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NEUTRONICS COMPUTATIONAL APPLICATIONS OF SYMMETRY ALGEBRAS

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ABSTRACT

Lie 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 multigroup diffusion equations and the "FLIP form" of the P_L equations. It is shown how Lie 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 groups 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 defined and found. Examples of invariant difference schemes are constructed from the basic difference equation invariance conditions and shown to be exact.

INTRODUCTION

The general objective of the ensuing 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 difference equations and the one-group diffusion equation. Ehrlich and Hurwitz[1] attribute to R. H. 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 2 Butler and Cook formulate 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 diffusion equation. Also, in the fourth chapter of reference 2 Gelbard considers double sweep algorithms for solving the P_L equations.

Additional discussions of double sweep algorithms appear in references 3-7. In Section 31 of reference 3 Gelfand and Fomin 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-Lokutsiyevskii method of chasing, are explored in the ninth chapter of reference 4. Double sweep algorithms for solving second order difference equations are developed in references 4-7.

Double sweep algorithms for both differential and difference equations that are discussed in references 1-7 are thought of in terms of the factorization method, of fields for second order differential equations, 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 8-13 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 invariant 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 Shokin[14] 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 Shokin[14] 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 $(x,y_1,y_2,\ldots,y_G)$ of one independent variable, x, and G dependent variables, y_g, $g=1,2,\ldots,G$, that are defined by $G+1$ independent functions, namely,

$$\bar{x} = f(x,y_1,y_2,\ldots,y_G;a_1,a_2,\ldots,a_r), \tag{1}$$

and

$$\bar{y}_g = f_g(x, y_1, y_2, \ldots, y_G; a_1, a_2, \ldots, a_r). \tag{2}$$

Each set of values of the parameters, $a_1, a_2, \ldots, a_r$, in (1) and (2) labels a different point transformation in the set, and these parameters are assumed to be essential. The transformations (1) and (2) comprise an r-parameter group of point transformations under the binary operation of performing two successive transformations if they satisfy the four basic group axioms , namely, (1) closure, (2) existence of an identity transformation in the set, (3) existence of an inverse transformation for each transformation in the set, and (4) associativity for the binary operation. This section provides the determination of r-parameter groups of point transformations that are admitted by the multigroup diffusion equations taken in the form,

$$x^{-N} D_x(x^N D_1 D_x y_1) - \sigma_{R,1} y_1 + S_1 = 0, \tag{3}$$

and

$$x^{-N} D_x(x^N D_g D_x y_g) - \sigma_{R,g} y_g + \sum_{h=1}^{g-1} \sigma(h \rightarrow g) y_h + S_g = 0, \tag{4}$$

for g=2,3,...,G. In (3) and (4) the parameter N is a geometric parameter (N=0 for slabs, N=1 for cylinders, and N=2 for spheres), and the source terms, S_g, may also include fission and/or external sources. As written, equation (4) contains only down-scattering terms, but up-scattering may also be included.

A group of point transformations admitted by a system of differential equations transforms one solution into another and leaves the system itself invariant, that is, the system has the same form in the new coordinates as it did in the original coordinates. Such an invariance property of a system of differential equations is also called a symmetry property of the system. Symmetry properties of systems of multigroup diffusion equations can be found systematically by determining the vector fields,

$$\underline{U}_s = X_s \partial_x + \sum_{g=1}^{G} Y_{gs} \partial_{y_g}, \tag{5}$$

which are called group generators and are said to represent the infinitesimal transformations of the group around the identity for which

$$X_s(x, y_1, \ldots, y_G) = \partial_{a_s} f \Big|_{\underline{a}=\underline{a}_o}, \tag{6}$$

and

$$Y_{gs}(x, y_1, \ldots, y_G) = \partial_{a_s} f_g \Big|_{\underline{a}=\underline{a}_o}, \tag{7}$$

for s=1,2,...,r. The group generators may be regarded as the basis of an r-dimensional vector space, close under the Lie bracket or commutator operation, and comprise the Lie algebra, or symmetry algebra, of a system of differential equations. The functions, X_s and Y_{gs}, are smooth and are called the coordinate functions of the group generator.

