LA-13499

Construction of Difference Equations Using Lie Groups

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CONTENTS

CONSTRUCTION OF DIFFERENCE EQUATIONS USING LIE GROUPS

by

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ABSTRACT

The theory of prolongations of the generators of groups of point transformations to the grid point values of dependent variables and grid spacings is developed and applied to the construction of group invariant numerical algorithms. The concepts of invariant difference operators and generalized discrete sources are introduced for the discretization of systems of inhomogeneous differential equations and shown to produce exact difference equations. Invariant numerical flux functions are constructed from the general solutions of first order partial differential equations that come out of the evaluation of the Lie derivatives of conservation forms of difference schemes. It is demonstrated that invariant numerical flux functions with invariant flux or slope limiters can be determined to yield high resolution difference schemes. The introduction of an invariant flux or slope limiter can be done so as not to break the symmetry properties of a numerical flux function.

1. INTRODUCTION

The technical meaning of the term, "invariant difference scheme", is not unique in numerical analysis literature. In Shokin [1] a difference scheme is said to be invariant if its first differential approximation in parabolic form admits the same transformation group as the system of differential equations that is being discretized. This definition is the basis of the Shokin classification of difference schemes into one of two types, namely, (1) schemes that satisfy group axioms and (2) schemes that do not satisfy group axioms in the sense of an invariant first differential approximation. In Dorodnitsyn [2,3] an invariant difference scheme is conceived of as a scheme whose functional form in terms of difference derivative invariants is the same as the functional form of the system of differential equations written out in terms of the differential invariants of a transformation group.

In this study invariant difference schemes of a more general character are constructed in terms of invariant difference operators and generalized discrete sources and in terms of invariant numerical flux functions. These two methods require the evaluation of the Lie derivatives of the grid point values of the dependent variables and the grid spacings. Such evaluations are based upon formulae that give the group action on derivatives up to infinite order rather than up to some finite order as is the case for invariant first differential approximations, which are the same as modified equations [4, 5] of difference schemes.

Prolongations of the generators of groups of point transformations to the grid point values of dependent variables and grid spacings are derived in Section 2. Once the prolongations of this more general type have been found, it is possible to calculate the extensions of group generators to various types of ordinary and partial difference derivatives. However, the theory of invariant difference operators and of invariant numerical flux functions is based upon the direct application of the prolongations to the grid point values of the dependent variables and the grid spacings.

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The concept of invariant difference operators is developed in Section 3 and applied to the construction of invariant difference schemes with generalized discrete sources. This development is done for systems of inhomogeneous first and second order ordinary differential equations. The resulting invariant difference schemes are shown to be exact; that is, their exact solutions predict the exact solutions of the differential equations for arbitrary size grid spacings.

The theory of invariant numerical flux functions is worked out in Section 4 and applied to the construction of invariant difference schemes in conservation form. When the Lie derivative of the conservation form of a difference scheme written in terms of the numerical flux function is evaluated, it is shown that the flux function must satisfy a first order partial differential equation to ensure the existence of an invariant difference scheme. The general solution of the invariant-numerical-flux-function partial differential equation is an arbitrary function of the solutions of its characteristic equations. This fact implies the existence of an infinite number of invariant numerical flux functions with either low order or high order. It is shown that numerical flux functions can be constructed with invariant flux limiters or slope limiters. Hence, the introduction of flux or slope limiters to develop high resolution difference scheme can be done so as not to break symmetry. The minmod function slope limiter, for example, preserves invariance properties of conservative difference schemes for both the advection equation and the inviscid Burgers equation.

2. DISCRETIZED PROLONGATIONS OF GROUP GENERATORS

The generators of multiparameter groups must be extended to grid spacings, grid point values of dependent variables, and difference derivatives to construct invariant numerical schemes. In the case of differential equations, prolongation of group generators need be carried out only to the highest order derivatives that appear in the system of differential equations. Determining the Lie derivatives of the grid point values of dependent variables and difference derivatives requires a knowledge of the group action on ordinary or partial derivatives up to infinite order. Accordingly, in this section the Lie derivatives of ordinary and partial derivatives of arbitrary order are found and used to obtain the Lie derivatives of grid point values of dependent variables. Once these are known, the Lie derivatives of difference derivatives can be computed.

Variables in physical problems are classified as dependent and independent. This distinction should be kept in mind when working out the prolongations of group generators for invariant numerical schemes. Four cases of group generation prolongations are considered below, namely,

(1) one dependent and one independent variable,
(2) one dependent and n independent variables,
(3) m dependent and one independent variable, and
(4) m dependent and n independent variables.

The group generator prolongations found for each of these four cases are applicable to the construction of invariant numerical schemes for (1) ordinary differential equations, (2) partial differential equations, (3) systems of ordinary differential equations, and (4) systems of partial differential equations, respectively. A discretized prolongation is defined as a group generator prolongation to grid spacings, grid point values of dependent variables, and difference derivatives.

2.1 Lie Derivatives of Adjacent Grid Point Values of Dependent Variables

In this section extensions of group generators to grid point values are determined under the assumption that only a single independent variable is incremented. This type of extension is sufficient for explicit difference schemes.

2.1.1 Case 1. Discretized Prolongations with One Dependent Variable and One Independent Variable

With the kth order derivative denoted by

$$u_k = \frac{d^k u(x)}{dx^k} \quad , \tag{2.1}$$

the total derivative operator is

$$\hat{D} = \frac{\partial}{\partial x} + \sum_{k=0}^{\infty} u_{k+1} \frac{\partial}{\partial u_k} \quad , \tag{2.2}$$

and the shift operator to the right is

$$\hat{S}^{+} = \sum_{k=0}^{\infty} \frac{h^k}{k!} \hat{D}^k = e^{h\hat{D}} \quad , \tag{2.3}$$

where h is the grid spacing. Also, the shift operator to the left is

$$\hat{S}^{-} = e^{-h\hat{D}} \quad . \tag{2.4}$$

If the grid spacing is not uniform, let h^+ denote the grid spacing to the right of a grid point, and let h^- denote the grid spacing to the left of a grid point. Then the shift operator to the right is

$$\hat{S}^{+} = e^{h^{+}\hat{D}} \quad , \tag{2.5}$$

and that to the left is

$$\hat{S}^{-} = e^{-h^{-}\hat{D}} \quad . \tag{2.6}$$

Shift operators acting on the dependent variable $u(x)$ yield

$$\hat{S}^{+}(u(x)) = u(x+h) \quad , \tag{2.7}$$

and

$$\hat{S}^{-}(u(x)) = u(x-h) \tag{2.8}$$

for uniform grids, or

$$\hat{S}^{+}(u(x)) = u\left(x+h^{+}\right) \quad , \tag{2.9}$$

and

$$\hat{S}^{-}(u(x)) = u\left(x-h^{-}\right) \quad , \tag{2.10}$$

for nonuniform grids.

