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A NEW PERSPECTIVE ON SOME APPROXIMATIONS USED IN NEUTRON TRANSPORT MODELING

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Abstract

In this contribution, we will use the *Maxwell-Cartesian spherical harmonics* (introduced in [1, 2]) to derive a system of partial differential equations governing transport of neutrons within an interacting medium. This system forms an alternative to the well known P_N approximation, which is based on the expansion into tesseral spherical harmonics ([3, p. 197]). In comparison with this latter set of equations, the Maxwell-Cartesian system posesses a much more regular structure, which may be used for various simplifications that could be advantageous from computational point of view.

1. Introduction

Consider the monoenergetic, steady-state neutron transport problem with fixed volumetric sources[1] in a domain $V \subset \mathbb{R}^3$ filled with isotropic medium interacting with the neutrons. Solution of this problem describes the stationary distribution of neutrons within V together with their motion directions and is called *angular neutron flux density* (or shortly *angular flux*). In standard notation, the angular flux is expressed by function $\psi(\mathbf{r}, \boldsymbol{\Omega})$ where $\mathbf{r} = [x, y, z]^T \in V$ and components of the direction vector are given in spherical coordinates as

$$\boldsymbol{\Omega} = \begin{bmatrix} \Omega_x \\ \Omega_y \\ \Omega_z \end{bmatrix} = \begin{bmatrix} \sin\vartheta\cos\varphi \\ \sin\vartheta\sin\varphi \\ \cos\vartheta \end{bmatrix} = \boldsymbol{\Omega}(\vartheta, \varphi), \quad \vartheta \in [0, \pi],\ \varphi \in [0, 2\pi).$$

Angular neutron flux is therefore a function defined in a five-dimensional domain $V \times S_2$ (S_2 denoting the unit 2-sphere). Numerical methods that can be used to determine the solution of practically significant neutron transport problems are usually constructed by first semi-discretizing the governing equation with respect to the angular variable $\boldsymbol{\Omega}$, yielding a system of PDE's in space, and using standard numerical methods like the finite volume or finite element methods to solve this system.

[1] The extension to energy- or time-dependent problems would be straightforward.

In this paper, we will be interested only in the angular semi-discretization of the neutron transport equation. One of the most popular method to accomplish this task is the *method of spherical harmonics*. In this method, the angular flux is expanded into a series of tesseral spherical harmonics ([3, p. 197]) which form a complete orthonormal basis of the space $L^2(S_2)$ of functions square-integrable with respect to $\mathbf{\Omega}$. By considering only spherical harmonics of degrees $n \leq N$ [2] and performing the Galerkin projection (with respect to $\mathbf{\Omega}$) of the neutron transport equation onto the subspace spanned by those functions, a system of first-order hyperbolic PDE's in space, conventionally referred to as the P_N system, is obtained[3]. However, the resulting system is quite complicated, strongly coupled through differential terms and lacks the invariance with respect to change of coordinate axes.

We therefore propose to use a different set of expansion functions to perform the angular semi-discretization. In [7], the author arrived at a "far more symmetric and compact" ([7, p. 1455]) form of the angularly semi-discretized system of equations governing the distribution of plasma by using an expansion of the solution in terms of special spherical harmonic tensors rather than the usual sets of tesseral spherical harmonics. Although the derivation and properties of the spherical harmonic tensors were not described in much detail in the paper, they are actually equal (up to a normalization) to the *Maxwell-Cartesian spherical harmonic tensors*, rigorously developed in [1]. Use of these tensors have so far proven to be advantageous in solving various electro-magnetics and quantum-mechanical problems ([1, 2]). Nevertheless, they have not been used for neutron transport problems until very recently ([5]).

In section 2, we will introduce the neutron transport equation and basic notation. Section 3 provides a brief review of the Maxwell-Cartesian spherical harmonic tensors, leaving the details to the original papers [1, 2]. The alternative to the P_N system is derived in section 4; the derivation is different from that of [5] and, in our opinion, provides more insight into the structure of the equations. How this insight can be used to obtain in a new way some known (but not yet completely understood) approximations used in neutron transport methods is suggested in the conclusion.

