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$\begin{array}{c} {\rm Exterior~calculus~note~on~the~additive~separation} \\ {\rm of~variables~3D~solution~to~a~dynamical~neutron~diffusion~BVP} \end{array}$

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Abstract

The boundary value approach to dynamic optimization is still an active area of research in many domains of process engineering. The particular domain of interest in the present work is a certain nonlinear optimization problem, constrained by a 3D neutron diffusion partial differential equation (PDE) and controlled, in time, by the boundary conditions. An analytical solution to the associated linear boundary value problem (BVP), which is a principal activity of this optimization, has been reached in 2019 by this author, based on application of an additive separation of variables (ASOV) principle, and was published in the International Journal of Dynamical Systems and Differential Equations.

The sole objective of this paper is to examine and verify the consistency of the ASOV method in solving the BVP of this optimization process. The justification of this method is based on reversibility of a pertaining generalized Euclidean transformation, and on asserting this reversibility in the context of an exterior differential framework for the BVP.

Keywords: additive separation of variables, dynamical neutron diffusion, cancer therapy, boundary value problem, Euclidean transformation, exterior analysis

1 Introduction

The panoramic picture of the research, addressed in this paper, overlooks a non-linear dynamic optimization [10, 12] problem, constrained [9] by (i) a source-free 3D neutron diffusion PDE and (ii) parametrized time control in some boundary equality constraints, [12, 14, 16, 20], of an associated linear BVP. The presented research is a contribution to the boundary value approach to dynamic optimization, reported in [12], which distinctively employs explicit parametrization, [10, 12]. The motivation for it comes from the fact that dynamical neutron fluxes happen to penetrate a (B/Gd)-loaded cancerous region better [11] than alternative stationary fluxes. A result that brings about a possible improvement in the nonlinear therapeutic objectives, to be optimized.

The present paper focuses, however, only on one detail of this picture, namely on the consistency of the analytical solvability of this dynamical BVP by the ASOV method, reported in [9]. It is well known that the availability of an analytical differentiable solution, [9], to the posing unique BVP is of crucial importance, [24, 27]. It happens to allow for an explicit nonlinearly parametrized Pareto optimization, [10, 12], that is employable instead of alternative optimization via Pontryagin's Maximum Principle [24], or Bellman's Dynamic Programming, with their implicit-only parametrization and their other intrinsic difficulties [29].

The 3D dynamical BVP of neutron cancer therapy, reported in [9], models the irradiation of a cancerous region R of an $R \cup (\Lambda \cup \Omega \cup \mho)$ composite in a patient by three orthogonal time-modulated beams of thermal neutrons. Its dynamical output variable is the neutron flux $\Phi(\mathbf{r},t)$, which satisfies the following monoenergetic volumetric source-free neutron diffusion PDE

(1)
$$\mathcal{L}(t, \mathbf{r}, \Phi, \Phi^{(2)}) = \frac{1}{v} \frac{\partial}{\partial t} \Phi(x, y, z, t) - \nabla \cdot \mathbf{D} \nabla \Phi(x, y, z, t) + \Sigma_a \Phi(x, y, z, t) = 0,$$

on a paralellipepedal region R (with a zero surface U that contains the (0,0,0) corner, an extrapolated region \overline{R} , see e.g. [15], and an extrapolated surface \overline{V} that contains the $(\overline{a}, \overline{b}, \overline{c})$ corner) with $\mathbf{r} = (x, y, z) \in \overline{R}$, $t \in [0, \infty)$, $(\mathbf{r}, t) \in \Re$, Σ_a as the neutron absorption macroscopic cross section [15], and \mathbb{D} as a neutron diffusion tensor defined via

(2)
$$\nabla \cdot \mathbf{D} \nabla = \nabla \cdot \left[D(x) \frac{\partial}{\partial x} \mathbf{i} + D(y) \frac{\partial}{\partial y} \mathbf{j} + D(z) \frac{\partial}{\partial z} \mathbf{k} \right]$$

= $D_{\parallel} \frac{\partial^{2}}{\partial x^{2}} + D_{\vdash} \frac{\partial^{2}}{\partial y^{2}} + D_{\perp} \frac{\partial^{2}}{\partial z^{2}}$,

in which $\{\mathbf{i}, \mathbf{j}, \mathbf{k}\}$ is a basis for \overline{R} .

The constraints are represented by the three dimensional vector equation $\mathbf{B}(t, \mathbf{r}, \Phi, \Phi^{(1)}) = \mathbf{b} \ (t, \mathbf{r})$:

$$(3) \quad \Phi(\mathbf{r},t) \mid_{\mathbf{r} \in \overline{V}} = 0,$$

$$(4) \nabla \Phi(\mathbf{r}, t) |_{\mathbf{r} \in U} = \begin{cases} -\frac{\varkappa_{\parallel}}{D_{\parallel}} S(t), & x = 0 \ (y - z \ plane \ \text{adjacent to} \ \Lambda) \\ -\frac{\varkappa_{\vdash}}{D_{\vdash}} S(t), & y = 0 \ (x - z \ plane \ \text{adjacent to} \ \Omega) \\ -\frac{\varkappa_{\perp}}{D_{\perp}} \check{S}(t), & z = 0 \ (x - y \ plane \ \text{adjacent to} \ \mho), \end{cases}$$

$$(5) \quad \Phi(\mathbf{r},0) \mid_{\mathbf{r} \in \overline{R}} = \begin{cases} \varphi(x), \ y-z \ plane \\ \emptyset(y), \ x-z \ plane \\ \varnothing(z), \ x-y \ plane, \end{cases}$$

In this BVP S(t), S(t) and S(t) are assumed to be a periodic boundary temporal surface source functions of even symmetry, D_{\parallel} , D_{\vdash} and D_{\perp} are the directional diffusion coefficients, with $\varkappa_{\parallel} = \varkappa_{R\parallel;\Lambda} = \frac{\varrho_{\Lambda}}{\varrho_{R\parallel} + \varrho_{\Lambda}}$, $\varkappa_{\vdash} = \varkappa_{R\vdash;\Omega} = \frac{\varrho_{\Omega}}{\varrho_{R\vdash} + \varrho_{\Omega}}$, and $\varkappa_{\perp} = \varkappa_{R\perp;\mho} = \frac{\varrho_{\mho}}{\varrho_{R\perp} + \varrho_{\mho}}$ as coupling factors, defined in [9], of the R region with the Λ , Ω and \mho slabs in an $R \cup (\Lambda \cup \Omega \cup \mho)$ composite. Here ϱ_{Λ} , ϱ_{Ω} , and ϱ_{\mho} are regional albedos while $\varrho_{R\parallel;}$, $\varrho_{R\perp}$ and $\varrho_{R\vdash}$ are directional albedos, [9], of the cancerous region R.