The coordinate functions of the group generators for the multigroup diffusion equations can be obtained as follows. We introduce the second order jet space whose coordinates represent the independent variable, x, the dependent variables, y_g, the first order derivatives, y_g', and the second order derivatives, y_g''. The multigroup equations are regarded as a set of smooth functions,

$$F_g(x;y_1,\dots,y_G;y_1',\dots,y_G';y_1'',\dots,y_G'') = 0, \tag{8}$$

for g=1,2,...,G, which defines a smooth map from this second order jet space to a G-dimensional Euclidean space. The multigroup equations determine a subvariety of the jet space because they indicate where this map vanishes. A group of point transformations whose second order prolongation leaves the subvariety invariant is a symmetry group of the multigroup equations. The second order prolongation of the vector field, $\underline{U}_s$, which will be denoted by $pr^{(2)}\underline{U}_s$, acts on the second order jet space and is given by

$$pr^{(2)}\underline{U}_s = X_s\,\partial_x + \sum_{g=1}^{G} Y_{gs}\,\partial_{y_g} + \sum_{g=1}^{G} \phi_{gs}^{(1)}\,\partial_{y_g'} + \sum_{g=1}^{G} \phi_{gs}^{(2)}\,\partial_{y_g''}, \tag{9}$$

where

$$\phi_{gs}^{(1)} = D_x Y_{gs} - y_g' D_x X_s, \tag{10}$$

and

$$\phi_{gs}^{(2)} = D_x \phi_{gs}^{(1)} - y_g'' D_x X_s. \tag{11}$$

A necessary and sufficient infinitesimal invariance condition that the group generators $\underline{U}_s$ represent an r-parameter group of point transformations admitted by the multigroup diffusion equations is that

$$pr^{(2)}\underline{U}_s(F_g) = 0,\ g=1,2,\dots,G, \text{ and } s=1,2,\dots,r, \tag{12}$$

whenever F_g=0. When written out in full equation (12) becomes a system of linear first order partial differential equations, which are called the determining equations of the group, for the coordinate functions X_s and Y_{gs} of the group generators.

The invariance condition (12) together with the second prolongation formulae (9)-(11) allow for the simultaneous transformation of all independent and dependent variables. Somewhat less general but very useful groups of point transformations for the multigroup diffusion equations can be found from (12) by restricting the action of the group to the dependent variables, that is, to the scalar fluxes of each energy group. In this case the independent spatial variable is not transformed under the group action, so X_s=0, for s=1,2,...,r. A second simplifying restriction is that the dependent variable coordinate functions are functions only of the independent variable. That is,

$$Y_{gs}(x,y_1,\dots,y_G) = Y_{gs}(x). \tag{13}$$

With these two restrictions the second order prolongation of the vector field $\underline{U}_s$ given by (9) reduces to

$$\mathrm{pr}^{(2)}\underline{U}_s = \sum_{g=1}^{G} Y_{gs}\,\partial_{y_g} + \sum_{g=1}^{G} D_x Y_{gs}\,\partial_{y'_g} + \sum_{g=1}^{G} D_x^2 Y_{gs}\,\partial_{y''_g} \,. \tag{14}$$

With the definition of the mapping functions F_g in (8) implied by the multigroup diffusion equations (3) and (4), evaluating the infinitesimal invariance condition (12) with the second order prolongation (14) produces the following set of differential equations satisfied by the dependent variable coordinate functions, $Y_{gs}(x)$;

$$x^{-N} D_x(x^N D_1 D_x Y_{1s}) - \sigma_{R,1} Y_{1s} = 0, \tag{15}$$

and

$$x^{-N} D_x(x^N D_g D_x Y_{gs}) - \sigma_{R,g} Y_{gs} + \sum_{h=1}^{g-1} \sigma(h\rightarrow g) Y_{hs} = 0, \tag{16}$$

for $g=2,3,\ldots,G$. That is, groups of point transformations that leave the inhomogeneous multigroup diffusion equations invariant can be found from solutions of the homogeneous multigroup diffusion equations when the group action is restricted to the dependent variables and the dependent variable coordinate functions, Y_{gs}, have the restricted form (13). Since (15) and (16) comprise a system of 2G second order differential equations, their solution provides at most a 2G-parameter group of point transformations admitted by the inhomogeneous multigroup diffusion equations and a 2G-dimensional Lie algebra of group generators, $\underline{U}_s$. Because all Lie brackets vanish, this algebra is Abelian. In the case of arbitrarily spatially dependent physical properties, group generators can be obtained by integrating (15) and (16) numerically. In the case of spatially uniform or piecewise constant properties in composite domains, group generators can be found by solving (15) and (16) analytically.