2. Mathematical model

The equation governing transport of neutrons, also known as the linear Boltzmann's transport equation (shortly BTE), reads (in standard notation, as e.g. in [11, Sec. 9.7]):

$$\mathbf{\Omega} \cdot \nabla\psi(\mathbf{r},\mathbf{\Omega}) + \sigma_t(\mathbf{r})\psi(\mathbf{r},\mathbf{\Omega}) - \int_{S_2} \left[\sigma_s(\mathbf{r},\mathbf{\Omega}\cdot\mathbf{\Omega}') + \frac{\nu(\mathbf{r})\sigma_f(\mathbf{r})}{4\pi}\right] \psi(\mathbf{r},\mathbf{\Omega}')\,\mathrm{d}\mathbf{\Omega}' = q(\mathbf{r},\mathbf{\Omega}), \tag{1}$$

where $\mathbf{r} \in V$, $\mathbf{\Omega} \in S_2$. The σ functions are called *macroscopic cross-sections* for a particular interaction, distinguished by the subscripts (t for the total probability

[2] Note that there are $2n+1$ tesseral harmonics of given degree $n \geq 0$.

[3] Detailed description is given in many classical books on nuclear reactor physics, like [11, 4].

of collision of any type with nuclei at $\mathbf{r}$, s for scattering from direction $\mathbf{\Omega}'$ to $\mathbf{\Omega}$ upon the collision and finally f for the collision which results in fissioning the target nucleus and releasing an average number of ν neutrons in the process). We will assume that all the macroscopic cross-sections are given bounded measurable functions and look for a non-negative $\psi \in L^2(V \times S_2)$ [4] given the volumetric distribution of neutron sources $q \in L^2(V \times S_2)$. Boundary conditions will not be considered here – we may remark, however, that the developments in this work make the incorporation of the well-known *Marshak approximation* of the boundary conditions (e.g., [11, p. 340]) straightforward.

3. Maxwell-Cartesian spherical harmonics

A general linear combination of tesseral harmonics of given degree n is called *surface spherical harmonic* of degree n. As shown in [1], a surface spherical harmonic of degree n can also be uniquely represented by a totally symmetric traceless Cartesian tensor of rank n [5] . Moreover, that paper presents a systematic way of obtaining a TST tensor of any rank n whose components are surface spherical harmonics of degree n in Cartesian frame of reference as defined by Maxwell in [8, p. 160]. Specifically, Maxwell's spherical harmonics based on Cartesian axes can be obtained (up to a normalization constant) as components of $\mathbb{P}^{(n)}(\mathbf{\Omega}) = \mathscr{D}_n\mathbf{\Omega}^n$ where $\mathscr{D}_n$ is the so-called *detracer operator* which projects a general totally symmetric tensor of rank n into the space of TST tensors of rank n (definition and various properties of this operator are given in [1, Sec. 5]; we use here the "projection version" of the operator, as discussed in the note in [1, p. 4311]).

We note that projection of $\mathbb{P}^{(n)}$ along, say, z-axis (or any other because of the symmetry) yields (up to a normalization factor) the Legendre polynomials P_n (cf. Tab. 1):

$$\mathbb{P}^{(n)}(\mathbf{\Omega}) \cdot \mathbf{e}_z^n = P^{(n)}_{\alpha_1\ldots\alpha_n}(\mathbf{\Omega})\delta_{3\alpha_1}\cdots\delta_{3\alpha_n} = P^{(n)}_{33\ldots3}(\mathbf{\Omega}) = \frac{n!}{(2n-1)!!}P_n(\Omega_z) \equiv C_nP_n(\Omega_z) \tag{2}$$

[4] We denote by $L^2(V \times S_2)$ the space of square-integrable functions with respect to the measure $\mathrm{d}\mu(V \times S_2) = \mathrm{d}\mathbf{r}\,\mathrm{d}\mathbf{\Omega} = \mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z\,\sin\vartheta\mathrm{d}\vartheta\,\mathrm{d}\varphi$.

[5] We will indicate a Cartesian tensor of rank n by superscribed (n) and index its 3^n components by a sequence of n Greek letters in subscript (each attaining value 1, 2, or 3, corresponding to Cartesian axes x, y, z, respectively); for vectors (rank-1 tensors), we will keep using conventional bold-face letters. Einstein's summation convention will be used whenever same indices appear in a tensor expression written in component notation. When a tensor is invariant under any permutation of its indices, it is called *totally symmetric*; contraction of two tensors of same rank is a number $\mathbb{A}^{(n)} \cdot \mathbb{B}^{(n)} := A^{(n)}_{\gamma_1\ldots\gamma_n}B^{(n)}_{\gamma_n\ldots\gamma_1}$, contraction of a tensor $\mathbb{P}^{(n)}$ in first index pair is defined as $P^{(n)}_{\alpha\alpha\gamma_3\ldots\gamma_n}$ and called *trace* in that index pair. Totally symmetric tensor whose trace in any index pair vanishes is called *totally symmetric traceless* (abbr. TST). The tensor product $\mathbb{C}^{(n+m)} = \mathbb{A}^{(n)} \otimes \mathbb{B}^{(m)}$ has components $C^{(n+m)}_{\alpha_1\ldots\alpha_n\beta_1\ldots\beta_m} = A^{(n)}_{\alpha_1\ldots\alpha_n}B^{(m)}_{\beta_1\ldots\beta_m}$ and the m-th power of a rank-n tensor is defined as $\mathbb{A}^{(n)} \otimes \mathbb{A}^{(n)} \otimes \cdots \otimes \mathbb{A}^{(n)}$ (m-times). Finally, we will consider the differential operator ∇ as a vector $[\frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z}]^T$, but keep writing $\nabla\mathbb{A}^{(n)}$ for $\nabla \otimes \mathbb{A}^{(n)}$.

