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NEUTRONICS COMPUTATIONAL APPLICATIONS OF SYMMETRY ALGEBRA*

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Author(s) Roy A. Axford, X DO

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Lawrence Livermore National Laboratory
Livermore, California 94550

NEUTRONICS COMPUTATIONAL APPLICATIONS OF SYMMETRY ALGEBRAS

Roy A. Anford

Los Alamos National Laboratory, Los Alamos, N. M. 87545
University of Illinois at Urbana-Champaign
103 S. Goodwin, Urbana, Illinois 61801

ABSTRACT

The groups of point transformations and their corresponding symmetry algebras are determined for a general system of second order differential equations, special cases of which include the multipgroup diffusion equations and the "EIP form" of the P_3 equations. It is shown how the symmetry algebras can be used to motivate, formulate and simplify double sweep algorithms for solving two point boundary value problems that involve systems of second order differential equations. A matrix Riccati equation that appears in double sweep algorithms is solved exactly by regarding a set of first integrals of the second order system as a set of first order differential invariants of the group of point transformations that is admitted by the system. A second computational application of symmetry algebras is the determination of invariant difference schemes which are defined as difference schemes that admit the same group of point transformations as those admitted by the differential equations that they simulate. Prolongations of symmetry algebra vector fields that are required to construct invariant difference equations are derived and found. Examples of invariant difference schemes are constructed from the basic difference equations, invariance conditions and shown to be exact.

INTRODUCTION

The general objective of the present paper is to define and to examine group theoretical foundations of computational algorithms that can be applied to obtain either analytic or numerical solutions of two point boundary value problems that involve systems of differential equations formulated from the neutron transport equation. The scope of this paper is limited to developing the theoretical aspects of the topic, and analytic solutions of elementary examples are included to illustrate the theoretical points.

Double sweep algorithms have been reported in the reactor physics literature for solving both second order differential equations and the one group difference equations. Ehrlich and Berkowitz attribute to R. W. Stark a double sweep algorithm for handling second order difference equations in diffusion theory and point out the computational advantages that are realized with this algorithm when solving two point boundary value problems. In the first chapter of reference 1, Ehrlich and Berkowitz relate from the point of view of the factorization method a double sweep algorithm for solving two point boundary value problems that involve the one group difference equation. Also, in the fourth chapter of reference 2, Gold and Berkowitz describe a sweep algorithm for solving the P_3 equations

tions.

Additional discussions of double sweep algorithms appear in references 4-7. In Section 31 of reference 3 Gelfand and Lomin show how an inward-outward sweep algorithm for solving two-point boundary value problems that entail a single inhomogeneous second order differential equation can be obtained from the concept of a field of a second order differential equation. Computational advantages of this algorithm, which is referred to as the Gelfand-Lokutsivetski method of chasing, are explored in the ninth chapter of reference 8. Double sweep algorithms for solving second order difference equations are developed in references 9-7.

Double sweep algorithms for both differential and difference equations that are discussed in references 4-7 are thought of in terms of the factorization method, of fields for second order differential equation, and of translating the left-hand boundary condition through the interior points to the right-hand boundary. A different point of view for understanding and formulating double sweep algorithms for systems of second order differential equations is introduced and developed in this paper. We show how knowledge of a Lie algebra of group generators of a system of second order differential equations can be used to understand, motivate, formulate and simplify double sweep algorithms for such systems. Other applications of Lie groups and symmetry algebras to differential equations, which include obtaining similarity solutions, special classes of exact solutions, and partially invariant solutions, are presented in references 8-12 in which, however, no computational applications appear. The simplification in a double sweep algorithm that can be achieved with a Lie algebra is particularly important because of the fact that the exact solution of a matrix Riccati equation can be found with the group generators.

A second computational application of symmetry algebras considered in this paper is that of constructing systems of difference equations that are exact and under the same group of point transformations as that admitted by the system of differential equations being simulated. Invariant difference schemes in the sense of first differential approximations have been studied by Shokri¹³ in the field of gas dynamics. Since the fact that the first differential approximation is invariant does not necessarily imply that all higher order differential approximations are invariant, the method of constructing so-called invariant difference schemes studied by Shokri¹³ can not lead to exact difference equations. Accordingly, we introduce and develop a concept of invariant difference equations that is the direct analog to the concept of invariant differential equations and that is capable of yielding exact difference equations. Specific neutronics examples of systems of group invariant difference equations that are exact have been found and are reported herein.