Throughout this paper, it would be assumed that the neutron flux intensity J(x,y,z,t), at $x=0^+$ through the $\Lambda \cap R$ plane, at $y=0^+$ through the $\Omega \cap R$ plane, and at $z=0^+$ through the $\Omega \cap R$ plane, should respectively satisfy

$$J(0^+, y, z, t) = \varkappa_{R\parallel;\Lambda} S(x, t),$$

 $J(x, 0^+, z, t) = \varkappa_{R\vdash;\Omega} S(y, t),$
 $J(x, y, 0^+, t) = \varkappa_{R\perp;\mho} S(z, t).$

In this BVP, the PDE is homogeneous (source free), and its BC's are of the same kind in each of the tree spatial variables. In particular, the spatial Dirichlet's BC(i) is homogeneous while the temporal Dirichlet's BC(iii) is nonhomogeneous. The Neumann BC(ii) is also nonhomogeneous, but periodic in time.

This problem has analytically been solved in [9] by an additive separation of variables (ASOV) method, and our main concern in this work is the establishment of the consistency of this method for this application.

It is well known that identification of a symmetry group G for a linear non-homogeneous boundary value problem (BVP)

(6)
$$\begin{cases} \mathcal{L}(\mathbf{x}, \Phi, \Phi^{(K)}) = f(\mathbf{x}) \\ \mathbf{B}(\mathbf{x}, \Phi, \Phi^{(K-1)}) = \mathbf{b}(\mathbf{x}), \end{cases}$$

where the partial differential and boundary vector operators, \mathcal{L} and \mathbf{B} , are both linear on \mathbb{R}^n and depend at most on the K-the partial derivative $\Phi^{(K)}$ of Φ , leads to an efficient method for its solution, [1, 2, 18]. Indeed, the symmetry group, generally speaking, is a Lie group, [23], and a Lie algebra is always associated with a Lie group. Moreover, a Lie algebra, having at least one infinitesimal generator, has a given dimension, and whenever the Lie algebra is solvable, the BVP is solvable. So the existence of a symmetry group for (6) can possibly be utilized to establish the irreducible components for the $\Phi^{(K)}$ and $\mathbf{x} = (x_1, x_2, x_3,, x_n) \in \mathbb{R}^n$ variables, then to deduce a solution. This happens to lead, [13], to a separated variable system BVP

(7)
$$\begin{cases} \mathbf{G}(\mathbf{x}, \mathbf{u}, \mathbf{u}^{(K)}) = \mathbf{g}(\mathbf{x}) \\ \mathbf{Q}(\mathbf{x}, \mathbf{u}, \mathbf{u}^{(K-1)}) = \mathbf{q}(\mathbf{x}), \end{cases}$$

by means of a $\mathbf{u} \mapsto \Phi$ transformation $\Phi = \gamma(\mathbf{u})$, or $\mathbf{u} = \gamma^{-1}(\Phi)$, that defines an accompanying (indexed with γ) nonsingular linear operator Γ_{γ} viz

(8)
$$\Gamma_{\gamma} \begin{pmatrix} \mathcal{L} - f \\ \mathbf{B} - \mathbf{b} \end{pmatrix} = \begin{pmatrix} \mathbf{G} - \mathbf{g} \\ \mathbf{Q} - \mathbf{q} \end{pmatrix}$$
.

Relation (7) indicates that symmetry adapted solutions to partial differential equations (PDE's) from knowledge of their Lie symmetries is an example of orthogonal variable separation, see e.g. [22]. In particular, W. Miller has highlighted in [22] many points of contact between separation of variables methods and Lie symmetries of a PDE, including their possible ties with the mathematics of the rather old Stäckel form, [26]. It should be noted, however, that symmetry-based methods have not been widely used, [4], for solving BVP's. The reason being that the pertaining boundary conditions (BC's) are usually not invariant under most similarity transformations, i.e. they do not admit the symmetries of the governing PDE's. Probably, the first rigorous definition of Lie's invariance for BVP's was formulated by G. W. Bluman, [4], in 1974. In fact there are still many realistic BVP's that cannot be solved using any definition, [2], of Lie's invariance of a BVP. Hence definitions involving more general types of symmetries, like Lie-Bäcklund non-point symmetries, are currently being investigated.

Despite all the previously stated, solving BVP's by separation of variables is both an art and science, which may seem to be only adhoc in nature. For linear PDE's, a multivariate solution $\Phi(\mathbf{x})$, in separated variable form, has widely been attempted by applying representations of $\Phi(\mathbf{x})$ as products or sums of single variable functions $P^{(i)}(x_i)$ or $S^{(i)}(x_i)$ viz

(9)
$$\Phi(\mathbf{x}) = \prod_{i=1}^{n} P^{(i)}(x_i),$$

or

(10)
$$\Phi(\mathbf{x}) = \sum_{i=1}^{n} S^{(i)}(x_i),$$

respectively.

The form (9) is multiplicative separation of variables, while (10) is additive. It is moreover straightforward to verify that each of them can only apply iff $\frac{\partial \Phi}{\partial x_i}$ / Φ or $\frac{\partial \Phi}{\partial x_i}$ / $S^{(i)}$ depend respectively only on x_i , $\forall i$.