($\mathbf{e}_z = [0,0,1]^T$, δ_{ij} is the Kronecker delta); also, the well-known formulas for Legendre polynomials could be extended within the tensorial framework to obtain explicit formulas for $\mathbb{P}^{(n)}$([3, Chap. VI]). This feature of Maxwell-Cartesian tensors makes the resulting angular discretization a natural multidimensional extension of the 1D P_N system (which is actually based on a Legendre expansion of angular flux), having an analogous form as the latter.

n	$\mathbb{Y}^n(\mathbf{\Omega}) \propto$	$\mathbb{P}^{(n)}(\mathbf{\Omega})$	$C_n P_n(\Omega_z)$
0	1	1	1
1	$\Omega_x,\ \Omega_y, \Omega_z$	$\Omega_x,\ \Omega_y,\ \Omega_z$	Ω_z
2	$-\Omega_x^2 - \Omega_y^2 + 2\Omega_z^2,\ \Omega_y\Omega_z,$ $\Omega_z\Omega_x,\ \Omega_x\Omega_y,\ \Omega_x^2 - \Omega_y^2$	$\Omega_x^2 - \frac{1}{3},\ \Omega_x\Omega_y,\ \Omega_x\Omega_z,$ $\Omega_y^2 - \frac{1}{3},\ \Omega_y\Omega_z,\ \Omega_z^2 - \frac{1}{3}$	$\Omega_z^2 - \frac{1}{3}$

Table 1: Tesseral and Maxwell-Cartesian sph. harmonics and Legendre polynomials.

4. The MCP_N approximation

Using the results of [3, Art. 114], the expansion of angular neutron flux in terms of surface spherical harmonics could be written as

$$\psi(\mathbf{r}, \mathbf{\Omega}) = \sum_{n=0}^{\infty} \frac{2n+1}{4\pi} \int_{S_2} \psi(\mathbf{r}, \mathbf{\Omega}') P_n(\mathbf{\Omega} \cdot \mathbf{\Omega}') \, \mathrm{d}\mathbf{\Omega}' \,. \tag{3}$$

As shown in [1, Sec. 7, Corollary II], Maxwell-Cartesian tensors appear in the following form of "addition theorem" for Legendre polynomials P_n:

$$\mathbb{P}^{(n)}(\mathbf{\Omega}) \cdot \mathbb{P}^{(n)}(\mathbf{\Omega}') = C_n P_n(\mathbf{\Omega} \cdot \mathbf{\Omega}') \tag{4}$$

(C_n defined in (2)). Combining the two results, we obtain

$$\psi(\mathbf{r}, \mathbf{\Omega}) = \sum_{n=0}^{\infty} \psi^{(n)}(\mathbf{r}) \cdot \mathbb{P}^{(n)}(\mathbf{\Omega}), \tag{5}$$

where we defined

$$\psi^{(n)}(\mathbf{r}) := \frac{2n+1}{4\pi C_n} \int_{S_2} \psi(\mathbf{r}, \mathbf{\Omega}) \mathbb{P}^{(n)}(\mathbf{\Omega}) \, \mathrm{d}\mathbf{\Omega} \,. \tag{6}$$

To find the relations that must be satisfied by the angular expansion moments $\psi^{(n)}(\mathbf{r})$ in order for (5) (or equivalently (3)) to be the solution of the BTE, we insert the expansion (5) into (1) (with source term represented in terms of angular expansion moments analogously to (6)). Applying eq. (4) to the generalized Fourier-series expansion of the scattering term in terms of the Legendre polynomials, we obtain:

$$\begin{aligned}\int_{S_2} \sigma_s(\mathbf{r}, \boldsymbol{\Omega}\cdot\boldsymbol{\Omega}')\psi(\mathbf{r},\boldsymbol{\Omega}')\,\mathrm{d}\boldsymbol{\Omega}' &= \sum_{n=0}^{\infty}\frac{2n+1}{4\pi}\sigma_{sn}(\mathbf{r})\int_{S_2} P_n(\boldsymbol{\Omega}'\cdot\boldsymbol{\Omega})\psi(\mathbf{r},\boldsymbol{\Omega}')\,\mathrm{d}\boldsymbol{\Omega}' \\ &= \sum_{n=0}^{\infty}\sigma_{sn}(\mathbf{r})\psi^{(n)}(\mathbf{r})\cdot\mathbb{P}^{(n)}(\boldsymbol{\Omega}).\end{aligned}$$