To construct an invariant numerical scheme to integrate the second order ordinary differential equation,

$$f(x,u,u',u'')=0 \quad , \tag{2.11}$$

assumed to admit the group of point transformation generated by

$$\hat{U}=\xi(x,u)\frac{\partial}{\partial x}+\eta(x,u)\frac{\partial}{\partial u} \quad , \tag{2.12}$$

the group is extended to grid spacings and the grid point values $u(x \pm h)$ of the dependent variable. The coordinate function $\xi(x,u)$ is the Lie derivative,

$$\frac{\delta x}{\delta a}=\xi(x,u) \quad , \tag{2.13}$$

and the coordinate function $\eta(x,u)$ is the Lie derivative

$$\frac{\delta u}{\delta a}=\eta(x,u) \quad , \tag{2.14}$$

where a is the group parameter. The prolongation of the group generator is

$$\hat{U}^{(G)}=\xi\frac{\partial}{\partial x}+\eta\frac{\partial}{\partial u}+\frac{\delta h}{\delta a}\frac{\partial}{\partial h}+\frac{\delta u(x+h)}{\delta a}\frac{\partial}{\partial u(x+h)}+\frac{\delta u(x-h)}{\delta a}\frac{\partial}{\partial u(x-h)} \quad . \tag{2.15}$$

To obtain the Lie derivative of the grid spacing first note that

$$h=x+h-x=\hat{S}^{+}(x)-x \quad . \tag{2.16}$$

Taking the Lie derivative of this equation yields

$$\frac{\delta h}{\delta a}=\frac{\delta}{\delta a}\hat{S}^{+}(x)-\frac{\delta x}{\delta a}=\hat{S}^{+}(\xi)-\xi \quad . \tag{2.17}$$

The Lie derivative of the grid point value $u(x+h)$ can be evaluated by several methods, the most direct of which starts from

$$u(x+h)=\sum_{k=o}^{\infty}\frac{h^k}{k!}u_k \quad . \tag{2.18}$$

The Lie derivative of this series is

$$\frac{\delta u}{\delta a}(x+h)=\frac{\delta u(x)}{\delta a}+\sum_{k=1}^{\infty}\left[\frac{h^{k-1}}{(k-1)!}\frac{\delta h}{\delta a}u_k+\frac{h^k}{k!}\frac{\delta u_k}{\delta a}\right] \quad , \tag{2.19}$$

in which the Lie derivative of the grid spacing is given in (2.17). The Lie derivative of the kth order derivative u_k is found from those of the sequence of one forms,

$$du = u_1\, dx \quad , \tag{2.20}$$

$$du_1 = u_2\, dx \quad , \tag{2.21}$$

$$du_2 = u_3\, dx \quad , \tag{2.22}$$

$$\vdots$$

$$du_{k-1} = u_k\, dx \quad , \tag{2.23}$$

$$du_k = u_{k+1}\, dx \quad . \tag{2.24}$$

That is, taking the Lie derivative of this sequence gives

$$\frac{\delta}{\delta a} du = \frac{\delta u_1}{\delta a} dx + u_1 \frac{\delta}{\delta a} dx \quad , \tag{2.25}$$

$$\frac{\delta}{\delta a} du_1 = \frac{\delta u_2}{\delta a} dx + u_2 \frac{\delta}{\delta a} dx \quad , \tag{2.26}$$

$$\vdots$$

$$\frac{\delta}{\delta a} u_{k-1} = \frac{\delta u_k}{\delta a} dx + u_k \frac{\delta}{\delta a} dx \quad . \tag{2.27}$$

Since the differential and Lie derivative operators are commutative, we have

$$\frac{\delta u_1}{\delta a} = \frac{d}{dx}\left(\frac{\delta u}{\delta a}\right) - u_1 \frac{d}{dx}\left(\frac{\delta x}{\delta a}\right) \quad , \tag{2.28}$$

$$\frac{\delta u_2}{\delta a} = \frac{d}{dx}\left(\frac{\delta u_1}{\delta a}\right) - u_2 \frac{d}{dx}\left(\frac{\delta x}{\delta a}\right) \quad , \tag{2.29}$$

$$\vdots$$

$$\frac{\delta u_k}{\delta a} = \frac{d}{dx}\left(\frac{\delta u_{k-1}}{\delta a}\right) - u_k \frac{d}{dx}\left(\frac{\delta x}{\delta a}\right) \quad . \tag{2.30}$$

These equations become

$$\frac{\delta u_1}{\delta u} = \hat{D}\eta - u_1 \hat{D}\xi = \hat{D}(\eta - u_1\xi) + u_2\xi \quad , \tag{2.31}$$

$$\frac{\delta u_2}{\delta a} = \hat{D}\left(\frac{\delta u_1}{\delta a} - u_2\xi\right) + u_3\xi = \hat{D}^2(\eta - u_1\xi) + u_3\xi \quad , \tag{2.32}$$

$$\vdots$$

$$\frac{\delta u_k}{\delta a} = \hat{D}^k(\eta - u_1\xi) + u_{k+1}\xi, (k = 1, 2, 3, ..., \infty) \quad . \tag{2.33}$$

Upon substituting (2.33) into (2.19) there follows

$$\frac{\delta u}{\delta a}(x+h) = \frac{\delta u}{\delta a}(x) + \sum_{k=1}^{\infty}\left\{\frac{h^{k-1}}{(k-1)!}\frac{\delta h}{\delta a}u_k + \frac{h^k}{k!}\left[\hat{D}^k(\eta - u_1\xi) + u_{k+1}\xi\right]\right\} \quad . \tag{2.34}$$

The summations in (2.34) are simplified as follows:

$$\sum_{k=1}^{\infty}\frac{h^{k-1}}{(k-1)!}\frac{\delta h}{\delta a}u_k = \left[\hat{S}^+(\xi) - \xi\right]\sum_{j=0}^{\infty}\frac{h^j}{j!}u_{j+1} = \left[\hat{S}^+(\xi) - \xi\right]\hat{S}^+(u_1) \tag{2.35}$$

$$\sum_{k=1}^{\infty}\frac{h^k}{k!}\hat{D}^k(\eta - u_1\xi) = u_1\xi - \eta + \hat{S}^+(\eta) - \hat{S}^+(u_1\xi) \tag{2.36}$$

$$\sum_{k=1}^{\infty}\frac{h^k}{k!}u_{k+1}\,\xi = \xi\,\hat{S}^+(u_1) - u_1\xi \quad . \tag{2.37}$$