Although all solutions of (15) and (16) provide 2G-dimensional Lie algebras of the inhomogeneous multigroup diffusion equations, there are G-dimensional subalgebras of group generators that generate G-parameter groups of point transformations which have been found to be useful in the construction of double sweep algorithms as discussed in the next section. Specific results for G-dimensional subalgebras in the case of spatially uniform physical properties can be expressed in terms of the basis functions, $V_s(x)$, defined as follows for slabs, cylinders, and spheres, respectively;

$$V_s(x) = \begin{cases} \cosh(B_s x), & \text{for } N=0, \\ I_o(B_s x), & \text{for } N=1, \\ \sinh(B_s x)/x, & \text{for } N=2, \end{cases} \tag{17}$$

where $B_s^2 = \sigma_{R,s}/D_s$. The group generators of the G-dimensional subalgebras take the same general form in each geometry, namely,

$$\underline{U}_s = V_s(x)\,\partial_{y_s} + V_s(x) \sum_{g=s+1}^{G} Q_{sg}\,\partial_{y_g} \,, \tag{18}$$

for $s=1,2,\ldots,G-2$,

$$\underline{U}_{G-1} = V_{G-1}(x)\,\partial_{y_{G-1}} + V_{G-1}(x)\,Q_{G-1,G}\,\partial_{y_G}, \tag{19}$$

and

$$\underline{U}_G = V_G(x)\,\partial_{y_G}\ . \tag{20}$$

The non-zero elements of the matrix Q_{sg} that appears in (18) and (19) are given by the following formulae;

$$Q_{s,s+1}(B^2_{s+1} - B^2_s) = \sigma(s \to s+1)/D_{s+1}, \tag{21}$$

for s=1,2,...,G-1, and

$$Q_{sg}(B^2_g - B^2_s) = D^{-1}_g\left[\sigma(s \to g) + \sum_{j=s+1}^{g-1} \sigma(j \to g)Q_{sj}\right], \tag{22}$$

for s=1,2,...,G-1 and g=s+2,s+3,...,G. The G-dimensional subalgebras cited in (18)-(22) are obtained simply by solving analytically the homogeneous multi-group diffusion equations for the case of spatially uniform physical properties. The full 2G-dimensional Lie algebra of generators can be written out directly by adding the G additional vector fields in which the functions, $V_s(x)$, in (18) through (20) are replaced by the functions, $R_s(x)$, defined by

$$R_s(x) = \begin{cases} \sinh(B_s x), & \text{for } N=0, \\ K_o(B_s x), & \text{for } N=1, \\ \cosh(B_s x)/x, & \text{for } N=2. \end{cases} \tag{23}$$

In the cylindrical and spherical geometry cases the singular nature of these functions limits their utility. Linear combinations of the functions, $V_s(x)$ and $R_s(x)$, defined in (17) and (23) can also be used in the explicit construction of G-dimensional subalgebras of group generators.

GROUP THEORY OF DOUBLE SWEEP ALGORITHMS

In this section it is shown how knowledge of the Lie algebra of a system of second order differential equations can be applied to the problem of deriving double sweep algorithms which can be used to obtain either analytic or numerical solutions of two-point boundary value problems that entail such systems. We consider two-point boundary value problems for the second order system of differential equations,

$$x^{-N}D_x(x^N D_g D_x y_g) + \sum_{h=1}^{G} A_{gh}y_h + S_g = 0, \tag{24}$$

for g=1,2,...,G. This system is somewhat more general than the multigroup system (3)-(4) which can be recovered from (24) with the identifications,

$$A_{gg} = -\sigma_{R,g}, \tag{25}$$

and

$$A_{gh} = \begin{cases} \sigma(h \rightarrow g), & \text{for } 1 \leq h \leq g-1, \\ 0, & \text{for } h > g. \end{cases} \tag{26}$$

More general systems of the form (24) arise, for example when solving for the scalar fluxes in a subcritical assembly due to an external source and when solving for the even Legendre moments of the directed flux in the P_L approximation of the neutron transport equation. For the latter, see, for example, Gelbard's discussion of the "FLIP form" of the P_L equations, which is (24) with N=0, in the fourth chapter of reference 2 and reference 15.