SYMMETRY GROUPS AND ALGEBRAS OF MULTIGROUP DIFFUSION MODELS

We consider sets of point transformations in the space $(x, y, z, \dots, y_1, \dots, y_n)$ of $n+1$ independent variables, x , and n dependent variables, y_1, \dots, y_n , that are defined by n independent functions, namely,

$$\bar{y}_i = f_i(x, y_1, \dots, y_n), \quad i=1, 2, \dots, n, \quad (1)$$

and

$$\bar{V}_E = T_E(N_1, V_1, V_2, \dots, V_G; a_1, a_2, \dots, a_r). \quad (1)$$

Each set of values of the parameters, a_1, a_2, \dots, a_r , and T labels a different point transformation in the set, and these parameters are assumed to be essential. The transformations T and T' comprise an operator for point transformations under the binary operation of performing two successive transformations if they satisfy the formal group axioms. Namely, the closure, the existence of an identity transformation in the set, the existence of an inverse transformation for each transformation in the set, and associativity for the binary operation. This set then provides the representation of a parameter set of point transformations that are subject to the matrix group-diffusion equation taken in the form

$$X \frac{\partial X}{\partial X_i} \frac{\partial X}{\partial V_j} \frac{\partial X}{\partial V_k} = \sigma_{ijk} X \quad (2)$$

or

$$X \frac{\partial X}{\partial X_i} \frac{\partial X}{\partial V_j} \frac{\partial X}{\partial V_k} = \sigma_{ijk} X + \sum_{l=1}^r \sigma_{ljk} X \frac{\partial X}{\partial a_l} \quad (3)$$

where σ_{ijk} and σ_{ljk} are the parameters N is an essential parameter N is the value $N = 1$ is considered and $N = 0$ is the case where $N = 0$ may also be considered and is excluded from the set. A similar equation for T' may also be derived containing terms that are omitted from the above.

A group of point transformations with the above system of differential equations that they are subject to, are called an invariant system. Also, invariant means that the system is the same for all the new coordinates as it is for the old coordinates, that is, that the value of the value of differential coefficients is not changed in a symmetry property of the system. Symmetry properties of the system are defined as follows: if the system is invariant for all the transformations of the system, then

$$X \frac{\partial X}{\partial X_i} \frac{\partial X}{\partial V_j} \frac{\partial X}{\partial V_k} = \sum_{l=1}^r \gamma_{ljk} X \frac{\partial X}{\partial a_l} \quad (4)$$

where γ_{ljk} are called group generators and are said to represent the infinitesimal transformations of the group around the identity, for which

$$X \frac{\partial X}{\partial X_i} \frac{\partial X}{\partial V_j} \frac{\partial X}{\partial V_k} = \Delta_{ijk} X \quad (5)$$

or

$$X \frac{\partial X}{\partial X_i} \frac{\partial X}{\partial V_j} \frac{\partial X}{\partial V_k} = \Delta_{ijk} X + \sum_{l=1}^r \gamma_{ljk} X \frac{\partial X}{\partial a_l}$$

For convenience, the group generators may be regarded as the basis of an invariant system. Also, the group generators are the infinitesimal operators of the system. The invariance of symmetry algebra of a system of differential equations. The terms γ_{ljk} and Δ_{ijk} are the terms are called the generators for the group of the group generators.

The coordinate functions of the group generators for the multiprong differential equations can be obtained as follows. We introduce the second order jet space whose coordinates represent the independent variable, x , the dependent variables, y , the first order derivatives, y' , and the second order derivatives, y'' . The G -multiprong equations are treated as a set of smooth functions,

$$F_p(x, y, y', y'', \dots, y^{(n)}) = 0, \quad (1)$$

for $p=1, \dots, b$, which defines a submanifold from this second order jet space to a b -dimensional F -linear space. The multiprong equation determines a subvariety of the jet space because they indicate where this may vanish. A group of point transformations whose second order prolongation leaves this subvariety invariant is a symmetry group of the multiprong equation. The second order prolongation of the vector field, X , which will be denoted by $p_2 X$, is a field on the second order jet space which is given by

$$p_2 X = X + \sum_{p=1}^b \xi_p \partial_{y_p'} + \sum_{p=1}^b \phi_p \partial_{y_p''} + \sum_{p=1}^b \phi_p^{(1)} \partial_{y_p^{(1)'}} \quad (2)$$

where

$$\xi_p = \xi(x, y, y', y''), \quad \phi_p = \phi(x, y, y', y''), \quad (3)$$

and

$$\phi_p^{(1)} = \xi_p \xi + \phi_p \xi', \quad (4)$$

where ξ and ϕ are not necessarily linear functions. It is assumed that the group is point, that is, ξ and ϕ are a particular function of the form $\xi = \xi(x, y)$ and $\phi = \phi(x, y, y')$ with no derivatives of x or y .