As

$$\hat{S}^+(u_1\xi) = \hat{S}^+(u_1)\hat{S}^+(\xi) \quad . \tag{2.38}$$

combining (2.34), (2.35), (2.36) and (2.37) produces, for the Lie derivative of the grid point value $u(x+h)$, the result

$$\frac{\delta u}{\delta a}(x+h) = \hat{S}^+(\eta) \quad . \tag{2.39}$$

The Lie derivative of the grid point value $u(x-h)$ is found by a similar derivation to be

$$\frac{\delta u}{\delta a}(x-h) = \hat{S}^-(\eta) \quad . \tag{2.40}$$

To obtain (2.40), we note that

$$h = x - (x-h) = x - \hat{S}^-(x) \quad , \tag{2.41}$$

so that, alternatively, the grid spacing Lie derivative is

$$\frac{\delta h}{\delta a} = \xi - \hat{S}^{-}(\xi) \quad . \tag{2.42}$$

In view of (2.17), (2.39), and (2.40) the prolongation of the group generator to grid spacings and grid point values of the dependent variable takes the form,

$$\hat{U}^{(G)} = \xi\frac{\partial}{\partial x} + \eta\frac{\partial}{\partial u} + \left[\hat{S}^{+}(\xi) - \xi\right]\frac{\partial}{\partial h} + \hat{S}^{+}(\eta)\frac{\partial}{\partial u(x+h)} + \hat{S}^{-}(\eta)\frac{\partial}{\partial u(x-h)} \quad . \tag{2.43}$$

for a uniformly spaced grid. For the case of a nonuniform grid with grid spacing h^{+} to the right of a grid point and a grid spacing h^{-} to the left, the prolonged group generator is

$$\hat{U}^{(G)} = \xi\frac{\partial}{\partial x} + \eta\frac{\partial}{\partial u} + \left[\hat{S}^{+}(\xi) - \xi\right]\frac{\partial}{\partial h^{+}} + \left[\xi - \hat{S}^{-}(\xi)\right]\frac{\partial}{\partial h^{-}}$$

$$+\hat{S}^{+}(\eta)\frac{\partial}{\partial u\left(x+h^{+}\right)} + \hat{S}^{-}(\eta)\frac{\partial}{\partial u\left(x+h^{-}\right)} \quad , \tag{2.44}$$

where the right and left shift operators $\hat{S}^{+}$ and $\hat{S}^{-}$ are given by (2.5) and (2.8), respectively.

With the Lie derivative results for the grid point values $u(x+h)$ and $u(x-h)$ found in (2.39) and (2.40), respectively, it is possible to calculate the Lie derivatives of difference derivatives. The forward difference operator is defined by

$$\hat{\Delta}^{+} = \frac{1}{h}\left[\hat{S}^{+} - 1\right] \quad , \tag{2.45}$$

and the backward difference operator by

$$\hat{\Delta}^{-} = \frac{1}{h}\left[1 - \hat{S}^{-}\right] \quad . \tag{2.46}$$

The forward difference derivative is

$$\hat{\Delta}^{+}(u) = \frac{1}{h}\left[\hat{S}^{+}(u) - u\right] = \frac{1}{h}\left[u(x+h) - u(x)\right] \quad . \tag{2.47}$$

and the backward difference derivative is

$$\hat{\Delta}^{-}(u) = \frac{1}{h}\left[u - \hat{S}^{-}(u)\right] = \frac{1}{h}\left[u(x) - u(x-h)\right] \quad . \tag{2.48}$$

The Lie derivative of (2.47) yields

$$\frac{\delta}{\delta a}\hat{\Delta}^{+}(u)=\frac{1}{h}\left[\frac{\delta u}{\delta a}(x+h)-\frac{\delta u}{\delta a}(x)\right]-\frac{1}{h}[u(x+h)-u(x)]\frac{1}{h}\frac{\delta h}{\delta a}$$

$$=\frac{1}{h}\left[\hat{S}^{+}(\eta)-\eta\right]-\frac{1}{h}[u(x+h)-u(x)]\frac{1}{h}\left[\hat{S}^{+}(\xi)-\xi\right] \tag{2.49}$$

or

$$\frac{\delta}{\delta a}\hat{\Delta}^{+}(u)=\hat{\Delta}^{+}(\eta)-\hat{\Delta}^{+}(u)\hat{\Delta}^{+}(\xi)\quad . \tag{2.50}$$

This result for the Lie derivative of the forward difference derivative is the finite difference equivalent to the Lie derivative of the first order deriative given in (2.31). Also, the Lie derivative of (2.48) is

$$\frac{\delta\hat{\Delta}^{-}}{\delta a}(u)=\frac{1}{h}\left[\frac{\delta u}{\delta a}(x)-\frac{\delta u}{\delta a}(x-h)\right]-\frac{1}{h}[u(x)-u(x-h)]\frac{1}{h}\frac{\delta h}{\delta a}$$

$$=\frac{1}{h}\left[\eta-\hat{S}^{-}(\eta)\right]-\frac{1}{h}[u(x)-u(x-h)]\frac{1}{h}\left[\xi-\hat{S}^{-}(\xi)\right] \tag{2.51}$$

or

$$\frac{\delta\hat{\Delta}^{-}}{\delta a}(u)=\hat{\Delta}^{-}(\eta)-\hat{\Delta}^{-}(u)\hat{\Delta}^{-}(\xi)\quad . \tag{2.52}$$

In terms of the forward and backward difference operators defined in (2.45) and (2.46), the three-point central difference approximation of a second order derivative is

$$\hat{\Delta}^{-}\hat{\Delta}^{+}(u)=\hat{\Delta}^{+}\hat{\Delta}^{-}(u)=\frac{1}{h^{2}}[u(x+h)+u(x-h)-2u(x)]\quad . \tag{2.53}$$