The basis of a G-dimensional Lie algebra of generators of a G-parameter group of point transformations that leaves the system (24) invariant is given by

$$\underline{U}_s = \sum_{g=1}^{G} Y_{gs} \partial_{y_g}, \quad \text{for } s=1,2,\ldots,G, \tag{27}$$

in which the coordinate functions, Y_{gs}, are solutions of the homogeneous set

$$x^{-N} D_x(x^N D_g D_x Y_{gs}) + \sum_{h=1}^{G} A_{gh} Y_{hs} = 0, \text{ for } g,s=1,2,\ldots,G. \tag{28}$$

The first order prolongation of this group is

$$pr^{(1)}\underline{U}_s = \sum_{g=1}^{G} Y_{gs} \partial_{y_g} + \sum_{g=1}^{G} D_x Y_{gs} \partial_{y'_g} . \tag{29}$$

Every infinitesimal transformation of the group can be written in the form,

$$\underline{U} = \sum_{s=1}^{G} e_s \underline{U}_s, \tag{30}$$

in which each e_s is a constant, and all first order prolongations can be expressed as

$$pr^{(1)}\underline{U} = \sum_{s=1}^{G} e_s pr^{(1)}\underline{U}_s. \tag{31}$$

To establish an outward and inward double sweep algorithm to solve two-point boundary value problems that involve the system (24) we seek a set of G first integrals of (24), namely,

$$W_g = -C_N x^N D_g y'_g + \sum_{j=1}^{G} \alpha_{gj} y_j, \text{ for } g=1,2,\ldots,G, \tag{32}$$

in which the geometric constants C_N are $C_0=1$, $C_1=2\P$, and $C_2=4\P$. The functions, $W_g(x)$ and $\alpha_{gj}(x)$, in (32) are solutions of differential equations obtained by substituting (32) into (24) and making use of the fact that the resulting relations must be identities in the dependent variables, y_g. That is, the set (32) must imply the system (24). It is found that the matrices, $\alpha_{gj}(x)$, must be solutions of the matrix Riccati system,

$$D_x\alpha_{gj} + (C_N x^N)^{-1}\sum_{k=1}^{G}\alpha_{gk}\alpha_{kj}/D_k + C_N x^N A_{gj} = 0, \qquad (33)$$

for g=1,2,...,G and j=1,2,...,G. Once these matrices are known, the first integrals are obtained by solving the linear first order system,

$$D_x W_g + (C_n x^N)^{-1}\sum_{j=1}^{G}\alpha_{gj}W_j/D_j = C_N x^N S_g, \quad \text{for } g=1,2,\dots,G. \qquad (34)$$

The two systems (33) and (34) are both integrated in an outward sweep with initial conditions chosen so that (32) satisfies the left-hand boundary conditions specified for the dependent variables, y_g. A typical example is $W_g(0) = 0$ and $\alpha_{gj}(0) = 0$. Following these two outward sweeps the solution of the system (24) is found by integrating (32), regarded as a first order linear system, in an inward sweep with initial conditions that incorporate the right-hand boundary conditions satisfied by the dependent variables, y_g.

In principle, the double sweep algorithm described above can be carried out completely with numerical integrations of the systems (32)-(34). However, a simplification can be achieved by obtaining the exact analytic solution of matrix Riccati system (33) in the following way. We first note that the set of first integrals (32) can be regarded as a set of first order differential invariants of the G-parameter group of point transformations generated by the basis of group generators (27). This fact implies that the first integrals are annihilated by the first order prolongation of the group given by (31), that is, that

$$pr^{(1)}\underline{U}(C_N x^N D_g y'_g + W_g - \sum_{j=1}^{G}\alpha_{gj}y_j) = 0. \qquad (35)$$

By combining (29) and (31) with (35) it is found that

$$\sum_{s=1}^{G} e_s(C_N x^N D_g D_x Y_{gs} - \sum_{j=1}^{G}\alpha_{gj}Y_{js}) = 0. \qquad (36)$$