$$p_2 X^2 = \xi^2 \partial_x^2 + 2\xi \xi' \partial_x \partial_y + \xi'^2 \partial_y^2 + \dots \quad (5)$$

wherever $F_p = 0$, which written out in full, yields a system of linear, but first order partial differential equations, $\mathcal{P}_1 \mathcal{P}_2$ are called the determining equations of the group for the coordinate functions, ξ_p and ϕ_p , of the p -prong generator.

The invariance condition (1) together with the second prolongation term (2) will allow for the simplification of the functions of all independent and dependent variables. In particular, a particularly very useful group of point transformations for the multiprong differential equations can be found from (1) by restricting the action of the group to the dependent variables, that is, by the condition $\xi = 0$ for each p . In this case, the independent spatial variables are not treated as linear for the group action, so $\xi_p = 0$ for $s=1, \dots, b$. A second simplifying restriction is that the dependent variable coordinate functions are functions only of the independent variables. That is,

$$y_p = y_p(x, y, y', y''), \quad (6)$$

with these two restrictions, the second order prolongation of the vector field X is given by $p_2 X$ in (2).

$$\frac{d}{dt} \begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix} = A \begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix} + \begin{bmatrix} b_1 \\ \vdots \\ b_n \end{bmatrix}$$

at:

$$\frac{d}{dt} \begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix} = A \begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix}$$

The nonzero elements of the matrix A_{ij} that appear in (1) and (2) are given by the following relations:

$$A_{ij} = \begin{cases} -k_{ij} & \text{if } i \neq j \\ k_{ij} & \text{if } i = j \end{cases}$$

where k_{ij} is defined as:

$$k_{ij} = \begin{cases} \sum_{k=1}^n k_{ijk} & \text{if } i \neq j \\ \sum_{k=1}^n k_{ijk} & \text{if } i = j \end{cases}$$

where k_{ijk} is the rate constant for the reaction $i \rightarrow j + k$. The rate constants k_{ijk} and k_{ij} are obtained simply by solving analytically the rate equations for the corresponding elementary reactions. The full dimensional rate equations of general form can be written, if desired, by adding the additional mass balance relations for the species x_i and x_j to the n equations that define the matrix A in (1) and (2).

$$A_{ij} = \begin{cases} -k_{ij} & \text{if } i \neq j \\ k_{ij} & \text{if } i = j \end{cases}$$

In the case of all elementary reactions, the usual procedure of the present paper for the calculation of the matrix A and b is defined in (1) and (2) and can be used in the study of steady-state and dimensional substrates of general reactions.

GENERALIZATION OF THE DOUBLE SWEEP ALGORITHM

In this section it is shown how knowledge of the fast algebra of a system of second-order differential equations can be applied to the present double-sweep algorithm which can be used to obtain either analytical or numerical solutions of two-point boundary value problems that result from systems. We consider two-point boundary value problems for the second-order system of differential equations:

$$A \frac{d^2 y}{dx^2} + B \frac{dy}{dx} + C y = F(x)$$

for $a \leq x \leq b$. This system is somewhat more general than the matrix system (1) in that it can be represented by (1) with the identification:

$$A_{ij} = \begin{cases} 0 & \text{if } i \neq j \\ A_{ij} & \text{if } i = j \end{cases}$$

at

Let $\{a_n\}$ be a sequence of real numbers. Then the sequence $\{a_n\}$ is bounded if and only if there exists a real number M such that $|a_n| \leq M$ for all n .

Proof: Suppose $\{a_n\}$ is bounded. Then there exists a real number M such that $|a_n| \leq M$ for all n . Conversely, suppose there exists a real number M such that $|a_n| \leq M$ for all n . Then $\{a_n\}$ is bounded.

Let $\{a_n\}$ be a sequence of real numbers. Then the sequence $\{a_n\}$ converges to a real number L if and only if for every $\epsilon > 0$, there exists a natural number N such that $|a_n - L| < \epsilon$ for all $n > N$.

Proof: Suppose $\{a_n\}$ converges to L . Then for every $\epsilon > 0$, there exists a natural number N such that $|a_n - L| < \epsilon$ for all $n > N$. Conversely, suppose for every $\epsilon > 0$, there exists a natural number N such that $|a_n - L| < \epsilon$ for all $n > N$. Then $\{a_n\}$ converges to L .