The theoretical basis for this separation of variables procedure happens to be constrained three fold. The first restriction on this basis comes from the possible nonuniqueness of $\Phi(\mathbf{x})$ satisfying (6). The second constraint is tied to whether the form (9), (10) or their other variants can satisfy the BVP. In this respect, it is well known that the additive separation of variables does not work for the Laplace equation $\Phi_{xx} + \Phi_{yy} + \Phi_{zz} = 0$ on R^3 ; as it cannot match the usual notion of a potential-it does not die at spatial infinity. In contrast, the multiplicative separation of variables works for this singular BVP. Then, the third constraint emerges from the approximate nature of representing $\Phi(\mathbf{x})$ in any of the separated variable forms. Ultimately, the Kolmogorov-Arnold representation theorem, which solves a more general form of Hilbert's thirteenth problem, [19], states that every continuous multivariate $\aleph(\mathbf{x})$ can be expressed as a finite composition of outer, F_q , and inner, $f_{q,p}$, continuous functions of a single variable x_p , with the binary operation of addition, viz

(11)
$$\aleph(\mathbf{x}) = \sum_{q=0}^{2n} F_q \left(\sum_{p=1}^n f_{q,p}(x_p) \right).$$

This fundamental theorem which is also applicable to the solution $\Phi(\mathbf{x})$ of (6), has however a number of other simpler variants. A further, even simpler situation, can occur when x_1 , say, and x_i , $\forall i > 1$, are subjected in the BVP to differential operators of varying orders, like say $\frac{\partial}{\partial x_1}$ and $\frac{\partial^2}{\partial x_i^2}$ (as in diffusional PDE's) on finite \overline{R} when there are weak grounds for assuming $x_1 - x_i$ separability, $\forall i > 1$. Here, one can recast (10) into the form

(12)
$$\Phi(\mathbf{x}) = \sum_{i=2}^{n} S^{(i)}(x_1, x_i),$$

where $S^{(i)}(x_1, x_i)$ is not necessarily x_1-x_i separable. This has been the ASOV principle, demonstrated in [9], to be applicable for a 3D closed form analytical solution to the dynamical BVP of neutron cancer therapy (NCT), via utilizing Laplace transforms in the $x_1 = t$ (time) variable instead of $t - x_i$ separability. Incidentally, the same Laplace transform approach had earlier been used in [8] for solving a 1D version of this BVP. It should be noted, moreover, that this 3D BVP is of unique symmetry due to its having the same kind of BC's in each of the three spatial variables, which can be of different spans. Actually, our aim in this work is to establish the consistency of this principle for solving this particular 3D BVP by exterior calculus arguments, without invoking the heavy machinery of Lie group symmetry.

The exterior analysis of the solvability of dynamical BVP's addresses variations of the BVP solution over differential volume elements $dt \wedge d\mathbf{r}$, with the wedge properties: $d\xi \wedge d\eta = -d\eta \wedge d\xi$; $d\xi \wedge d\xi = 0$, for any ξ and η . An analysis which is a natural geometric setting, as to be shown in sections 2 and 3, from which to initiate a consistency assessment of the ASOV principle, enabling a more concise and explicit evaluation than by an alternative symmetry-based assessment. A more detailed account on exterior differential analysis is provided in Appendix A.

The paper is organized as follows. After this introduction, section 2 reports on the main result of this work on separability and solvability of BVP's in general. In section 3, we review the ASOV solution of the 3D dynamical BVP of NCT, reported in [9]. Finally in section 4 we employ an exterior calculus approach to establish the consistency of the arguments for the ASOV principle in solving the considered BVP.

2 Solvability and additive separability

Recently in [25] Ramsey et al. studied the relation of symmetry to the multiplicative separability of the neutron diffusion equation. Using Lie group analysis, they found that the traditional space-time multiplicatively separable solution of the neutron diffusion BVP corresponds to time translation and flux scaling symmetries. In 1971, using the language of differential forms, Harrison and Estbrook, [13], formulated an alternative approach to traditional symmetry analysis meth-

ods. In this "isovectors" approach, all differential equations being analyzed are recast as exterior differential systems (EDS), and analysis of acting operators takes place in a manifold spanned by all independent and dependent variables of the associated BVP. An approach that is intended for applications where Lie symmetry analysis turns out to be prohibitively complicated or not to produce conclusive results.

The 3D dynamical BVP of neutron cancer therapy, of present interest, acts on a neutron diffusional flux

(13)
$$\Phi = \Phi(\mathbf{r}, t) = \Phi(x, y, z, t),$$

and may, in general be transformed, via γ of (8), by any kind of separation of variables. The associated Γ_{γ} nonsingular, $\Gamma_{\gamma}(\mathbf{0}) = \mathbf{0}$, operator is symbolic in its action of rearranging and redimensioning of the mapped vectors. The ASOV, (12), in particular, can be expressed here via

(14)
$$\Phi = \gamma(\phi) = \sum_{i=1}^{3} \phi_i = \phi_1(x, t) + \phi_2(y, t) + \phi_3(z, t), \ \phi = (\phi_1, \phi_2, \phi_3);$$

 $(\mathbf{r}, t) \in \Re.$

This γ happens remarkably to be closed under addition (of Φ and Ψ) and under scalar multiplication (of c by Φ), i.e. it is a linear $\Phi \mapsto \phi$ transformation. A linearity that obviously does not hold for multiplicative separation of variables; and is a reason for the focus of attention in this paper only on the ASOV transformation (14).

As a matter of notation, we shall refer to the BVP's (6) and (7) by $BVP(\Re, \mathcal{L}, \mathbf{B})$ and $BVP(\Re, \mathbf{G}, \mathbf{Q})$, respectively. Now we are able to advance the following basic results of this work.

Lemma 1 Let a solution Φ to a $BVP(\Re,\mathcal{L},\mathbf{B})$ of (6) be analyzable, $\Phi \to \phi$, by means of the ASOV transformation γ^{-1} of (14), with an accompanying nonsingular operator Γ_{γ} transforming (6) to a system $BVP(\Re,\mathbf{G},\mathbf{Q})$

(15)
$$\begin{cases} \mathbf{G}(\mathbf{x}, \phi, \phi^{(K)}) = \mathbf{g}(\mathbf{x}) \\ \mathbf{Q}(\mathbf{x}, \phi, \phi^{(K-1)}) = \mathbf{q}(\mathbf{x}). \end{cases}$$

Then the Lie symmetry solvability of (15) guaranties reversibility of these γ^{-1} and Γ_{γ} transformations to a solution $\Phi = \gamma(\phi)$ of the original BVP.