This relation must hold for all values of the constants, e_s, which shows that the matrices, α_{gj}, which satisfy the matrix Riccati system (33), are solutions of the set,

$$\sum_{j=1}^{G}\alpha_{gj}Y_{js} = C_N x^N D_g Y'_{gs}, \quad \text{for } g,j=1,2,\dots,G. \qquad (37)$$

Upon defining the determinant,

$$\Delta = \begin{vmatrix} Y_{11} & Y_{21} & \cdots & Y_{G1} \\ Y_{12} & Y_{22} & \cdots & Y_{G2} \\ \vdots & \vdots & & \vdots \\ Y_{1G} & Y_{2G} & \cdots & Y_{GG} \end{vmatrix}, \qquad (38)$$

it follows directly from Cramer's rule that the solution of (37) is given by

$$\alpha_{g1} = \frac{C_N x^N}{\Delta} \begin{vmatrix} D_g Y'_{g1} & Y_{21} & \cdots & Y_{G1} \\ D_g Y'_{g2} & Y_{22} & \cdots & Y_{G2} \\ \cdot & \cdot & & \cdot \\ \cdot & \cdot & & \cdot \\ D_g Y'_{gG} & Y_{2G} & \cdots & Y_{GG} \end{vmatrix}, \text{ for } g=1,2,\ldots,G, \tag{39}$$

$$\alpha_{g2} = \frac{C_N x^N}{\Delta} \begin{vmatrix} Y_{11} & D_g Y'_{g1} & \cdots & Y_{G1} \\ Y_{12} & D_g Y'_{g2} & \cdots & Y_{G2} \\ \cdot & \cdot & & \cdot \\ \cdot & \cdot & & \cdot \\ Y_{1G} & D_g Y'_{2G} & \cdots & Y_{GG} \end{vmatrix}, \text{ for } g=1,2,\ldots,G, \tag{40}$$

and so forth to the last column

$$\alpha_{gG} = \frac{C_N x^N}{\Delta} \begin{vmatrix} Y_{11} & Y_{21} & \cdots & D_g Y'_{g1} \\ Y_{12} & Y_{22} & \cdots & D_g Y'_{g2} \\ \cdot & \cdot & & \cdot \\ \cdot & \cdot & & \cdot \\ Y_{1G} & Y_{2G} & \cdots & D_g Y'_{gG} \end{vmatrix}, \text{ for } g=1,2,\ldots,G. \tag{41}$$

Accordingly, solving the matrix Riccati system (33) has been reduced to the explicit construction of a G-dimensional Lie algebra of a G-parameter group of point transformations admitted by the inhomogeneous differential system (24) and to the evaluation of the determinants (38)-(41). The double sweep algorithm, in turn, simplifies to integrating the linear first order system (34) with an outward sweep and to integrating the linear first order system (32) with an inward sweep.

Further simplifications in the above analysis occur when the system (24) is reduced to the multigroup diffusion equations (3)-(4) with the definitions (25)-(26). In this case the relevant Lie algebra of group generators is given by (18)-(20) for which

$$Y_{gs} = \begin{cases} 0, & \text{for } g < s, \\ V_g(x), & \text{for } g=s, \\ V_s(x) Q_{sg}, & \text{for } g > s, \end{cases} \tag{42}$$

$$\Delta = Y_{11} Y_{22} Y_{33} \cdots\cdots Y_{GG}, \tag{43}$$

and, therefore,

$$\alpha_{gs} = 0, \quad \text{for } g < s, \tag{44}$$

and

$$\alpha_{gg} = C_N x^N D_g Y'_{gg}/Y_{gg}. \tag{45}$$

In view of (44) and (45) the system (34) decouples and reduces to

$$D_x W_1 + \alpha_{11} W_1/(C_N x^N D_1) = C_N x^N S_1, \tag{46}$$

for g=1, and to

$$D_x W_g + \alpha_{gg} W_g/(C_N x^N D_g) = C_N x^N S_g - (C_N x^N)^{-1} \sum_{j=1}^{g-1} \alpha_{gj} W_j/D_g, \tag{47}$$

for g=2,3,...,G. The system (32) also decouples to

$$C_N x^N D_1 y'_1 - \alpha_{11} y_1 = -W_1, \tag{48}$$

for g=1, and to

$$C_N x^N D_g y'_g - \alpha_{gg} y_g = -W_g + \sum_{j=1}^{g-1} \alpha_{gj} y_j, \tag{49}$$