The Lie derivative of this equation is

$$\frac{\delta}{\delta a}\hat{\Delta}^{-}\hat{\Delta}^{+}(u)=\frac{1}{h^{2}}\left[\frac{\delta u}{\delta a}(x+h)+\frac{\delta u}{\delta a}(x-h)-2\frac{\delta u}{\delta a}(x)\right]$$

$$-2\frac{1}{h}\frac{\delta h}{\delta a}\frac{1}{h^{2}}[u(x+h)+u(x-h)-2u(x)]$$

$$=\frac{1}{h^{2}}\left[\hat{S}^{+}(\eta)+\hat{S}^{-}(\eta)-2\eta\right]-\frac{2}{h}\left[\hat{S}^{+}(\xi)-\xi\right]\hat{\Delta}^{-}\hat{\Delta}^{+}(u)\quad , \tag{2.54}$$

or

$$\frac{\delta}{\delta a}\hat{\Delta}^{-}\hat{\Delta}^{+}(u)=\hat{\Delta}^{-}\hat{\Delta}^{+}(\eta)-2\hat{\Delta}^{-}\hat{\Delta}^{+}(u)\hat{\Delta}^{+}(\xi)\quad , \tag{2.55}$$

which gives the group action on the three-point central difference formula. The two-point central difference formula approximation for the first order derivative is

$$\hat{\Delta}^{\pm}(u)=\frac{1}{2h}\left[u(x+h)-u(x-h)\right]=\frac{1}{2}\left[\hat{\Delta}^{+}(u)+\hat{\Delta}^{-}(u)\right] \quad . \tag{2.56}$$

The Lie derivative of this is

$$\frac{\delta}{\delta a}\hat{\Delta}^{\pm}(u)=\frac{1}{2}\left[\frac{\delta}{\delta a}\hat{\Delta}^{+}(u)+\frac{\delta}{\delta a}\hat{\Delta}^{-}(u)\right] \quad , \tag{2.57}$$

which in view of (2.50) and (2.52) becomes

$$\frac{\delta}{\delta a}\hat{\Delta}^{\pm}(u)=\frac{1}{2}\left[\hat{\Delta}^{+}(\eta)-\hat{\Delta}^{+}(u)\hat{\Delta}^{+}(\xi)+\hat{\Delta}^{-}(\eta)-\hat{\Delta}^{-}(u)\hat{\Delta}^{-}(\xi)\right] \quad , \tag{2.58}$$

and for a uniform grid this simplifies to

$$\frac{\delta}{\delta a}\hat{\Delta}^{\pm}(u)=\frac{1}{2}\left[\hat{\Delta}^{+}(\eta)+\hat{\Delta}^{-}(\eta)\right]-\hat{\Delta}^{+}(\xi)\frac{1}{2}\left[\hat{\Delta}^{+}(u)+\hat{\Delta}^{-}(u)\right] \quad , \tag{2.59}$$

or

$$\frac{\delta}{\delta a}\hat{\Delta}^{\pm}(u)=\hat{\Delta}^{\pm}(\eta)-\hat{\Delta}^{\pm}(u)\hat{\Delta}^{+}(\xi) \quad . \tag{2.60}$$

Lie derivatives of other finite difference approximations for first, second, and higher order derivatives can be derived by the methods used above which are based upon first finding the Lie derivatives of the grid spacings and the relevant grid point values of the dependent variables.

When the group of point transformations that is generated by (2.12) is extended to two neighboring grid point values, to forward and backward difference derivatives, and to two and three-point central difference formulas, the generator of the prolonged group is

$$\begin{aligned}\hat{U}^{(G)}=&\ \xi\frac{\partial}{\partial x}+\eta\frac{\partial}{\partial u}+\left[\hat{S}^{+}(\xi)-\xi\right]\frac{\partial}{\partial h}+\hat{S}^{+}(\eta)\frac{\partial}{\partial u(x+h)}\\&+\hat{S}^{-}(\eta)\frac{\partial}{\partial u(x-h)}+\left[\hat{\Delta}^{+}(\eta)-\hat{\Delta}^{+}(u)\hat{\Delta}^{+}(\xi)\right]\frac{\partial}{\partial\hat{\Delta}^{+}(u)}\\&+\left[\hat{\Delta}^{-}(\eta)-\hat{\Delta}^{-}(u)\hat{\Delta}^{-}(\xi)\right]\frac{\partial}{\partial\hat{\Delta}^{-}(u)}\\&+\left[\hat{\Delta}^{\pm}(\eta)-\hat{\Delta}^{\pm}(u)\hat{\Delta}^{+}(\xi)\right]\frac{\partial}{\partial\hat{\Delta}^{\pm}(u)}\\&+\left[\hat{\Delta}^{-}\hat{\Delta}^{+}(\eta)-2\hat{\Delta}^{-}\hat{\Delta}^{+}(u)\hat{\Delta}^{+}(\xi)\right]\frac{\partial}{\partial\hat{\Delta}^{-}\hat{\Delta}^{+}(u)}\end{aligned} \tag{2.61}$$

for uniform grid spacings. If a group of point transformations is given by specifying the two coordinate functions $\xi(x,u)$ and $\eta(x,u)$ for the independent and dependent variables, respectively, then by solving the linear first order partial differential equation formed with the prolonged generator (2.61), namely,

$$\hat{U}^{(G)}F = 0 \quad , \tag{2.62}$$

by the method of characteristics, the general forms of first and second order difference equations that are invariant under the group generated by (2.12) can be found. Since the general solution of a linear first order partial differential equation is an arbitrary function of the solutions of the characteristic equations, it is possible to construct, in principle, an infinite number of difference equations that are invariant under a given group. If the selected group of point transformations is also admitted by a first or second order ordinary differential equation, then difference equations that are invariant under the same group can be found by the above method.

For example, consider the scaling group generated by

$$\hat{U} = x\frac{\partial}{\partial x} + mu\frac{\partial}{\partial u} \quad . \tag{2.63}$$

The prolongation of this group generator to the grid spacing, forward grid point value of the dependent variable, and first order forward difference derivative is

$$\hat{U}^{(G)} = x\frac{\partial}{\partial x} + mu(x)\frac{\partial}{\partial u(x)} + \frac{\delta h}{\delta a}\frac{\partial}{\partial h} + \frac{\delta u(x+h)}{\delta a}\frac{\partial}{\partial u(x+h)} + \frac{\delta \hat{\Delta}^{+}u}{\delta a}\frac{\partial}{\partial \hat{\Delta}^{+}u} \tag{2.64}$$

in which the Lie derivatives are

$$\frac{\delta h}{\delta a} = h \quad , \tag{2.65}$$

$$\frac{\delta u(x+h)}{\delta a} = \hat{S}^{+}(\eta) = m\, u(x+h) \quad , \tag{2.66}$$

and

$$\frac{\delta \hat{\Delta}^{+}(u)}{\delta a} = (m-1)\hat{\Delta}^{+}(u) \quad . \tag{2.67}$$