Let $\{a_n\}$ be a sequence of real numbers. Then the sequence $\{a_n\}$ is Cauchy if and only if for every $\epsilon > 0$, there exists a natural number N such that $|a_n - a_m| < \epsilon$ for all $n, m > N$. The Cauchy criterion is equivalent to the convergence criterion.

Let $\{a_n\}$ be a sequence of real numbers. Then the sequence $\{a_n\}$ is bounded if and only if it is Cauchy.

Proof: Suppose $\{a_n\}$ is bounded. Then there exists a real number M such that $|a_n| \leq M$ for all n . Then $\{a_n\}$ is Cauchy.

Conversely, suppose $\{a_n\}$ is Cauchy. Then there exists a real number L such that $\{a_n\}$ converges to L . Then $\{a_n\}$ is bounded.

Let $\{a_n\}$ be a sequence of real numbers. Then the sequence $\{a_n\}$ converges to a real number L if and only if $\lim_{n \rightarrow \infty} a_n = L$.

Proof: Suppose $\{a_n\}$ converges to L . Then $\lim_{n \rightarrow \infty} a_n = L$. Conversely, suppose $\lim_{n \rightarrow \infty} a_n = L$. Then $\{a_n\}$ converges to L .

Let $\{a_n\}$ be a sequence of real numbers. Then the sequence $\{a_n\}$ is bounded if and only if $\limsup a_n < \infty$ and $\liminf a_n > -\infty$.

Proof: Suppose $\{a_n\}$ is bounded. Then $\limsup a_n < \infty$ and $\liminf a_n > -\infty$. Conversely, suppose $\limsup a_n < \infty$ and $\liminf a_n > -\infty$. Then $\{a_n\}$ is bounded.

Let $\{a_n\}$ be a sequence of real numbers. Then the sequence $\{a_n\}$ converges to a real number L if and only if $\limsup a_n = \liminf a_n = L$.

Proof: Suppose $\{a_n\}$ converges to L . Then $\limsup a_n = \liminf a_n = L$. Conversely, suppose $\limsup a_n = \liminf a_n = L$. Then $\{a_n\}$ converges to L .

$$a_{p_1} = \frac{C_{p_1}^{(1)} Y}{\lambda} \begin{pmatrix} Y_{p_1}^{(1)} Y_{p_1}^{(2)} \dots Y_{p_1}^{(n)} \\ Y_{p_1}^{(1)} Y_{p_1}^{(2)} \dots Y_{p_1}^{(n)} \\ \vdots \\ Y_{p_1}^{(1)} Y_{p_1}^{(2)} \dots Y_{p_1}^{(n)} \end{pmatrix}, \text{ for } p=1, \dots, n \quad (2.1)$$

$$a_{p_2} = \frac{C_{p_2}^{(1)} Y}{\lambda} \begin{pmatrix} Y_{p_2}^{(1)} Y_{p_2}^{(2)} \dots Y_{p_2}^{(n)} \\ Y_{p_2}^{(1)} Y_{p_2}^{(2)} \dots Y_{p_2}^{(n)} \\ \vdots \\ Y_{p_2}^{(1)} Y_{p_2}^{(2)} \dots Y_{p_2}^{(n)} \end{pmatrix}, \text{ for } p=1, \dots, n \quad (2.2)$$

and, therefore, the last term

$$a_{p_3} = \frac{C_{p_3}^{(1)} Y}{\lambda} \begin{pmatrix} Y_{p_3}^{(1)} Y_{p_3}^{(2)} \dots Y_{p_3}^{(n)} \\ Y_{p_3}^{(1)} Y_{p_3}^{(2)} \dots Y_{p_3}^{(n)} \\ \vdots \\ Y_{p_3}^{(1)} Y_{p_3}^{(2)} \dots Y_{p_3}^{(n)} \end{pmatrix}, \text{ for } p=1, \dots, n \quad (2.3)$$

A particular choice of the matrix P (its elements have been referred to the explicit construction of a particular Lie algebra of a superalgebra of n -point transformations admitted by the non-linear differential system) and to the evaluation of the determinant Δ (2.4) allow the double sweep algorithm to be simplified to integrate the linear first order system (2.1) with an initial sweep and to integrate the linear first order system (2.2) with an initial sweep.