for g=2,3,...,G. It follows directly from (45) and (46) that

$$D_x(Y_{11} W_1) = C_N x^N Y_{11} S_1, \tag{50}$$

and from (45) and (48) that

$$D_x(y_1/Y_{11}) = -W_1/(C_N x^N D_1 Y_{11}). \tag{51}$$

From (45) and (47) we obtain

$$D_x(Y_{gg} W_g) = C_N x^N S_g Y_{gg} - (C_N x^N)^{-1} Y_{gg} \sum_{j=1}^{g-1} \alpha_{gj} W_j/D_g, \tag{52}$$

for g=2,3,...,G. It can be shown by straightforward but tedious algebra that equation (52) can be expressed in the alternative form,

$$D_x(Y_{gg} W_g) = C_N x^N S_g Y_{gg} + C_N x^N Y_{gg} \sum_{h=1}^{g-1} \sigma(h \rightarrow g) y_h + D_x(Y_{gg} \sum_{j=1}^{g-1} \alpha_{gj} y_j). \tag{53}$$

From (45) and(49) it follows that

$$D_x(y_g/Y_{gg}) = -W_g/(C_N x^N D_g Y_{gg}) + (C_N x^N D_g Y_{gg})^{-1} \sum_{j=1}^{g-1} \alpha_{gj} y_j. \tag{54}$$

With equations (50)-(54) the integration of the multigroup diffusion equations (3)-(4) has been reduced to G outward sweep quadratures with (50) and (52) or (53) together with G inward sweep quadratures with (51) and (54). These quadratures are decoupled and may performed successively. This type of decoupling does not necessarily occur for the more general second order system (24).

The manner in which solutions of the multigroup diffusion equations (3)-(4) can be found with the quadratures implied in (50)-(54) 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

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

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

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

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_g, the double sweep algorithm that is defined by (50)-(54) 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 schemes 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 <u>first differential approximation</u> 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'n 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 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

$$pr^{(2D)}\underline{U}_s = \sum_{g=1}^{G} Y_{gs}\,\partial_{y_g(x)} + \sum_{g=1}^{G} Z_{gs}(+1)\,\partial_{y_g(x+1)} + \sum_{g=1}^{G} Z_{gs}(-1)\,\partial_{y_g(x-1)} \qquad (57)$$

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

$$\bar{x} = x + \delta a_s\, X_s(x,y_1,\ldots,y_G), \qquad (58)$$

$$\bar{y}_g(\bar{x}) = y_g(x) + \delta a_s\, Y_{gs}(x,y_1,\ldots,y_G), \qquad (59)$$

to

$$\bar{y}_g(\bar{x}+1) = y_g(x+1) + \delta a_s\, Z_{gs}(+1). \qquad (60)$$

But

$$\bar{y}_g(\bar{x}+1) = \bar{y}_g(\bar{x}) + \sum_{k=1}^{\infty} D_{\bar{x}}^k \bar{y}_g(\bar{x})/k!. \qquad (61)$$

The kth order derivative transforms according to

$$D_{\bar{x}}^k \bar{y}_g(\bar{x}) = D_x^k y_g(x) + \delta a_s\, Y_{gs}^{(k)}, \qquad (62)$$

where

$$Y_{gs}^{(1)} = D_x Y_{gs} - y_g' D_x X_s, \qquad (63)$$

$$Y_{gs}^{(k)} = D_x Y_{gs}^{(k-1)} - y_g^{(k)} D_x X_s, \quad \text{for } k=2,3,\ldots.. \qquad (64)$$

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

$$\bar{y}_g(\bar{x}+1) = y_g(x+1) + \delta a_s(Y_{gs} + \sum_{k=1}^{\infty} Y_{gs}^{(k)}/k!). \qquad (65)$$

Comparing (60) and (65) yields

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

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

$$Z_{gs}(-1) = Y_{gs} + \sum_{k=1}^{\infty} (-1)^k Y_{gs}^{(k)}/k! \ . \tag{67}$$