Proof: Consideration of (7)-(8) in the form

(16)
$$\begin{pmatrix} \mathbf{G} - \mathbf{g} \\ \mathbf{Q} - \mathbf{q} \end{pmatrix} = \Gamma_{\gamma} \begin{pmatrix} \mathcal{L} - f \\ \mathbf{B} - \mathbf{b} \end{pmatrix}$$

allows for rewriting it as a symbolic functional transformation $\begin{pmatrix} \mathcal{L} \\ \mathbf{B} \end{pmatrix} \mapsto$

$$\begin{pmatrix} \mathbf{G} \\ \mathbf{Q} \end{pmatrix}$$
, given by

(17)
$$\begin{pmatrix} \mathbf{G} \\ \mathbf{Q} \end{pmatrix} = \Gamma_{\gamma} \begin{pmatrix} \mathcal{L} \\ \mathbf{B} \end{pmatrix} + \begin{pmatrix} \mathbf{g}^* \\ \mathbf{q}^* \end{pmatrix}.$$

Locally, in the neighborhood of any fixed $\mathbf{x_0} = (x_0, y_0, z_0, t_0)$, $\Phi_0 = \Phi(\mathbf{x_0})$, $\gamma \to \gamma_0$ and $\Gamma_{\gamma} \to \Gamma_{\gamma_0}$. Then the previous vector equation becomes

(18)
$$\begin{pmatrix} \mathbf{G_0} \\ \mathbf{Q_0} \end{pmatrix} = \Gamma_{\gamma_0} \begin{pmatrix} \mathcal{L}_0 \\ \mathbf{B_0} \end{pmatrix} + \begin{pmatrix} \mathbf{g_0^*} \\ \mathbf{q_0^*} \end{pmatrix}$$

a generalized Euclidean transformation of \mathbb{R}^2 , which is almost always reversible.

A transformation of the type (18) forms a group (under the usual composition of generalized transformations) called an affine transformation group, [17], denoted as \Im^2 . Moreover, one would expect an affine group to consist of geometrical actions like "translations", "rotations" and "reflections" in R^2 . Indeed, such Euclidean transformations preserve the degree of subjected curves, thus mapping a "circle" to a "circle", preserve the ratio of distances, thus mapping centers of circles to centers of circles and preserve contact between existing curves. One can, therefore, claim that $\begin{pmatrix} \mathbf{G_0} \\ \mathbf{Q_0} \end{pmatrix}$ and $\begin{pmatrix} \mathcal{L}_0 \\ \mathbf{B_0} \end{pmatrix}$ belong in generalized affine symmetric spaces, and that linearity of the ASOV γ is an essential instrument for that. Extension of these features, however, globally to (17), i.e. claiming that $\begin{pmatrix} \mathbf{G} \\ \mathbf{Q} \end{pmatrix}$

and $\begin{pmatrix} \mathcal{L} \\ \mathbf{B} \end{pmatrix}$ of (17) also form an affine group, can only be a rough approximation, that calls for a deeper theoretical verification.

Anyhow, and without such a verification, if the system BVP (15) is Lie symmetry solvable, i.e. its algebra is solvable, then the system (15) itself, or its equivalent (17), are solvable. Moreover, solvability of (17) means solvability of (18), $\forall \mathbf{x_0}$, and reversibility of Γ_{γ_0} to a solution $\Phi_0 = \gamma(\phi_0)$ of the original BVP is guaranteed for every $\mathbf{x_0}$. Here the proof completes.

The expected complexity of solving a Lie symmetry algebra for the posing BVP (6) and its possible nonuniqueness motivates avoiding it by means of the simpler substitute result that follows.

Theorem 1 (Analysis-Synthesis) Let a solution Φ to a $BVP(\Re,\mathcal{L},\mathbf{B})$ of (6) be analyzable, $\Phi \to \phi$, by means of the ASOV transformation γ^{-1} of (14), with an accompanying nonsingular operator Γ_{γ} transforming (6) to a system $BVP(\Re, \mathbf{G}, \mathbf{Q})$ of (15). If this system is solvable for ϕ , and can be synthesized back to $\begin{pmatrix} \mathcal{L} - f \\ \mathbf{B} - \mathbf{b} \end{pmatrix}$ by means of the transformation

(19)
$$\Gamma_{\gamma}^{-1} \begin{pmatrix} \mathbf{G} - \mathbf{g} \\ \mathbf{Q} - \mathbf{q} \end{pmatrix} = \begin{pmatrix} \mathcal{L} - f \\ \mathbf{B} - \mathbf{b} \end{pmatrix}$$
,

then γ is additionally reversible to a solution $\Phi = \gamma(\phi)$ of the original BVP.

Proof: According to [21], a linear operator Υ is said to be symmetric for the BVP($\Re, \mathcal{L}, \mathbf{B}$) if

- 1. $\Upsilon: \Re \to \Re$, automorphic,
- 2. $\Upsilon \mathcal{L} = \mathcal{L} \Upsilon$, commutative,
- 3. $\Upsilon \mathbf{B} = \mathbf{B} \Upsilon$, commutative.

Obviously, the operators commuting with a given operator form a group. Let $\mathcal{E}_{\mathcal{L}}$ and $\mathcal{E}_{\mathbf{B}}$ stand for the group of operators commuting with \mathcal{L} and \mathbf{B} respectively, then the group $\mathcal{E} = \mathcal{E}_{\Re} \cap \mathcal{E}_{\mathcal{L}} \cap \mathcal{E}_{\mathbf{B}}$ is the symmetry group, [21], of the BVP($\Re, \mathcal{L}, \mathbf{B}$), where \mathcal{E}_{\Re} is the automorphism group of \Re . It is rather straightforward to verify that Γ_{γ} in (14), of the ASOV method, satisfies the properties of an Υ .

Moreover if Γ_{γ} is a symmetric operator for BVP($\Re, \mathcal{L}, \mathbf{B}$) and Γ_{γ}^{-1} is a symmetric operator for BVP($\Re, \mathbf{G}, \mathbf{Q}$), then BVP($\Re, \mathcal{L}, \mathbf{B}$) and BVP($\Re, \mathbf{G}, \mathbf{Q}$) are symmetries of each other. Consequently, BVP($\Re, \mathcal{L}, \mathbf{B}$) and BVP($\Re, \mathbf{G}, \mathbf{Q}$) can have the same solution, which is a necessary condition for reversibility of γ , defined in (14).

Finally, Γ_{γ}^{-1} cannot exist if γ does not exist. So the contrary can not be true.

It should be noted that γ of theorem 1 is not restricted to the ASOV transformation (14) but applies also to any other variant of it. Distinctively, Γ_{γ}^{-1} could e.g. involve some algebra with wedge products on associated manifolds; as to be illustrated in section 4.