Because of the orthogonality of $\mathbb{P}^{(n)}$ of different ranks ([1, Sec. 8.7]), the fission part will have the following form:

$$\int_{S_2}\frac{\nu(\mathbf{r})\sigma_f(\mathbf{r})}{4\pi}\psi(\mathbf{r},\boldsymbol{\Omega}')\,\mathrm{d}\boldsymbol{\Omega}' = \sum_{n=0}^{\infty}\frac{\nu(\mathbf{r})\sigma_f(\mathbf{r})}{4\pi}\psi^{(n)}(\mathbf{r})\cdot\int_{S_2}\mathbb{P}^{(n)}(\boldsymbol{\Omega}')\,\mathrm{d}\boldsymbol{\Omega}' = \nu(\mathbf{r})\sigma_f(\mathbf{r})\phi(\mathbf{r}), \tag{7}$$

where $\phi \equiv \psi^{(0)}$ is the *scalar flux*. Therefore, by inserting (5) into (1) and using these results we obtain

$$\sum_{n=0}^{\infty}\left[\boldsymbol{\Omega}\cdot\nabla\psi^{(n)} + \sigma_t\psi^{(n)} - \sigma_{sn}\psi^{(n)} - \delta_{n0}\nu\sigma_f\phi - q^{(n)}\right]\cdot\mathbb{P}^{(n)}(\boldsymbol{\Omega}) = 0 \tag{8}$$

where each term in the square brackets is dependent only on $\mathbf{r}$ (omitted for brevity).

Because of the linear dependence among certain functions in each $\mathbb{P}^{(n)}(\boldsymbol{\Omega})$ (owing to the requirement of vanishing trace), we cannot deduce from (8) that for each n, all components of the tensor in brackets must vanish. The angular discretization is further hampered by the advection term which still contains the angular variable $\boldsymbol{\Omega}$. However, using the *detracer exchange theorem* ([2, Sec. 5.2]) and total symmetry of $\psi^{(n)}$ (by definition (6)), we note that the expansion (5) is actually equivalent to a power series in $\boldsymbol{\Omega}$:

$$\psi(\mathbf{r},\boldsymbol{\Omega}) = \sum_{n=0}^{\infty}\psi^{(n)}(\mathbf{r})\cdot\boldsymbol{\Omega}^n. \tag{9}$$

Using this fact to simplify the advection term $(\boldsymbol{\Omega}\cdot\nabla)\psi^{(n)}\cdot\boldsymbol{\Omega}^n$, we may rewrite equation (8) as

$$\sum_{n=0}^{\infty}\left[\nabla\psi^{(n-1)} + \sigma_t\psi^{(n)} - \sigma_{sn}\psi^{(n)} - \delta_{n0}\nu\sigma_f\phi - q^{(n)}\right]\cdot\boldsymbol{\Omega}^n = 0 \tag{10}$$

with the term with $n < 0$ discarded.

Equation (10) expresses a vanishing linear combination of monomials restricted to the unit sphere. Even though the monomials of all degrees are completely linearly independent, once restricted to the unit sphere there exist nontrivial linear combinations, such as $\Omega_x^2+\Omega_y^2+\Omega_z^2-1=0$. Hence we still cannot deduce that the expression in square brackets in (10) must be a zero tensor. However, in view of the theorem in [1, Sec. 4.2], it is possible to eliminate these nontrivial linear combinations by requiring the coefficients of the combination to form TST tensors for each n. Since $\psi^{(n)}$ and $q^{(n)}$ are TST by definition, we only have to symmetrize and detrace the advection terms. We need to be careful, however, not to change the original equation. This can be done by a clever rearranging of the terms in the sum. After using the definition of the detracer operator, symmetrization by

$$\left[\mathbb{A}^{(n)}\right]_{\mathrm{sym}} = \widetilde{\mathbb{A}}^{(n)} \quad \text{with components} \quad \widetilde{A}^{(n)}_{\alpha_1\ldots\alpha_n} = \frac{1}{n!}\sum_{\pi(\alpha_1\ldots\alpha_n)} A^{(n)}_{\alpha_1\ldots\alpha_n}$$