The characteristic equations of the linear first order partial differential equation,

$$\hat{U}^{(G)}F = 0 \quad , \tag{2.68}$$

formed with the prolonged generator (2.64) are

$$\frac{dx}{x} = \frac{dh}{h} = \frac{du(x)}{mu(x)} = \frac{du(x+h)}{mu(x+h)} = \frac{d\Delta^{+}(u)}{(m-1)\Delta^{+}(u)} \quad . \tag{2.69}$$

The solutions of these characteristic equations are

$$\frac{x}{h} = \text{constant} \quad , \tag{2.70}$$

$$\frac{u(x)}{x^m} = \text{constant} \quad , \tag{2.71}$$

$$\frac{u(x+h)}{h^m} = \text{constant} \quad , \tag{2.72}$$

and

$$\frac{\hat{\Delta}^+ u}{x^{m-1}} = \text{constant} \quad . \tag{2.73}$$

Hence, it is found that

$$\hat{\Delta}^+(u) = x^{m-1} f\left(\frac{x}{h}, \frac{u(x)}{x^m}, \frac{u(x+h)}{h^m}\right) \quad , \tag{2.74}$$

where f is an arbitrary function of the indicated arguments, is the general form of a first order difference equation that is invariant under the scaling group generated by (2.63). This follows simply by solving the partial differential equation by the method of characteristics.

2.1.2 CASE 2. DISCRETIZED PROLONGATIONS WITH ONE DEPENDENT AND n INDEPENDENT VARIABLES

In this section discretized prolongations of the group generator,

$$\hat{U} = \sum_{i-1}^{n} \xi^i \frac{\partial}{\partial x^i} + \eta \frac{\partial}{\partial u} \quad , \tag{2.75}$$

are determined. Here the coordinate function for the ith independent variable x^i is

$$\frac{\delta x^i}{\delta a} = \xi^i\left(x^i, x^2, ..., x^n, u\right) \quad , \tag{2.76}$$

the Lie derivative of x^i, and the coordinate function for the dependent variable is

$$\frac{\delta u}{\delta a} = \eta\left(x^i, x^2, \; ...., \; x^n, u\right) \quad . \tag{2.77}$$

The derivation will assume uniform grids for which h_i is the grid spacing of the ith independent variable x^i. The removal of this assumption causes no fundamental difficulty.

The shift operator to the right for the ith independent variable is

$$\hat{S}_i^{+} = e^{h_i \hat{D}_i} \quad , \tag{2.78}$$

and the shift operator to the left is

$$\hat{S}_i^{-} = e^{-h_i \hat{D}_i} \quad . \tag{2.79}$$

In these last two equations the total derivative operator $\hat{D}_i$ with respect to the ith independent variable is defined as

$$\hat{D}_i = \frac{\partial}{\partial x^i} + u_i \frac{\partial}{\partial u} + \sum_{j=1}^{n} u_{ji} \frac{\partial}{\partial u_j} + \sum_{\ell=1}^{n} \sum_{j=1}^{n} u_{\ell ji} \frac{\partial}{\partial u_{\ell j}} + \dots \tag{2.80}$$

in which the partial derivatives are denoted by subscripts, that is

$$u_i = \frac{\partial u}{\partial x^i} \quad , \tag{2.81}$$

$$u_{ji} = \frac{\partial^2 u}{\partial x^j \partial x^i} \quad , \tag{2.82}$$

$$u_{\ell ji} = \frac{\partial^3}{\partial x^l \partial x^j \partial x^i} \quad , \tag{2.83}$$

and so forth. The forward partial difference derivative operator is

$$\hat{\Delta}_i^{+} = \frac{1}{h_i}\left(\hat{S}_i^{+} - 1\right) \tag{2.84}$$

and the backward partial difference derivative operator is

$$\hat{\Delta}_i^{-} = \frac{1}{h_i}\left(1 - \hat{S}_i^{-}\right) \quad , \tag{2.85}$$

both with respect to the ith independent variable. Shift operators acting on the dependent variable produce

$$u\left(x^1, x^2, \dots, x^i + h_i, \dots, x^n\right) = \hat{S}_i^{+}\left(u\left(x^1, x^2, \dots, x^i, \dots, x^n\right)\right) \quad , \tag{2.86}$$

and

$$u\left(x^1, x^2, \dots, x^i - h_i, \dots, x^n\right) = \hat{S}_i^{-}\left(u\left(x^1, x^2, \dots, x^i, \dots, x^n\right)\right) \quad . \tag{2.87}$$

Since

$$h_i = x^i + h_i - x^i = \hat{S}_i^{+}\left(x^i\right) - x^i \quad , \tag{2.88}$$

the Lie derivative of the grid spacing for the i th independent variable is

$$\frac{\delta h_i}{\delta a} = \hat{S}_i^{+}\left(\xi^i\right) - \xi^i \ , \tag{2.89}$$

where (2.88) has been used. Alternately from

$$h_i = x^i - \left(x^i - h_i\right) = x^i - \hat{S}_i^{-}\left(x^i\right) \ , \tag{2.90}$$

it follows that

$$\frac{\delta h_i}{\delta a} = \xi^i - \hat{S}_i^{-}\left(\xi^i\right) \ . \tag{2.91}$$

For nonuniform grids, the Lie derivatives of the grid spacing to the right, h_i^+, and to the left, h_i^-, are given by (2.89) and (2.91), respectively.

