection method.

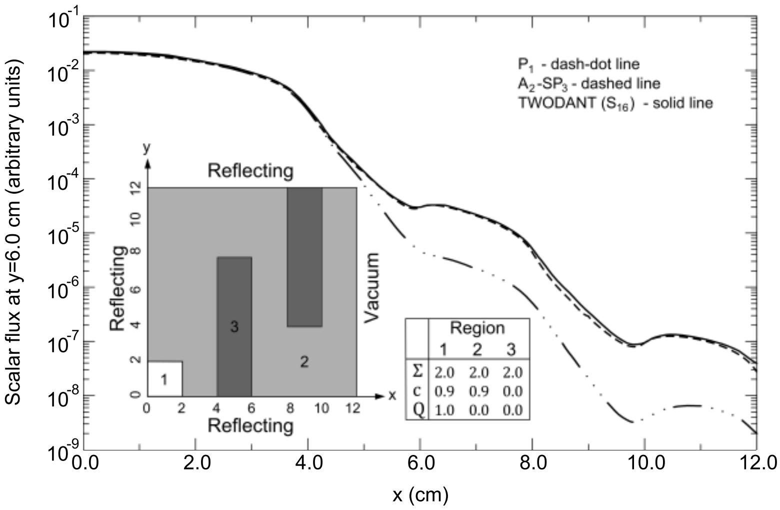


Fig. 1. – Scalar flux distribution along the horizontal cut $y = 6.0\,\mathrm{cm}$. Geometry and material characteristics of the problem are also shown. Data from [9].

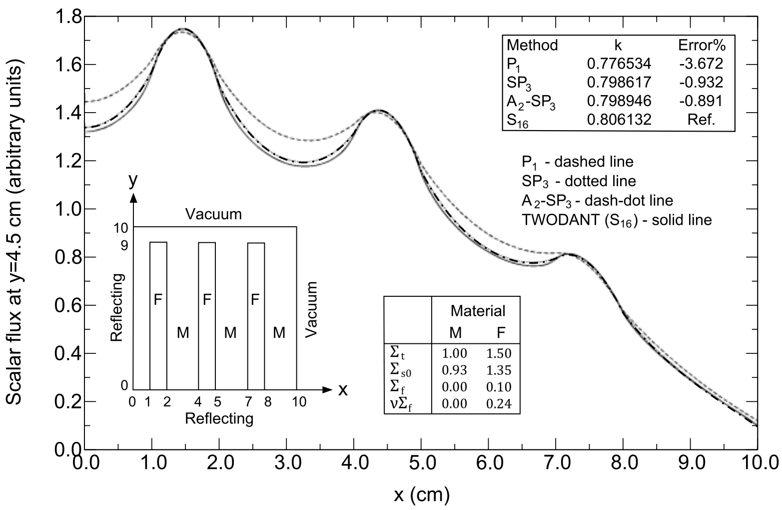


Fig. 2. – Scalar flux along $y = 4.5\,\mathrm{cm}$ and estimates of the fundamental eigenvalue for the 2D one-group eigenvalue problem. Geometry and material characteristics are also shown. As expected, the curves referring to the $SP_3$ method and to the $A_2$-$SP_3$ method are overlapping almost exactly. Data from [10].