(where the sum is over all permutations of the tensor indices) and regrouping the sum by $\mathbf{\Omega}^n$, we arrive at the final equation (with $\Sigma_n := \sigma_t\psi^{(n)} - \sigma_{sn}\psi^{(n)} - \delta_{n0}\nu\sigma_f$)

$$\sum_{n=0}^{\infty}\left\{\left[\nabla\psi^{(n-1)} - \frac{n-1}{2n-1}\mathbb{I}\otimes\nabla\cdot\psi^{(n-1)}\right]_{\mathrm{sym}} + \frac{n+1}{2n+3}\nabla\cdot\psi^{(n+1)} + \Sigma_n\psi^{(n)} - q^{(n)}\right\}\cdot\mathbf{\Omega}^n = 0, \tag{11}$$

which implies that each component of the TST coefficient tensor of rank n in curly brackets must vanish.

5. Conclusion and outlook

By truncating the expansion (9) (or (5)) at $n = N$ for some $N \geq 0$, we obtain from eq. (11) an alternative set to the ordinary P_N equations which could be called an *MCP_N approximation* (because its solution represents the expansion of angular flux into Maxwell-Cartesian surface spherical harmonics of degrees up to N). The symmetric and traceless structure of the MCP_N equations could be used to provide new perspectives on some other widely used approximations or to create new ones. For instance, by projecting each tensor along any chosen axis, we obtain one dimensional equations equivalent with the 1D P_N equations (after suitable normalization of $\psi_z^{(n)}$). This indicates the possibility to investigate the original ad-hoc derivation of the popular SP_N approximation (by formal extension of the 1D P_N equations into 3D, [6]) in the current tensorial framework. Similarly, a different normalization of $\psi^{(n)}$ leads to the system derived in [5]. However, the derivation in [5] is partially formal and does not take into account all the important properties of spherical harmonic tensors (in particular their tracelessness and linear dependence for given degree).

There is also an interesting link to an old article of Selengut ([10]) in which the full multidimensional P_3 solution is obtained by solving a set of two coupled diffusion equations[6] with special interface conditions in presence of multiple heterogeneous regions. Selengut's derivation of the set is however quite puzzling (see also commentary

[6]much like in the SP_3 approximation, but apparently without restrictions on dimensionality or cross-sections other than the usual isotropic scattering and volumetric source assumptions

in [9, Sec. 5.2]) and his equations have never been either analyzed or at least numerically tested. On the other hand, we have been able to derive Selengut's equation for scalar flux (even with anisotropic scattering) by combining the MCP_3 equations into an equation for $\psi^{(2)}$ and adding a *compatibility condition* of vanishing trace of $\psi^{(2)}$. Further work in this direction is currently under way.

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References

[1] Applequist, J.: Traceless cartesian tensor forms for spherical harmonic functions: new theorems and applications to electrostatics of dielectric media. J. Phys. A **22** (1989), 4303–4330.

[2] Applequist, J.: Maxwell-Cartesian spherical harmonics in multipole potentials and atomic orbitals. Theoretical Chemistry Accounts **107** (2002), 103–115.

[3] Byerly, W. E.: *An elementary treatise on Fourier's series and spherical, cylindrical and ellipsoidal harmonics, with applications to problems in mathematical physics.* Ginn and Co., Boston, USA, 1893, 2nd edn.

[4] Cacuci, D. G.: *Handbook of nuclear engineering, Volume I: Nuclear engineering fundamentals.* Springer Science + Business Media LLC, 2010.

[5] Coppa, G. G. M.: Deduction of a symmetric tensor formulation of the P_n method for the linear transport equation. Progress in Nuclear Energy **52** (2010), 747–752.

[6] Gelbard, E. M.: Application of spherical harmonics methods to reactor problems. Tech. Rep. WAPD-BT-20, Bettis Atomic Power Laboratory, 1960.

[7] Johnston, T. W.: General spherical harmonic tensors in the Boltzmann equation. J. Math. Phys. **7** (1966), 1453–1458.

[8] Maxwell, J. C.: *A treatise on electricity and magnetism*, vol. I. Clarendon Press, Oxford, UK, 1873.

[9] McClarren, R. G.: Theoretical aspects of the simplified P_n equations. Transport Theory Statist. Phys. **39** (2011), 73–109.

[10] Selengut, D. S.: A new form of the P3 approximation. Transactions of American Nuclear Society **13** (1970), 625–626.

[11] Stacey, W. M.: *Nuclear reactor physics.* John Wiley & Sons, Inc., New York, 2007, 2nd edn.