In the case of evolutionary vector fields (X_s=0) the kth order derivative coordinate functions simplify to

$$Y_{gs}^{(k)} = D_x^k Y_{gs}, \tag{68}$$

so that (66) and (67) become

$$Z_{gs}(\pm) = Y_{gs}(x\pm 1). \tag{69}$$

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

$$pr^{(2D)}\underline{U}_s = \sum_{g=1}^{G} Y_{gs}(x)\,\partial_{y_g(x)} + \sum_{g=1}^{G} Y_{gs}(x+1)\,\partial_{y_g(x+1)} + \sum_{g=1}^{G} Y_{gs}(x-1)\,\partial_{y_g(x-1)}. \tag{70}$$

With the prolongations (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

$$H_g[x,y_1(x),\ldots,y_G(x),y_1(x+1),\ldots,y_G(x+1),y_1(x-1),\ldots,y_G(x-1)] = 0, \tag{71}$$

for g=1,2,...,G. This system is said to be invariant under the r-parameter group generated by the vector fields $\underline{U}_s$ (27) with the prolongations (57) provided that

$$pr^{(2D)}\underline{U}_s(H_g) = 0, \text{ for } g=1,2,\ldots,G \text{ and } s=1,2,\ldots,r, \tag{72}$$

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 Shokin in reference 14 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 diffusion equations in slab geometry admit a two-parameter group of point transformations with the two-dimensional Lie algebra,

$$\underline{U}_1 = \cosh(B_1 x)\,\partial_{y_1} + Q_{12}\cosh(B_1 x)\,\partial_{y_2}, \tag{73}$$

$$\underline{U}_2 = \cosh(B_2 x)\,\partial_{y_2}, \tag{74}$$

where

$$Q_{12} = \sigma(1\rightarrow 2)/[D_2(B_2^2 - B_1^2)]. \tag{75}$$

Let the grid points be $x_n = nh$, where h is the mesh spacing, and let grid point values of the dependent variables be $y_g(x_n) = y_{g,n}$. Then the prolongations required to construct invariant second order difference equations can be expressed as

$$\begin{aligned} pr^{(2D)}\underline{U}_1 = {} & \cosh(nhB_1)\,\partial_{y_{1,n}} + \cosh[(n+1)hB_1]\,\partial_{y_{1,n+1}} \\ & + \cosh[(n-1)hB_1]\,\partial_{y_{1,n-1}} + \cosh(nhB_1)Q_{12}\,\partial_{y_{2,n}} \\ & + \cosh[(n+1)hB_1]Q_{12}\,\partial_{y_{2,n+1}} + \cosh[(n-1)hB_1]Q_{12}\,\partial_{y_{2,n-1}}, \end{aligned} \tag{76}$$

and

$$\begin{aligned} pr^{(2D)}\underline{U}_2 = {} & \cosh(nhB_2)\,\partial_{y_{2,n}} + \cosh[(n+1)hB_2]\,\partial_{y_{2,n+1}} \\ & + \cosh[(n-1)hB_2]\,\partial_{y_{2,n-1}}. \end{aligned} \tag{77}$$

Thinking 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,

$$H_1 = E_n(y_{1,n+1} + y_{1,n-1} - 2y_{1,n}) - B_1^2 y_{1,n} + S_1/D_1 - T_1(h) = 0 \tag{78}$$

$$\begin{aligned} H_2 = {} & F_n(y_{2,n+1} + y_{2,n-1} - 2y_{2,n}) - B_2^2 y_{2,n} + S_2/D_2 \\ & + [\sigma(1\rightarrow 2)/D_2]y_{1,n}G_n - T_2(h) = 0 \end{aligned} \tag{79}$$

and apply the three invariance conditions,

$$pr^{(2D)}\underline{U}_1(H_1) = 0, \tag{80}$$

$$pr^{(2D)}\underline{U}_1(H_2) = 0, \tag{81}$$

and

$$pr^{(2D)}\underline{U}_2(H_2) = 0. \tag{82}$$

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

$$\frac{y_{1,n+1} + y_{1,n-1} - 2y_{1,n}}{(4/B_1^2)\sinh^2(B_1h/2)} - B_1^2 y_{1,n} + S_1/D_1 = 0, \tag{83}$$

and

$$\frac{y_{2,n+1} + y_{2,n-1} - 2y_{2,n}}{(4/B_2^2)\sinh^2(B_2h/2)} - B_2^2 y_{2,n} + S_2/D_2 + \sigma(1\rightarrow 2)\, G_n y_{1,n}/D_2$$

$$= (G_n - 1)S_1\sigma(1\rightarrow 2)/(B_1^2 D_1 D_2), \tag{84}$$

where

$$G_n = \frac{B_2^2}{B_2^2 - B_1^2}\left[1 - \frac{\sinh^2(B_1h/2)}{\sinh^2(B_2h/2)}\right]. \tag{85}$$