From (2.86) the forward grid point value of the dependent variable with respect to the i th independent variable is

$$u\left(x^1, x^2, \ldots, x^i + h_i, \ldots, x^n\right) = u\left(x^1, x^2, \ldots, x^i, \ldots, x^n\right) + \sum_{k=1}^{\infty} \frac{h_i^k}{k!} u_i^{(k)} \ , \tag{2.92}$$

in which $u_i^{(k)}$ denotes the kth other derivative with respect to the i th independent variable. Let H_i^+ denote the Lie derivative of the forward grid point value, that is,

$$H_i^+ = \frac{\delta u}{\delta a}\left(x^1, x^2, \ldots, x_i + h^i, \ldots, x^n\right) \ . \tag{2.93}$$

Taking the Lie derivative of (2.92) yields

$$H_i^+ = \frac{\delta u}{\delta a} + \sum_{k=1}^{\infty}\left[\frac{h_i^{k-1}}{(k-1)!}\frac{\delta h_i}{\delta a} u_i^{(k)} + \frac{h_i^k}{k!}\frac{\delta u_i^{(k)}}{\delta a}\right] \ . \tag{2.94}$$

By a straightforward but long calculation the Lie derivative of the kth order derivative with respect to the i th independent variable is found to be given by

$$\frac{\delta u_i^{(k)}}{\delta a} = \hat{D}_i^k\left(\eta - \sum_{j=1}^{n} u_j \xi^j\right) + \sum_{j=1}^{n} \frac{\partial^k u_j}{\partial\left(x^i\right)^k}\xi^j \ . \tag{2.95}$$

Combining (2.14), (2.89), (2.95), and (2.94) yields

$$H_i^+ = \eta + \sum_{k=1}^{\infty} \frac{h_i^k}{k!}\hat{D}_i^k(\eta) + \left[\hat{S}_i^{+}\left(\xi^i\right) - \xi^i\right]\sum_{k=1}^{\infty}\frac{h_i^{k-1}}{(k-1)!}u_i^{(k)}$$

$$-\sum_{k=1}^{\infty}\frac{h_i^k}{k!}\sum_{j=1}^{n}\hat{D}_i^k\left(u_j\xi^j\right)+\sum_{k=1}^{\infty}\frac{h_i^k}{k!}\sum_{j=1}^{n}\frac{\partial^k u_j}{\partial\left(x^i\right)^k}\xi^j \quad . \tag{2.96}$$

The summations in (2.96) may be simplified as follows:

$$\hat{S}_i^+(\eta)=\eta+\sum_{k=1}^{\infty}\frac{h_i^k}{k!}\hat{D}_i^k(\eta) \tag{2.97}$$

$$\sum_{k=1}^{\infty}\frac{h_i^{k-1}}{(k-1)!}u_i^{(k)}=\sum_{k=0}^{\infty}\frac{h_i^k}{k!}u_i^{(k+1)}=\hat{S}_i^+\left(u_i\right) \quad . \tag{2.98}$$

$$\sum_{k=1}^{\infty}\frac{h_i^k}{k!}\sum_{j=1}^{n}\hat{D}_i^k\left(u_j\xi^j\right)=\sum_{k=1}^{\infty}\frac{h_i^k}{k!}\left[\hat{D}_i^k\left(u_i\xi^i\right)+\sum_{\substack{j=1\\ j\neq i}}^{n}\hat{D}_i^k\left(u_j\xi^j\right)\right]$$

$$=\hat{S}_i^+\left(u_j\xi^j\right)-u_j\xi^j+\sum_{\substack{j=1\\ j\neq i}}^{n}\hat{S}_i^+\left(u_j\xi^j\right)-\sum_{\substack{j=1\\ j\neq i}}^{n}u_j\xi^j \quad . \tag{2.99}$$

$$\sum_{k=1}^{\infty}\frac{h_i^k}{k!}\sum_{j=1}^{n}\frac{\partial^k u_j}{\partial\left(x^i\right)^k}\xi^j=\sum_{k=1}^{\infty}\frac{h_i^k}{k!}\left[\frac{\partial^k u_i}{\partial\left(x^i\right)^k}\xi^i+\sum_{\substack{j=1\\ j\neq i}}^{n}\frac{\partial^k u_j}{\partial\left(x^i\right)^k}\xi^j\right]$$

$$=\xi^i\left[-u_i+\hat{S}_i^+\left(u_i\right)\right]-\sum_{\substack{j=1\\ j\neq i}}^{n}u_j\xi^j+\sum_{\substack{j=1\\ j\neq i}}^{n}\xi^j\hat{S}_i^+\left(u_j\right) \quad . \tag{2.100}$$

By combining (2.96), (2.97), (2.98), (2.99), and (2.100), it is found that the Lie derivative of the forward grid point value of the dependent variable with respect to the ith independent variable is given by

$$H_i^+=\hat{S}_i^+(\eta)-\sum_{\substack{j=1\\ j\neq i}}^{n}\hat{S}_i^+\left(u_j\right)\left[\hat{S}_i^+\left(\xi^j\right)-\xi^j\right] . \tag{2.101}$$

Let H_i^- denote the Lie derivative of the backward grid point value of the dependent with respect to the ith independent variable, that is,

$$H_i^-=\frac{\delta u}{\delta a}\left(x^i,x^2,\ldots,x^i-h_i,\ldots,x^n\right) \quad . \tag{2.102}$$

A derivation similar to that giving (2.100) produces

$$H_i^- = \hat{S}_i^-(\eta) + \sum_{\substack{j=1 \\ j\neq i}}^{n} \hat{S}_i^-(u_j)\left[\xi^j - \hat{S}_i^-(\xi^j)\right] \quad . \tag{2.103}$$

With the Lie derivatives obtained in (2.89) and (2.103), the prolongation of the group generator (2.75) to backward and forward neighboring grid point values of the dependent variable and grid spacing is

$$\hat{U}^{(G)} = \sum_{i=1}^{n} \xi^i \frac{\partial}{\partial x^i} + \eta \frac{\partial}{\partial u} + \sum_{i=1}^{n} \left[\hat{S}_i^+(\xi^i) - \xi^i\right] \frac{\partial}{\partial h_i}$$

$$+ \sum_{i=1}^{n} H_i^+ \frac{\partial}{\partial u(x^i + h_i)} + \sum_{i=1}^{n} H_i^- \frac{\partial}{\partial u(x^i - h_i)} \quad , \tag{2.104}$$

where

$$u(x^i + h_i) = u(x^i, x^2, \ldots, x^i + h_i, \ \ldots, x^n) \quad , \tag{2.105}$$

and

$$u(x^i - h_i) = u(x^i, x^2, \ \ldots, x^i - h_i, \ \ldots, x^n) \quad . \tag{2.106}$$

Prolongations of the type found in (2.104) are used to find invariant difference schemes for partial differential equations.