Further simplifications in the above analysis occur when the system (2.1) is referred to the multigroup differential equations (2.1) with the definition (2.5)-(2.6). In this case the relevant Lie algebra of group generators is given by (2.7)-(2.8) for which

$$Y_{p_1} = \begin{cases} a_{p_1} & \text{for } p=1, \\ Y_{p_1}^{(1)} & \text{for } p=2, \\ Y_{p_1}^{(1)} \times Y_{p_1}^{(2)} & \text{for } p=3, \end{cases} \quad (2.9)$$

$$\Delta = Y_{p_1}^{(1)} Y_{p_1}^{(2)} \dots Y_{p_1}^{(n)} \quad (2.10)$$

and, therefore,

$$a_{p_1} = 0, \text{ for } p=1, \quad (2.11)$$

and

$$\mathbf{a}_{EF} = C_N^N D_E Y_{EP}^* / Y_{EP}^* \quad (4.5)$$

In view of (4.4) and (4.5) the system (4.3) decouples and reduces to

$$D_X^N \mathbf{w}_1 + \mathbf{a}_{11} \mathbf{w}_1 / (C_N^N D_1) = C_N^N S_1, \quad (4.6)$$

for $p=1$, and to

$$D_X^N \mathbf{w}_p + \mathbf{a}_{EP} \mathbf{w}_p / (C_N^N D_p) = C_N^N S_p - (C_N^N D_p)^{-1} \sum_{j=1}^{p-1} \mathbf{a}_{Ej} \mathbf{w}_j / D_j, \quad (4.7)$$

for $p=2, 3, \dots, G$. The system (3.2) also decouples to

$$C_N^N D_{11}^N v_1^* - \mathbf{a}_{11} v_1^* = -\mathbf{w}_1, \quad (4.8)$$

for $p=1$, and to

$$C_N^N D_{pE}^N v_p^* - \mathbf{a}_{EP} v_p^* = -\mathbf{w}_p + \sum_{j=1}^{p-1} \mathbf{a}_{Ej} v_j^*, \quad (4.9)$$

for $p=2, 3, \dots, G$. It follows directly from (4.6) and (4.8) that

$$D_X^N (Y_{11}^* \mathbf{w}_1) = C_N^N Y_{11}^* S_1, \quad (4.10)$$

and from (4.7) and (4.9) that

$$D_X^N (Y_{pE}^* \mathbf{w}_p) = -\mathbf{w}_p / (C_N^N D_p) + \mathbf{a}_{EP} v_p^*. \quad (4.11)$$

From (4.10) and (4.11) we obtain

$$D_X^N (Y_{pE}^* \mathbf{w}_p) = C_N^N Y_{pE}^* S_p - C_N^N Y_{pE}^* \sum_{j=1}^{p-1} \mathbf{a}_{Ej} v_j^* / D_j, \quad (4.12)$$

for $p=2, 3, \dots, G$. It can be shown by straightforward but tedious algebra that equation (4.12) can be expressed in the alternative form

$$D_X^N (Y_{pE}^* \mathbf{w}_p) = C_N^N Y_{pE}^* S_p + C_N^N Y_{pE}^* \sum_{h=1}^{p-1} \sigma(C_N^N D_h) v_h^* + D_X^N (Y_{pE}^* \sum_{j=1}^{p-1} \mathbf{a}_{Ej} v_j^*), \quad (4.13)$$

from (4.11) and (4.9) it follows that

$$D_X^N (Y_{pE}^* \mathbf{w}_p) = -\mathbf{w}_p / (C_N^N D_p) + C_N^N Y_{pE}^* \sum_{j=1}^{p-1} \mathbf{a}_{Ej} v_j^*. \quad (4.14)$$

With equations (4.13) and (4.14) the integration of the multigroup diffusion equations (3.1) has been reduced to a set of two quadratures with (4.13) and (4.14) or (4.11) and (4.9) together with a second-order quadrature with (4.11) and (4.9). The quadratures are decoupled and may be performed separately. This type of decoupling has not previously been reported for the more general second-order system (3.1).