3 The 3D BVP ASOV solution

Here we briefly review the ASOV solution to the posing BVP when the Neumann BC(ii) is periodic in time, with

(20)
$$\begin{cases} S(t) = \frac{a_0}{2} + \sum_{\substack{m=1 \ \infty}}^{\infty} a_m \cos m\omega t, \\ S(t) = \frac{b_0}{2} + \sum_{\substack{m=1 \ \infty}}^{\infty} b_m \cos m\omega (t + \varepsilon), \\ \check{S}(t) = \frac{c_0}{2} + \sum_{\substack{m=1 \ \infty}}^{\infty} c_m \cos m\hat{w} (t + \widehat{\varepsilon}). \end{cases}$$

Clearly the unique symmetry of this 3D BVP (due to its having the same kind of BC's in each of the three spatial variables, which can be of different spans) should facilitate the application of the ASOV principle for the solution. Hence in the associated manifold, the ASOV principle (11) allows for writing

(21)
$$\Phi(x, y, z, t) = \phi(x, t) + \psi(y, t) + \Xi(z, t),$$

where each of $\phi(x,t)$, $\psi(y,t)$ and $\Xi(z,t)$ can satisfy simpler BCs than $\Phi(x,y,z,t)$.

Next, let us assume validity of (14) by the solution of (13-17) to rewrite (13) as

$$(22) \ \frac{1}{v} \frac{\partial}{\partial t} (\phi + \psi + \Xi) - \left[D_{\parallel} \frac{\partial^2}{\partial x^2} + D_{\vdash} \frac{\partial^2}{\partial y^2} + D_{\perp} \ \frac{\partial^2}{\partial z^2} \right] (\phi + \psi + \Xi) \ +$$

$$\Sigma_a (\phi + \psi + \Xi) = 0.$$

This can readily be reduced to

$$(23) \begin{cases} \frac{1}{v} \frac{\partial}{\partial t} \phi(x,t) - D_{\parallel} \frac{\partial^{2}}{\partial x^{2}} \phi(x,t) + \Sigma_{a} \phi(x,t) \\ = -\frac{1}{v} \frac{\partial}{\partial t} [\psi(y,t) + \Xi(z,t)] + \left[D_{\vdash} \frac{\partial^{2}}{\partial y^{2}} \psi(y,t) + D_{\perp} \frac{\partial^{2}}{\partial z^{2}} \Xi(z,t) \right] \\ - \Sigma_{a} \left[\psi(y,t) + \Xi(z,t) \right] = \lambda(t), \end{cases}$$

with $\lambda(t)$ as an unknown functional parameter, in the sense of [7], of the time variable.

For
$$\times = \frac{x}{\sqrt{vD_{\parallel}}} \ge 0$$
,
the mixed-type BVP becomes

(24)
$$\begin{cases} \frac{\partial}{\partial t}\phi(\mathbf{x},t) - \frac{\partial^{2}}{\partial \mathbf{x}^{2}}\phi(\mathbf{x},t) + v\Sigma_{a} \ \phi(\mathbf{x},t) = v\lambda(t), \\ (\mathrm{i}) \ \phi(\sqrt{vD_{\parallel}}\widehat{a},t) = 0, \\ (\mathrm{ii}) \ \frac{\partial}{\partial \mathbf{x}} \ \phi(\mathbf{x},t) \mid_{\mathbf{x} = 0} = -\sqrt{\frac{v}{D_{\parallel}}} \varkappa_{\parallel} \left[\frac{a_{0}}{2} + \sum_{m=1}^{\infty} a_{m} \cos m\omega t \right], \\ (\mathrm{iii}) \ \phi(\mathbf{x},0) = \varphi(\mathbf{x}), \end{cases}$$

while for $\acute{y} = \frac{y}{\sqrt{vD_{\vdash}}} \geq 0$, we have

(25)
$$\begin{cases} \frac{\partial}{\partial t}\psi(\acute{y},t) - \frac{\partial^{2}}{\partial \acute{y}^{2}}\psi(y,t) + \Sigma_{a} \psi(\acute{y},t) = v\zeta(t), \\ (i) \quad \psi(\sqrt{vD_{\vdash}}\widehat{b},t) = 0, \\ (ii) \quad \frac{\partial}{\partial \acute{y}} \psi(\acute{y},t)|_{\acute{y} = 0} = -\sqrt{\frac{v}{D_{\vdash}}}\varkappa_{\vdash} \left[\frac{b_{0}}{2} + \sum_{m=1}^{\infty} b_{m}\cos m\varpi(t+\varepsilon)\right], \\ (iii) \quad \psi(\acute{y},0) = \emptyset(\acute{y}), \end{cases}$$

with $\zeta(t)$ as an unknown functional parameter different from $\lambda(t)$.

Then for $z = \frac{z}{\sqrt{vD_{\perp}}} \ge 0$, the associated mixed-type BVP must be

(26)
$$\begin{cases} \frac{\partial}{\partial t}\Xi(\dot{z},t) - \frac{\partial^{2}}{\partial \dot{z}^{2}}\Xi(\dot{z},t) + v\Sigma_{a}\Xi(\dot{z},t) = -v\lambda(t) - v\zeta(t), \\ (i) \quad \Xi(\sqrt{vD_{\perp}}\widehat{c},t) = 0, \\ (ii) \quad \frac{\partial}{\partial \dot{z}}\Xi(\dot{z},t)|_{\dot{z}=0} = -\sqrt{\frac{v}{D_{\perp}}}\varkappa_{\perp}\left[\frac{c_{0}}{2} + \sum_{m=1}^{\infty} c_{m}\cos m\hat{w}(t+\widehat{\varepsilon})\right], \\ (iii) \quad \Xi(\dot{z},0) = \varnothing(\dot{z}). \end{cases}$$

All these three BVPs , now with nonhomogeneous PDF's, are structurally identical and coupled by means of the unknown $\lambda(t)$ and $\xi(t)$ functions. They contain yet unknown individual initial conditions $\varphi(x)$, $\emptyset(y)$ and $\varnothing(z)$ in their temporal nonhomogeneous Dirichlet's BC (iii).

The existence of a unique solution to the posing BVP, via the ASOV principle (9), turns out to require the imposition of an additional "complementarity"-like condition that

(27)
$$\phi(0,t) = \psi(0,t) = \Xi(0,t)$$
.