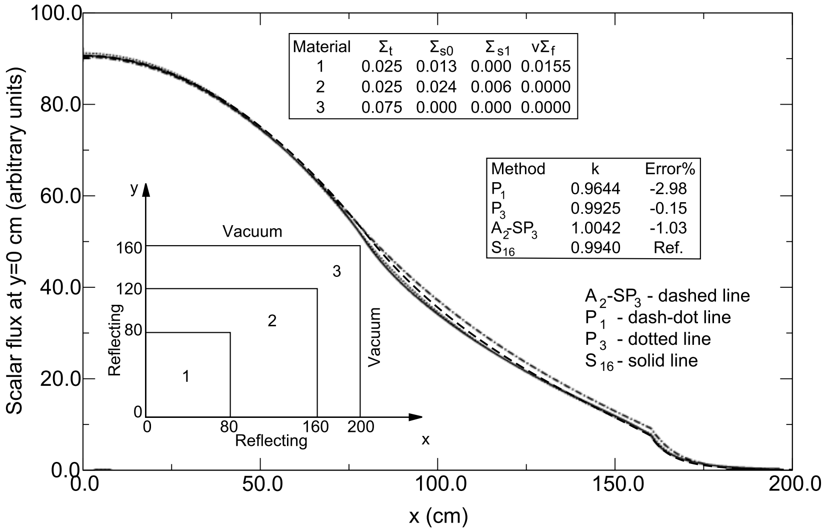


Fig. 3. – Scalar flux along $y = 0.0$ cm and estimates of the fundamental eigenvalue for the 2D heterogeneous eigenvalue problem with anisotropic scattering. Geometry and material characteristics are also shown. Data from [11].

The first example is a 2D problem considering a localized source and pure absorbers in the source-free scattering region. Figure 1, in which the geometry and material characteristics are also shown, compares the scalar flux distribution obtained by the $A_2$-$SP_3$ method in correspondence of $y = 6.0$ cm with the flux distributions reported in [9]. The excellent agreement between the $A_2$-$SP_3$ and TWODANT($S_{16}$) results is evident. The second example is a 2D one-group, isotropic scattering, eigenvalue problem. The comparison of the scalar flux distribution obtained by the $A_2$-$SP_3$ method with the results reported in [10] is shown in fig. 2, together with the geometry and the material characteristics. The agreement still turns out to be very good. Moreover, fig. 2 reports also the estimate of the fundamental eigenvalue obtained by the different methods and, again, the equivalence between the $A_2$-$SP_3$ and the $SP_3$ methods is supported by the results. The third example concerns a 2D heterogeneous eigenvalue problem with anisotropic scattering. As for the foregoing examples, fig. 3 both shows the geometry and the material

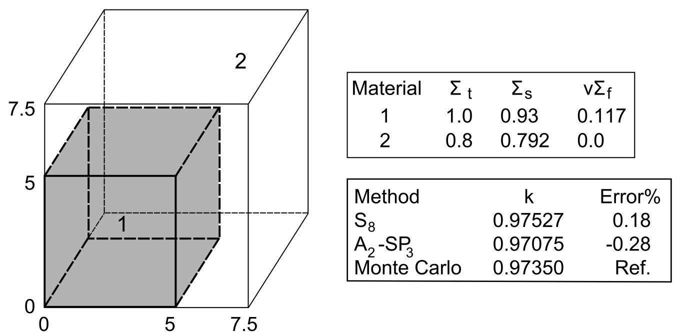


Fig. 4. – Estimates of the fundamental eigenvalue for the 3D simplified reactor. Geometry and material characteristics are also shown. Data from [12].

characteristics of the problem and compares the scalar flux distribution in correspondence of $y = 0.0$ cm as obtained by $A_2$-$SP_3$ method with the distributions resulting from other methods, as reported in [11]. The last example is a one-group eigenvalue problem for a 3D simplified reactor [12]. The calculated fundamental eigenvalue is shown in fig. 4, together with the reactor geometry (thanks to the symmetry, only one-eighth of the core needs to be modeled) and the material properties.

## 5. – Conclusion

If applied to the $A_2$-$SP_3$ equations, the Boundary Element-Response Matrix method has been shown to yield satisfactory solutions of 2D and 3D source and criticality benchmark problems, both with isotropic and linearly anisotropic scattering. As expected, the $A_2$-$SP_3$ calculations shown above turned out to be remarkably more accurate than those based on diffusion (or $P_1$) theory, with an increment of the computational burden of only a factor two. With respect to the $SP_N$ equation system, $A_N$ has the advantage of having a very simple structure. This could suggest increasing the calculation order to, *e.g.*, $N = 3$ or 4, at least for the diffusing systems in which the cross-sections (in particular the total cross-section) do not undergo a very strong variation.

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