The manner in which solutions of the multigroup diffusion equations (3.1) can be found with the quadratures involved in (4.13) and (4.14) can be illustrated with

an elementary two-group example. In the case of a sphere with radius, R , spatially uniform properties and spatially uniform sources in the both the fast and slow energy groups, the fast group scalar flux obtained directly from (50) and (51) with elementary closed-form integrations is

$$y_1 = (S_1/B_1^2 D_1) [1 - R \sinh(B_1 x)/x \sinh(B_1 R)], \quad (55)$$

and the slow flux obtained directly from (53) and (54), also with elementary closed-form integrations, is

$$y_2 = \frac{S_2}{B_2^2 D_2} \left[1 - \frac{R \sinh(B_2 x)}{x \sinh(B_2 R)} \right] + \frac{\sigma(1-\beta)}{B_2^2 D_2} \frac{S_1}{B_1^2 D_1} \left[1 + \frac{B_1^2}{B_2^2 - B_1^2} \frac{R \sinh(B_2 x)}{x \sinh(B_2 R)} - \frac{B_1^2}{B_2^2 - B_1^2} \frac{R \sinh(B_1 x)}{x \sinh(B_1 R)} \right] \quad (56)$$

when Dirichlet boundary conditions are applied on the outer surface. Multiple region solutions with piecewise constant properties can be obtained analytically in the same way. With an obvious interpretation of the sources, S_i , the double sweep algorithm that is defined by (50)-(56) can also be applied to the determination of the effective multiplication factor of an assembly with the source iteration method.

GROUP INVARIANT DIFFERENCE SCHEMES

Because of the many analogies between differential and difference equations, the notion of group invariant difference scheme arises quite naturally in the sense that difference equations formulated to provide solutions of differential equations should have the same invariance properties as the differential equations themselves. An approach to formulating group invariant difference equations is discussed in this section. The objective is to transfer invariance properties of the solutions of systems of differential equations to their finite difference simulations.

Although difference equations with the same invariance properties as their corresponding differential equations are called "invariant difference schemes", there are different definitions of what is actually meant by an invariant difference scheme. In reference 14 Shokin defines a difference scheme to be invariant under a group of point transformations if its first differential approximation admits this group. However, Shokin's definition implies that the actions of the prolongations of the group generators is on the space whose coordinates include the independent and dependent variables, the independent variable grid spacings, and all derivatives up to order one greater than appear in the system of differential equations. Consequently, Shokin's definition of an invariant difference scheme can not lead to exact difference equations whose exact solutions agree with the exact solutions of the differential equations simulated as invariance of the first differential approximation does not necessarily imply invariance of all higher order differential approximations. Even though Shokin's definition of an invariant difference scheme does not yield exact difference equations, it does produce significantly improved difference equations for solving the gas dynamics equations as discussed

cussed in reference 14.

A second definition of an invariant difference scheme is that a difference scheme is said to be invariant under a group of point transformations if it admits the prolongation of the group to the grid point values that appear as unknowns in the difference equations. This definition implies that the prolongations of the group generators act on the space whose coordinates are the independent variables and the dependent variables evaluated at the grid points. Also, this definition, which introduces a new type of prolongation, is capable of producing exact difference equations.

To construct explicitly invariant second order difference equations for the system (24), it is necessary to determine the prolongations of the vector fields (27) to the dependent variables evaluated at $x+1$ and at $x-1$. We denote these prolongations by

$$pr^{(2D)} \underline{u}_s = \sum_{E=1}^G Y_{Es} \partial_{v_E}(x) + \sum_{E=1}^G Z_{Es}^{(+1)} \partial_{v_E}(x+1) + \sum_{E=1}^G Z_{Es}^{(-1)} \partial_{v_E}(x-1) \quad (57)$$

in which the coordinate functions, $Z_{Es}^{(+1)}$ and $Z_{Es}^{(-1)}$, for the dependent variables with displaced arguments can be found in the following way. We extend the s th infinitesimal transformation,

$$\bar{x} = x + \delta a_s X_s(x, v_1, \dots, v_G), \quad (58)$$

$$\bar{v}_E(\bar{x}) = v_E(x) + \delta a_s Y_{Es}(x, v_1, \dots, v_G), \quad (59)$$

to

$$\bar{v}_E(\bar{x}+1) = v_E(x+1) + \delta a_s Z_{Es}^{(+1)}. \quad (60)$$

But

$$\bar{v}_E(\bar{x}+1) = v_E(x) + \sum_{k=1}^{\infty} D_{\bar{x}}^k \bar{v}_E(\bar{x}) / k!. \quad (61)$$

The k th order derivative transforms according to

$$D_{\bar{x}}^k \bar{v}_E(\bar{x}) = D_{x,E}^k v_E(x) + \delta a_s Y_{Es}^{(k)}, \quad (62)$$

where

$$Y_{Es}^{(1)} = D_{x,E} v_E + v_E' D_{x,s} X_s, \quad (63)$$

$$Y_{Es}^{(p)} = D_{x,E} Y_{Es}^{(p-1)} + v_E^{(p)} D_{x,s} X_s, \quad \text{for } p = 2, 3, \dots \quad (64)$$