This is a physically quite reasonable condition, see [9], equivalent to the continuity of the neutron flux (or density) through the (0,0,0) corner interface of R.

Because of the linearity of the nonhomogeneous PDE in (8) and of its associated BC's, we may determine $\varphi(\times)$ by the following boundary decomposition principle. Consider first a steady state neutron diffusional process generated only by the stationary term (m=0 mode) of the Neumann BC(ii). Since the two remaining BCs are time-independent and so are the coefficients Σ_a , D_{\parallel} and v of the PDE, then $\frac{\partial}{\partial t}\phi=0$, $\lambda(t)$ becomes a constant λ and $\phi(\times,t)$ becomes $\varphi(\times)$ that satisfies the auxiliary ordinary BVP:

$$\begin{cases}
\frac{d^{2}}{dx^{2}}\varphi(\times) - v\Sigma_{a} \varphi(\times) = -v\lambda, \\
(i) \quad \varphi(\sqrt{vD_{\parallel}}\widehat{a}) = 0, \\
(ii) \quad \frac{d}{dx}\varphi(\times)|_{\times=0} = -\sqrt{\frac{v}{D_{\parallel}}}\varkappa_{\parallel}\frac{a_{0}}{2}.
\end{cases}$$

The solution $\varphi(\times)$ of the auxiliary BVP can be derived in detail via formula (32) in [9] which contains the unknown coupling factor λ . This $\varphi(\times)$ can be substituted back into BC(iii) of (26) to complete its statement prior to its subsequent solution for $\phi(\times,t)$ by means of the Laplace transformation in the t-domain. In a similar fashion $\emptyset(\mathring{y})$ can be determined via (49) of [9] and to contain $\mathcal{F} = \zeta(0)$, while $\varnothing(\mathring{z})$ contains $(\lambda + \mathcal{F})$, via (67) of [9]. These λ and \mathcal{F} coupling factors are shown to be computable by means of the nonlinear process (71) of [9].

Furthermore, invertible Laplace transforms of the coupling functions $\lambda(t)$ and $\zeta(t)$ turn out also to be computable by a modal expansion approach via the complex nonlinear process (94) of [9]. Both of the nonlinear processes (71) and (94) are actually based on (27). Then the entire ASOV solution for this BVP is obtained, via repeated inversions of Laplace transforms, in the closed analytical form reported in [9].

4 Exterior analysis

To simplify notation in this analysis, let us represent the three PDE's , in the posing BVP, that are separated according to the ASOV principle viz

(28)
$$\phi_t - \phi_{\times \times} + g_1(t, \times) \phi = 0$$
,

(29)
$$g_1(t,x) = v\Sigma_a - v\lambda(t)\phi^{-1}(x,t),$$

(30)
$$\psi_t - \psi_{\acute{y}\acute{y}} + g_2(t, \acute{y}) \psi = 0,$$

(31)
$$g_2(t, \acute{y}) = v\Sigma_a - v\zeta(t)\psi^{-1}(\acute{y}, t),$$

(32)
$$\Xi_t - \Xi_{zz} + q_3(t, z) \Xi = 0$$
,

(33)
$$g_3(t, \acute{z}) = v\Sigma_a + v[\lambda(t) + \zeta(t)]\Xi^{-1}(\acute{z}, t).$$

Nowadays, the isovector method is developed in rigorous detail and applied to many problems in science and engineering, see e.g. [5, 28]. Inspired by these works, let revisit the BVP (24), of the \times - variable, and reduce it to a first-order differential system BVP, by assuming

(34)
$$\rho = \rho(x,t) = \frac{\partial}{\partial x} \phi(x,t),$$

then multiplying the BVP by the differential volume element $dt \wedge d \times \wedge d\acute{y} \wedge d\acute{z}$, where the operator \wedge means wedge (or exterior) product, to write

$$\rho \ dt \wedge \ d \times \wedge \ d\acute{y} \wedge d\acute{z} + \ d\phi \wedge \ dt \wedge \ d\acute{y} \wedge d\acute{z} = 0,$$

$$d\phi \wedge \ d \times \wedge \ d\acute{y} \wedge d\acute{z} + \ d\rho \wedge \ dt \wedge \ d\acute{y} \wedge d\acute{z} + \ g_1 \phi \ dt \wedge \ d \times \wedge \ d\acute{y} \wedge d\acute{z} = 0,$$

$$\phi(\times,0) \ dt \wedge \ d \times \wedge \ d\acute{y} \wedge d\acute{z} - \varphi(\times) \ dt \wedge \ d \times \wedge \ d\acute{y} \wedge d\acute{z} = 0,$$

$$\rho(0,t) \ dt \wedge \ d \times \wedge \ d\acute{y} \wedge d\acute{z} + \sqrt{\frac{v}{D_{\parallel}}} \varkappa_{\parallel} \ S(t) \ dt \wedge \ d \times \wedge \ d\acute{y} \wedge d\acute{z} = 0,$$

$$\phi(\sqrt{vD_{\parallel}}\widehat{a},t) \ dt \wedge \ d \times \wedge \ d\acute{y} \wedge d\acute{z} = 0,$$

$$\phi(0,t) \ dt \wedge \ d \times \wedge \ d\acute{y} \wedge d\acute{z} - \psi(0,t) \ dt \wedge \ d \times \wedge \ d\acute{y} \wedge d\acute{z} = 0,$$

with the last equation representing the complementarity corner continuity condition, to define the unknown ASOV parameter $\lambda = \lambda(t)$ standing in $g_1 = g_1(t, \times)$, of (29). Application of similar steps to the BVP's (25) and (26), while assming,