2.1.3 CASE 3. DISCRETIZED PROLONGATIONS WITH m DEPENDENT AND ONE INDEPENDENT VARIABLE

The generators of groups of point transformations that are admitted by systems of ordinary differential equations take the form,

$$\hat{U} = \xi \frac{\partial}{\partial x} + \sum_{\nu=1}^{m} \eta^\nu \frac{\partial}{\partial u^\nu} \quad , \tag{2.107}$$

in which the Lie derivative of the independent variable is

$$\frac{\delta x}{\delta a} = \xi(x, u^1, u^2, \ldots, u^m) \quad , \tag{2.108}$$

and the Lie derivative of the νth dependent variable is

$$\frac{\delta u^\nu}{\delta a} = \eta^\nu(x, u^1, u^2, \ldots, u^m) \quad . \tag{2.109}$$

In terms of the total derivative operator,

$$\hat{D} = \frac{\partial}{\partial x} + \sum_{k=0}^{\infty} \sum_{\nu=1}^{m} u_{k+1}^\nu \frac{\partial}{\partial u_k^\nu} \quad , \tag{2.110}$$

the shift operator to the right is

$$\hat{S}^{+} = e^{h\hat{D}} \quad , \tag{2.111}$$

and the shift operator to the left is

$$\hat{S}^{-} = e^{-h\hat{D}} \quad . \tag{2.112}$$

Extending the group generator (2.107) to neighboring grid point values of all of the dependent variables is done by calculating the Lie derivatives of $u^{\nu}(x \pm h)$ for $\nu = 1, 2, ..., m$. As

$$u^{\nu}(x+h) = \hat{S}^{+}(u^{\nu}) = \sum_{k=0}^{\infty} \frac{h^k}{k!} u_k^{\nu}(x) \quad , \tag{2.113}$$

the Lie derivative is

$$\frac{\delta u^{\nu}}{\delta a}(x+h) = \frac{\delta u^{\nu}}{\delta a} + \sum_{k=1}^{\infty} \left[\frac{h^{k-1}}{(k-1)!} \frac{\delta h}{\delta a} u_k^{\nu} + \frac{h^k}{k!} \frac{\delta u_k^{\nu}}{\delta a} \right] \quad . \tag{2.114}$$

The Lie derivative of the grid spacing is

$$\frac{\delta h}{\delta a} = \hat{S}^{+}(\xi) - \xi \quad , \tag{2.115}$$

and the Lie derivative of the kth order derivative of the νth dependent variable is

$$\frac{\delta u_k^{\nu}}{\delta a} = \hat{D}^k(\eta^{\nu} - u_1^{\nu}\xi) + u_{k+1}^{\nu}\, \xi \quad . \tag{2.116}$$

Hence, equation (2.114) becomes

$$\frac{\delta u^{\nu}}{\delta a}(x+h) = \eta^{\nu} + \left[\hat{S}^{+}(\xi) - \xi\right]\hat{S}^{+}(u_1^{\nu})$$
$$+ \sum_{k=1}^{\infty} \frac{h^k}{k!} \hat{D}^k(\eta^{\nu} - u_1^{\nu}\xi) + \sum_{k=1}^{\infty} \frac{h^k}{k!}\, \xi\, u_{k+1}^{\nu} \quad , \tag{2.117}$$

which, as in the derivation of (2.39), simplifies to

$$\frac{\delta u^{\nu}}{\delta a}(x+h) = \hat{S}^{+}(\eta^{\nu}) \tag{2.118}$$

to yield the Lie derivative of the forward grid point value. In the same way the Lie derivative of the backward grid point value of the νth dependent variable is

$$\frac{\delta u^{\nu}}{\delta a}(x-h)=\hat{S}^{-}(\eta^{\nu}) \quad . \tag{2.119}$$

With the results (2.118) and (2.119), the prolongation of the group generator (2.107) to neighboring grid point values of all of the dependent variables and the grid spacing is

$$\hat{U}^{(G)}=\xi\frac{\partial}{\partial x}+\sum_{\nu=1}^{m}\eta^{\nu}\frac{\partial}{\partial u^{\nu}}+\sum_{\nu=1}^{m}\hat{S}^{+}(\eta^{\nu})\frac{\partial}{\partial u^{\nu}(x+h)}$$

$$+\left[\hat{S}^{+}(\xi)-\xi\right]\frac{\partial}{\partial h}+\sum_{\nu=1}^{m}\hat{S}^{-}(\eta^{\nu})\frac{\partial}{\partial u^{\nu}(x-h)} \quad . \tag{2.120}$$

Further extension of this generator to forward and backward difference derivatives, to two-point central difference derivatives, and to three-point central difference derivatives can be done as in CASE 1 above.

2.1.4 CASE 4. DISCRETIZED PROLONGATIONS WITH m DEPENDENT AND n INDEPENDENT VARIABLES

Systems of partial differential equations in n independent variables $x^{i}, i=1,2, \ldots, n$, and m dependent variables $u^{\nu}, \nu=1,2,\ldots,m$, with symmetry properties admit groups of point transformations with generators of the form,

$$\hat{U}=\sum_{i=1}^{n}\xi^{i}\frac{\partial}{\partial x^{i}}+\sum_{\nu=1}^{m}\eta^{\nu}\frac{\partial}{\partial u^{\nu}} \quad , \tag{2.121}$$

in which the Lie derivative of the i th independent variable is

$$\frac{\delta x^{i}}{\delta a}=\xi^{i}\left(x^{1},x^{2},\ldots,x^{n},u^{1},u^{2},\ldots,u^{m}\right) \quad , \tag{2.122}$$

and the Lie derivative of the ν th dependent variable is

$$\frac{\delta u^{\nu}}{\delta a}=\eta^{\nu}\left(x^{1},x^{2},\ldots,x^{n},u^{1},u^{2},\ldots,u^{m}\right) \quad . \tag{2.123}$$

Forward and backward neighboring grid point values of the ν th dependent variable with respect to the i th independent variables are given by

$$u^{\nu}\left(x^{1},x^{2},\ldots,x^{i}\pm h_{i},\ldots,\ x^{n}\right)=\hat{S}_{i}^{\pm}\left(u^{\nu}\right) \quad , \tag{2.124}$$

where the right and left shift operators with respect to the i th independent variable are

$$\hat{S}_{i}^{\pm}=e^{\pm h_{i}\hat{D}_{i}} \tag{2.125}$$

in terms of the total derivative operator,

$$\hat{D}_i = \frac{\partial}{\partial x^i} + \sum_{\nu=1}^{m} u_i^\nu \frac{\partial}{\partial u^\nu} + \sum_{\nu=1}^{m} \sum_{j=1}^{n} u_{ji}^\nu \frac{\partial}{\partial u_j^u} + \dots \quad . \tag{2.126}$$

Here partial derivatives are denoted by subscripts, that is,

$$u_i^\nu = \frac{\partial u^\nu}{\partial x^i} \quad , \tag{2.127}$$

$$u_{ij}^\nu = \frac{\partial^2 u^\nu}{\partial x^i \partial x^j} \quad , \tag{2.128}$$

and so forth.