Upon substituting (59) and (62) into (61), it is found that

$$\bar{v}_E(\bar{x}+1) = v_E(x+1) + \delta a_s (Y_{Es} + \sum_{k=1}^{\infty} Y_{Es}^{(k)} / k!). \quad (65)$$

Comparing (60) and (65) yields

$$Z_{ES}^{(+1)} = Y_{ES} + \sum_{k=1}^{\infty} Y_{ES}^{(k)}/k! \quad (66)$$

for the sth basis transformation in a multiparameter group. In a similar way it can be shown that

$$Z_{ES}^{(-1)} = Y_{ES} + \sum_{k=1}^{\infty} (-1)^k Y_{ES}^{(k)}/k! \quad (67)$$

In the case of evolutionary vector fields ($X_S^{(0)}$) the kth order derivative coordinate functions simplify to

$$Y_{ES}^{(k)} = D_x^k Y_{ES} \quad (68)$$

so that (66) and (67) become

$$Z_{ES}^{(\pm)} = Y_{ES}(x \pm 1) \quad (69)$$

Accordingly, the vector field prolongations (57) can be expressed as

$$\begin{aligned} \text{Pr}^{(2D)}_{ES} &= \sum_{E=1}^G Y_{ES}(x) \partial_{V_E}(x) + \sum_{E=1}^G Y_{ES}(x+1) \partial_{V_E}(x+1) \\ &\quad + \sum_{E=1}^G Y_{ES}(x-1) \partial_{V_E}(x-1) \end{aligned} \quad (70)$$

With the prolongation (70) the definition of what is meant by an invariant system of second order difference equations can be quantified.

In analogy to the differential system (8) we denote an arbitrary system of second order difference equations by

$$H_g[x, v_1(x), \dots, v_G(x), v_1(x+1), \dots, v_G(x+1), v_1(x-1), \dots, v_G(x-1)] = 0, \quad (71)$$

for $g = 1, 2, \dots, G$. This system is said to be invariant under the r parameter group generated by the vector fields $\text{Pr}^{(2D)}_{ES}$ with the prolongations (57) provide that

$$\text{Pr}^{(2D)}_{ES} (H_g) = 0, \quad \text{for } g = 1, 2, \dots, G \text{ and } s = 1, 2, \dots, r, \quad (72)$$

whenever $H_g = 0$. This set of invariance conditions for a system of second order difference equations is the finite difference equivalent to the set (12) of invariance conditions for a system of second order differential equations and comprises a completely different definition of difference scheme invariance than that based on the first differential approximation as employed by Shokri in reference (1) for gas dynamics problems.

To illustrate how the invariance conditions (72) can be implemented in the construction of invariant difference schemes, we shall consider some elementary examples. As shown earlier, the two group deformation equations in slab geometry admit a two parameter group of point transformations with the two dimensional Lie algebra,

$$\underline{L}_1 = \cosh B_1 x^1 \partial_{v_1} + Q_{12} \cosh B_1 x^1 \partial_{v_2}, \quad (70)$$

$$\underline{L}_2 = \cosh h_2 x^2 \partial_{v_2}, \quad (71)$$

where

$$Q_{12} = \sigma(1-\sigma)/iD_1 h_1^2 - P_1^2/4. \quad (72)$$

Let the grid points be $x_i^j = ih_j$, where h_j is the mesh spacing, and let grid point values of the dependent variables be $v(x_i^j) = v_{i,j}^n$. Then the prolongations required to construct invariant second order difference equations can be expressed as

$$\begin{aligned} \text{pr}^{(2,0)} \underline{L}_1 &= \cosh(nhB_1) \partial_{v_{1,n}} + \cosh[(n+1)hB_1] \partial_{v_{1,n+1}} \\ &+ \cosh[(n-1)hB_1] \partial_{v_{1,n-1}} + \cosh(nhB_1) Q_{12} \partial_{v_{2,n}} \\ &+ \cosh[(n+1)hB_1] Q_{12} \partial_{v_{2,n+1}} + \cosh[(n-1)hB_1] Q_{12} \partial_{v_{2,n-1}}, \end{aligned} \quad (76)$$

and

$$\begin{aligned} \text{pr}^{(2,0)} \underline{L}_2 &= \cosh(nhB_2) \partial_{v_{2,n}} + \cosh[(n+1)hB_2] \partial_{v_{2,n+1}} \\ &+ \cosh[(n-1)hB_2] \partial_{v_{2,n-1}}. \end{aligned} \quad (77)$$