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, $G_n \longrightarrow 1$, so that (83) and (84) 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 (83)-(84) are accurate even for coarse meshes. In fact, they are exact. It can be shown directly that the exact solutions of (83) and (84) can be expressed as

$$y_{1,n} = \frac{S_1}{B_1^2 D_1}\left[1 - \frac{\cosh(nhB_1)}{\cosh(N_I hB_1)}\right], \tag{86}$$

and

$$y_{2,n} = \frac{S_2}{B_2^2 D_2}\left[1 - \frac{\cosh(nhB_2)}{\cosh(N_I hB_2)}\right]$$

$$+ \frac{S_1}{B_1^2 D_1}\,\frac{\sigma(1\rightarrow 2)}{B_2^2 D_2}\left[1 - \frac{B_2^2}{B_2^2 - B_1^2}\,\frac{\cosh(nhB_1)}{\cosh(N_I hB_1)} + \frac{B_1^2}{B_2^2 - B_1^2}\,\frac{\cosh(nhB_2)}{\cosh(N_I hB_2)}\right] \tag{87}$$

for the case of N_I spatial intervals and Dirichlet boundary conditions on the outer surface. The exact solutions (86) and (87) of the difference equations (83) and (84) agree with the exact solutions of the two-group diffusion equations when these are evaluated at the grid points of the finite difference mesh.

CONCLUSIONS

Lie 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 equations and the "FLIP form" of the P_L 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.

REFERENCES

1 R. Ehrlich and H. Hurwitz, Jr., "Multigroup Methods for Neutron Diffusion Problems," Nucleonics 12, No. 2 (1954), p 23.

2 H. Greenspan, C. N. Kelber, and D. Okrent (Eds.), Computing Methods in Reactor Physics, Gordon and Breach Science Publishers, New York, New York (1968).

3 I. M. Gelfand and S. V. Fomin, Calculus of Variations, Prentice-Hall, Inc., Englewood Cliffs, New Jersey (1963).

4 I. S. Berezin and N. P. Zhidkov, Computing Methods, Vol. II, Pergamon Press, Oxford, England (1965).

5 S. K. Godunov and V. S. Ryabenki, Theory of Difference Schemes; An Introduction, North-Holland Publishing Company, Amsterdam, Holland (1964).

6 S. K. Godunov and V. S. Ryabenki, Difference Schemes; An Introduction to the Underlying Theory, Elsevier Science Publishers, Amsterdam, Holland (1987).

7 V. K. Saul'yev, Integration of Equations of Parabolic Type by the Method of Nets, The Macmillan Company, New York, New York (1964).

8 G. W. Blumen and J. D. Cole, Similarity Methods for Differential Equations, Springer-Verlag, New York, New York (1974).

9 R. L. Anderson and N. H. Ibragimov, Lie-Backlund Transformations in Applications, SIAM Studies in Applied Mathematics, No. 1, Philadelphia, Pennsylvania (1979).

10 L. V. Ovsiannikov, Group Analysis of Differential Equations, Academic Press, New York, New York (1982).

11 N. H. Ibragimov, Transformation Groups Applied to Mathematical Physics, D. Reidel Publishing Company, Dordrecht, Holland (1985).

12 P. J. Olver, Applications of Lie Groups to Differential Equations, Springer-Verlag, New York, New York (1986).

13 W. I. Fushchich and A. G. Nikitin, Symmetries of Maxwell's Equations, D. Reidel Publishing Company, Dordrecht, Holland (1987).

14 Y. I. Shokin, The Method of Differential Approximation, Springer-Verlag, New York, New York (1983).

15 E. Gelbard, J. Davis and J. Pearson, "Iterative Solutions to the P_L and Double-P_L Equations," Nucl. Sci. and Engr. 5, No. 1 (1959), p 36.