(36)
$$\theta = \theta(\acute{y}, t) = \frac{\partial}{\partial \acute{y}} \psi(\acute{y}, t), \quad \beta = \beta(\acute{z}, t) = \frac{\partial}{\partial \acute{z}} \Xi(\acute{z}, t),$$

results with the following two respective exterior differential systems (EDS's)

$$\theta \ dt \wedge \ d \times \wedge \ d\acute{y} \wedge \ d\acute{z} - \ d\psi \wedge \ dt \wedge \ d \times \wedge \ d\acute{z} = 0,$$

$$d\psi \wedge \ d \times \wedge \ d\acute{y} \wedge \ d\acute{z} + \ d\theta \wedge \ dt \wedge \ d \times \wedge \ d\acute{z} + \ g_2 \psi \ dt \wedge \ d \times \wedge \ d\acute{y} \wedge \ d\acute{z} = 0,$$

$$\psi(\acute{y},0) \ dt \wedge \ d \times \wedge \ d\acute{y} \wedge \ d\acute{z} - \emptyset(\acute{y}) \ dt \wedge \ d \times \wedge \ d\acute{y} \wedge \ d\acute{z} = 0,$$

$$\theta(0,t) \ dt \wedge \ d \times \wedge \ d\acute{y} \wedge \ d\acute{z} + \sqrt{\frac{v}{D_{\vdash}}} \varkappa_{\vdash} \ \S(t) \ dt \wedge \ d \times \wedge \ d\acute{y} \wedge \ d\acute{z} = 0,$$

$$\psi(\sqrt{vD_{\vdash}} \widehat{b}, t) \ dt \wedge \ d \times \wedge \ d\acute{y} \wedge \ d\acute{z} = 0,$$

$$\psi(0,t) \ dt \wedge \ d \times \wedge \ d\acute{y} \wedge \ d\acute{z} - \Xi(0,t) \ dt \wedge \ d \times \wedge \ d\acute{y} \wedge \ d\acute{z} = 0,$$

$$\beta \ dt \wedge d \times \wedge d\acute{y} \wedge d\acute{z} + d\Xi \wedge dt \wedge d \times \wedge d\acute{y} = 0,$$

$$d\Xi \wedge d \times \wedge d\acute{y} \wedge d\acute{z} + d\beta \wedge dt \wedge d \times \wedge d\acute{y} + g_3\Xi \ dt \wedge d \times \wedge d\acute{y} \wedge d\acute{z} = 0,$$

$$\Xi(\acute{y},0) \ dt \wedge d \times \wedge d\acute{y} \wedge d\acute{z} - \varnothing(\acute{z}) \ dt \wedge d \times \wedge d\acute{y} \wedge d\acute{z} = 0,$$

$$\beta(0,t) \ dt \wedge d \times \wedge d\acute{y} \wedge d\acute{z} + \sqrt{\frac{v}{D_{\perp}}} \varkappa_{\perp} \ \check{S}(t) \ dt \wedge d \times \wedge d\acute{y} \wedge d\acute{z} = 0,$$

$$\Xi(\sqrt{vD_{\perp}}\widehat{c},t) \ dt \wedge d \times \wedge d\acute{y} \wedge d\acute{z} = 0,$$

$$\Xi(0,t) \ dt \wedge d \times \wedge d\acute{y} \wedge d\acute{z} - \varphi(0,t) \ dt \wedge d \times \wedge d\acute{y} \wedge d\acute{z} = 0.$$

The system (35)-(38) is a Grassman algebraic system (whose product is the wedge product) and its differential forms are mathematical objects that represent infinitesimal volumes of infinitesimal parallelepipeds and so can be integrated over volumes and higher order manifolds in a way that generalizes line integrals from calculus. They interestingly happen also to be common ingredients with infinitesimal Lie group symmetries.

The last equation in (37) accounts for the ASOV parameter ζ , standing in $g_2 = g_2(t, \acute{y})$, while the last equation in (38) accounts for $-(\lambda + \zeta)$ standing in $g_3 = g_3(t, \acute{z})$. It should not be overlooked, moreover, that $S(t) = S(t, \omega), \S(t) = \S(t, \varpi, \varepsilon)$ and $\check{S}(t) = \check{S}(t, \hat{w}, \widehat{\varepsilon})$.

4.1 First equations

The first equations in the EDS's (35), (37) and (38) sum up to

$$(\rho + \theta + \beta) dt \wedge d \times \wedge d\acute{y} \wedge d\acute{z} + [d\phi \wedge dt \wedge d\acute{y} \wedge d\acute{z} - d\psi \wedge dt \wedge d \times \wedge d\acute{z} + d\Xi \wedge dt \wedge d \times \wedge d\acute{y}] = 0,$$

which is the same as

$$\begin{split} (\rho + \theta + \beta) \ d \times \wedge \ d \circ \wedge \ d \circ \wedge \ d t - [d \phi \wedge d \circ \wedge \ d \circ \wedge \ d t - d \psi \wedge \ d \times \wedge \ d \circ \wedge \ d t \\ + d \Xi \wedge d \times \wedge d \circ \wedge \ d t] = 0, \end{split}$$

or

$$\{ (\rho + \theta + \beta) \ d \times \wedge \ d \circ \wedge d \circ - [d \phi \wedge d \circ \wedge d \circ - d \psi \wedge d \times \wedge \ d \circ + d \Xi \wedge d \times \wedge d \circ] \} \wedge dt = 0.$$

This relation is remarkably independent of the temporal differential element dt viz

(39)
$$(\rho + \theta + \beta) d \times \wedge d\acute{y} \wedge d\acute{z} - [d\phi \wedge d\acute{y} \wedge d\acute{z} - d\psi \wedge d \times \wedge d\acute{z} + d\Xi \wedge d \times \wedge d\acute{y}] = 0.$$

It should be noted however that the ρ , θ and β variables are of auxiliary nature, and do not appear explicitly in the original PDE.

4.2 Separated DE's

The second equations in the EDS's (35), (37) and (38) sum up to

$$(d\phi + d\psi + d\Xi) \ d \times \wedge \ d\acute{y} \wedge d\acute{z} + [d\rho \wedge \ dt \wedge \ d\acute{y} \wedge d\acute{z} + d\theta \wedge \ dt \wedge \ d \times \wedge \ d\acute{z}$$

 $+d\beta \wedge dt \wedge d \times \wedge d\acute{y}$] $+ [g_1\phi + g_2\psi + g_3\Xi] dt \wedge d \times \wedge d\acute{y} \wedge d\acute{z} = 0$, which is the same as

$$\frac{\partial}{\partial t}(\phi + \psi + \Xi) dt \wedge d \times \wedge d\acute{y} \wedge d\acute{z} - \left[\frac{\partial \rho}{\partial \times} + \frac{\partial \theta}{\partial \acute{y}} + \frac{\partial \beta}{\partial \acute{z}}\right] dt \wedge d \times \wedge d\acute{y} \wedge d\acute{z} + v\Sigma_a(\phi + \psi + \Xi) dt \wedge d \times \wedge d\acute{y} \wedge d\acute{z} = 0,$$

i.e.