Writing in terms of three-point central difference formulae for second order derivatives, we start from the following possible forms for a set of two second order difference equations,

$$H_1 = i_n^2 (v_{1,n+1} + v_{1,n-1} - 2v_{1,n}) + B_1^2 v_{1,n} + S_1/D_1 - T_1(h) = 0 \quad (78)$$

$$\begin{aligned} H_2 = i_n^2 (v_{2,n+1} + v_{2,n-1} - 2v_{2,n}) + B_2^2 v_{2,n} + S_2/D_2 \\ + [\sigma(1-\sigma)/D_2] v_{1,n} G_n - T_2(h) = 0 \end{aligned} \quad (79)$$

and apply the three invariance conditions,

$$\text{pr}^{(2,0)} V_1(H_1) = 0, \quad (80)$$

$$\text{pr}^{(2,0)} V_2(H_2) = 0 \quad (81)$$

and

$$\text{pr}^{(2,0)} V_2(H_1) = 0. \quad (82)$$

Following a straightforward but rather lengthy calculation, we obtain the two following second order difference equations for the slab geometry two group difference equations:

$$\frac{y_{1,n+1} + y_{1,n-1} - 2y_{1,n}}{(4/B_1^2)\sinh^2(B_1 h/2)} - B_1^2 v_{1,n} + S_1/D_1 = 0, \quad (8a)$$

and

$$\frac{y_{2,n+1} + y_{2,n-1} - 2y_{2,n}}{(4/B_2^2)\sinh^2(B_2 h/2)} - B_2^2 v_{2,n} + S_2/D_2 + \mathcal{O}(1 \rightarrow 2) G_n v_{1,n}/D_2 = (G_n - 1)S_1 \mathcal{O}(1 \rightarrow 2)/(B_1^2 D_1 D_2), \quad (8b)$$

where

$$G_n = \frac{B_2^2}{B_2^2 - B_1^2} \left[1 - \frac{\sinh^2(B_1 h/2)}{\sinh^2(B_2 h/2)} \right]. \quad (8c)$$

Similar results can be derived in the same way for spherical and cylindrical geometries by thinking of second order derivatives in terms of three-point central difference formulae and first order derivatives in terms of two-point central difference formulae. It is of interest to note that, in the limit of very small mesh spacing, $G_n \rightarrow 1$, so that (8a) and (8b) reduce to difference equations obtained with standard three-point difference formulae for second order derivatives in this limit.

It may also be noted that the difference equations (8a)-(8c) are accurate even for large mesh spacings. In fact, they are exact. It can be shown directly that the exact solutions of (8a) and (8b) can be expressed as

$$v_{1,n} = \frac{S_1}{B_1^2 D_1} \left[1 - \frac{\cosh(nhB_1)}{\cosh(N_1 hB_1)} \right], \quad (8d)$$

and

$$v_{2,n} = \frac{S_2}{B_2^2 D_2} \left[1 - \frac{\cosh(nhB_2)}{\cosh(N_1 hB_2)} \right] + \frac{S_1}{B_1^2 D_1} \frac{\mathcal{O}(1 \rightarrow 2)}{B_2^2 D_2} \left[1 - \frac{B_2^2}{B_2^2 - B_1^2} \frac{\cosh(nhB_1)}{\cosh(N_1 hB_1)} + \frac{B_1^2}{B_2^2 - B_1^2} \frac{\cosh(nhB_2)}{\cosh(N_1 hB_2)} \right] \quad (8e)$$

for the case of N_1 spatial intervals and Dirichlet boundary conditions on the outer surface. The exact solutions (8d) and (8e) of the difference equations (8a) and (8b) agree with the exact solutions of the two group diffusion equations when these are evaluated at the grid points of the finite difference method.

CONCLUSIONS

The symmetry algebras and their corresponding groups of point transformations have been determined for systems of second order differential equations of the type encountered in various approximations of the neutron transport equation, which include, but are not limited to, the multigroup diffusion equation and the "III form" of the P_1 equations. Two point boundary value problems that

involve these systems can be solved with double sweep algorithms that can be motivated, formulated, and simplified with a knowledge of their symmetry algebras. The concept of invariant systems of difference equations has been introduced, and it has been shown how symmetry algebras can be used to construct sets of difference equations that are also exact.

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