(40)
$$\left[\frac{\partial}{\partial t}\Phi - \nabla^2 \Phi + v\Sigma_a \Phi\right] dt \wedge d \times dy \wedge dz = 0.$$

This proves that satisfaction of the EDS's, resulting from application of the ASOV principle to a PDE, implies, as a must, solvability of this PDF.

4.3 The boundary conditions

The third equations in the EDS's (35), (37) and (38) sum up to

$$[\phi(\times,0) + \psi(\acute{y},0) + \Xi(\acute{y},0)]dt \wedge d \times \wedge d\acute{y} \wedge d\acute{z} - [\varphi(\times) + \emptyset(\acute{y}) + \varnothing(\acute{z})]dt \wedge d \times \wedge d\acute{y} \wedge d\acute{z} = 0,$$

which is the same as

$$(41) \left. \left\{ \Phi(\mathbf{r},0) \right|_{\mathbf{r} \in \overline{R}} \right. \\ \left. - [\varphi(\times) + \emptyset(\acute{y}) + \varnothing(\acute{z})] \right\} dt \wedge d \times \wedge d\acute{y} \wedge d\acute{z} = 0.$$

As for the fourth equations, their sum is

$$[\rho(0,t) + \theta(0,t) + \beta(0,t)] dt \wedge d \times \wedge d\mathring{y} \wedge d\mathring{z}$$

$$+ \left[\sqrt{\tfrac{v}{D_{\parallel}}} \varkappa_{\parallel} S(t) + \sqrt{\tfrac{v}{D_{\vdash}}} \varkappa_{\vdash} \S(t) + \sqrt{\tfrac{v}{D_{\perp}}} \varkappa_{\perp} \check{S}(t) \right] \, dt \, \wedge \, d \times \wedge \, d \circ \wedge \, d \circ = 0.$$

Clearly, this is same as or, in the context of the ASOV, as

Furthermore, the fifth equations add up to

$$\left[\phi(\sqrt{vD_{\parallel}}\widehat{a},t)+\psi(\sqrt{vD_{\vdash}}\widehat{b},t)+\Xi(\sqrt{vD_{\perp}}\widehat{c},t)\right]\,dt\wedge d\times\wedge d\acute{y}\wedge d\acute{z}=0\ ,$$
 which is the same as (8) in the form

Distinctively, the sixth equations in the EDS's (28),(30) and (31) add up to

$$(45) \quad 0 \ dt \wedge d \times \wedge d\acute{y} \wedge d\acute{z} = 0,$$

a constraint inactive on the original BVP and its solution Φ .

These facts, which satisfy the conditions of Theorem 1, establish the correctness of the ASOV principle in solving the 3D dynamical BVP of neutron cancer therapy. At this point, it should be underlined that:

- i) The ASOV solution to the present neutron diffusion BVP is the only existing closed form analytical solution to this newly formulated problem.
- ii) The alternative to ASOV hypothetical method of analytical solution could be a multiplicative separation of variables. This turned out, however, to be analytically intractable.
- iii) Moreover, possible numerical methods are irrelevant since the considered ASOV solution is meant for further inclusion in theoretical therapeutic optimization algorithms.
- iv) The reported in this paper consistency analysis of the ASOV solution to this dynamical BVP is unique and new. Moreover, the only possible alternative symmetry-based analysis (which has so far never been attempted) would certainly be useful, if it happens to be tractable.

Conclusion

In this paper, we have studied the consistency question related to the ASOV solution of the 3D dynamical BVP of NCT. The conclusive lemma 1 of this work indicates that any symmetry-based analysis, which is probably too involved analytically, is of limited practical value. Distinctively, the reported related isovetor analysis, of section 4 in the context of theorem 1, appears to be direct, concise and elegant in establishing this consistency.

5 Appendix A: Exterior differential analysis

An exterior differential system (EDS) is a system of equations on a manifold defined by equating to zero a number of exterior differential forms, see e.g. [3]. When all the forms are linear, it is called a Pfaffian system. The theory of exterior differential forms is coordinate (x, y, z, t) free and its related computations have a distinctive algebraic character. A system of PDE's of any number of independent

and dependent variables can be written as an EDS (an isovector system). PDE's and their Pfaffian EDS's are essentially the same, [3], in many respects.

The solutions of a BVP obtained by using Lie theory of continuous symmetry groups are called group-invariant solutions. Furthermore, the relation between Lie symmetries and prolongation structures, [1, 2], or EDS's, of field equations is widely recognized.

In exterior differential calculus, the isovectors are elements of a vector space; vectors may be added or multiplied by scalars. For the product, however, the wedge (Grassmann) product \wedge is used. This is a generalization of the cross product in 3D vector algebra. A product that introduces the notion of a multivector. In actual fact the \wedge product is the "correct" type of product to use in computing a volume element $d\mathbf{x}$ in a tensor field, see e.g. [6]. The infinitesimal volume element $d\mathbf{x}$ bounded by $dx_1 \cup dx_2 \cup dx_3 \cdot \cdots \cup dx_n$ has a volume given by $d\mathbf{x} = dx_1 \wedge dx_2 \wedge dx_3 \cdot \cdots \wedge dx_n$, instead of the symmetric product $dx_1 dx_2 dx_3 \cdots dx_n$. This is a technical refinement, often omitted in vector fields, though quite essential in tensor fields, encountered e.g. in the BVP (posed in this paper), which incorporates a neutron diffusion tensor.

Exterior differential calculus (isovector calculus) is primarily intended, [30], for calculation of invariance groups of EDS's. Unfortunately, however, the maximum number of determining equations for the isovectors of a given PDE can be very large. For typical 2D systems arising in fluid dynamics there may be as many as 1710 determining equations, [6, 30], This situation is expected to blow up significantly for the dynamical BVP posing in this work, in a way prohibiting its performance by hand. Moreover, the alternative symbolic computation, see e.g. [30], is not amongst our scheduled activities in the work.

For these reasons we have decided in this paper to abandon the classical symmetry-related analysis for the consistency of the ASOV principle. Nonetheless, the exterior differential calculus continues to provide a proper abstract framework for the treatment of geometrical vector (or tensor) operations that extend naturally through the t-variable to general 4-dimensions in \Re . Its concise concepts yield elegant and peculiarly coherent constructs (as with lemma1 and theorem 1) in contrast with the intricacies of Lie symmetries of the original BVP or its EDS.

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