The discretized prolongation of the generator (2.121) can be obtained by the method used to obtain the discretized prolongation given in (2.104). An alternative method of derivation follows. With overbars used to denote quantities transformed under the group action, we start with the infinitesimal transformation,

$$\bar{u}^\nu\left(\bar{x}^1, \bar{x}^2, \dots, \bar{x}^i + \bar{h}_i, \dots,\ \bar{x}^n\right) = u^\nu\left(x^1, x^2, \dots, x^i + h_i, \dots,\ x^n\right)$$

$$+\delta a \frac{\delta u^\nu}{\delta a}\left(x^1, x^2, \dots, x^i + h_i, \dots,\ x^n\right) \quad , \tag{2.129}$$

where the second term on the right contains the Lie derivative of the forward grid point value, the quantity being sought. Expanding the left side of (2.129) in a Taylor series gives

$$\bar{u}^\nu\left(\bar{x}^1, \bar{x}^2, \dots, \bar{x}^i + \bar{h}_i, \dots,\ \bar{x}^n\right) = \bar{u}^\nu\left(\bar{x}^1, \bar{x}^2, \dots, \bar{x}^i, \dots,\ \bar{x}^n\right)$$

$$+\sum_{k=1}^{\infty} \frac{\bar{h}_i^k}{k!} \frac{\partial^k \bar{u}^\nu}{\partial\left(\bar{x}^i\right)^k} \quad . \tag{2.130}$$

From the meaning of infinitesimal transformations of independent variables, dependent variables, and various order derivatives, we have

$$\bar{u}^\nu\left(\bar{x}^1, \bar{x}^2, \dots, \bar{x}^i, \dots,\ \bar{x}^n\right) = u^\nu\left(x^1, x^2, \dots, x^i, \dots,\ x^n\right) + \eta^\nu \delta a \tag{2.131}$$

$$\bar{x}^i = x^i + \xi^i\, \delta a \quad , \tag{2.132}$$

and

$$\frac{\partial^k \bar{u}^\nu}{\partial\left(\bar{x}^i\right)^k} = \frac{\partial^k u^\nu}{\partial\left(x^i\right)^k} + \delta a \frac{\delta}{\delta a}\left(\frac{\partial^k u^\nu}{\partial\left(x^i\right)^k}\right) \quad . \tag{2.133}$$

The Lie derivative of the kth order partial derivative with respect to the ith independent variable appearing in (2.133) can be determined by first evaluating the Lie derivative of the differential form,

$$du^{\nu} = \sum_{i=1}^{n} u_i^{\nu} dx^i \quad , \tag{2.134}$$

to obtain

$$\frac{\delta u_i^{\nu}}{\delta a} = \hat{D}_i\left(\eta^{\nu} - \sum_{j=1}^{n} u_j^{\nu}\xi^j\right) + \sum_{j=1}^{n} u_{ji}^{\nu}\,\xi^j \quad . \tag{2.135}$$

Next the Lie derivative of the differential form,

$$du_i^{\nu} = \sum_{j=1}^{n} u_{ij}^{\nu}\, dx^j \quad , \tag{2.136}$$

yields

$$\frac{\delta u_{ij}^{\nu}}{\delta a} = \hat{D}_j\left(\frac{\delta u_i^{\nu}}{\delta a} - \sum_{k=1}^{n} u_{ik}^{\nu}\,\xi^k\right) + \sum_{k=1}^{n} u_{ijk}^{\nu}\,\xi^k \quad , \tag{2.137}$$

which with (2.135) becomes

$$\frac{\delta u_{ij}^{\nu}}{\delta a} = \hat{D}_i\hat{D}_j\left(\eta^{\nu} - \sum_{k=1}^{n} u_k^{\nu}\,\xi^k\right) + \sum_{k=1}^{n} u_{ijk}^{\nu}\,\xi^k \quad . \tag{2.138}$$

The Lie derivative of the differential form,

$$du_{ij}^{\nu} = \sum_{k=1}^{n} u_{ijk}^{\nu} dx^k \quad , \tag{2.139}$$

is

$$\frac{\delta u_{ijk}^{\nu}}{\delta a} = \hat{D}_k\left(\frac{\delta u_{ij}^{\nu}}{\delta a} - \sum_{\ell=1}^{n} u_{ij\ell}^{\nu}\,\xi^{\ell}\right) + \sum_{\ell=1}^{n} u_{ijk\ell}^{\nu}\,\xi^{\ell} \quad , \tag{2.140}$$

so with (2.138) we obtain the Lie derivative of third order partial derivatives in the form,

$$\frac{\delta u_{ijk}^{\nu}}{\delta a} = \hat{D}_k\,\hat{D}_j\,\hat{D}_i\left(\eta^{\nu} - \sum_{\ell=1}^{n} u_{\ell}^{\nu}\xi^{\ell}\right) + \sum_{\ell=1}^{n} u_{ijk\ell}\xi^{\ell} \quad . \tag{2.141}$$

From this equation it is seen that the kth order partial derivative with respect to the ith independent variable has the Lie derivative,

$$\frac{\delta}{\delta a}\left(\frac{\partial^k u^\nu}{\partial (x^i)^k}\right) = \hat{D}_i^k\left(\eta^\nu - \sum_{j=1}^{n} u_j^\nu \xi^j\right) + \sum_{j=1}^{n} \frac{\partial^k u_j^\nu}{\partial (x^i)^k}\xi^j \quad . \tag{2.142}$$

The infinitesimal transformation for the grid spacing h_i of the i th independent variable is

$$\bar{h}_i = h_i + \frac{\delta h_i}{\delta a}\delta a \quad . \tag{2.143}$$

As

$$h_i = \hat{S}_i^+(x^i) - x^i \quad , \tag{2.144}$$

the Lie derivative of the grid spacing is

$$\frac{\delta h_i}{\delta a} = \hat{S}_i^+(\xi^i) - \xi^i \quad . \tag{2.145}$$

From the binomial theorem

$$\bar{h}_i^k = h_i^k + k\, h_i^{k-1}\frac{\delta h_i}{\delta a}\delta a + \ldots \tag{2.146}$$

to first order terms in δa. By taking into account (2.130), (2.133), (2.14), and (2.146), equation (2.129) reduces to

$$\begin{aligned}\bar{u}^\nu(\bar{x}^i, \bar{x}^2, \ldots, \bar{x}^i + \bar{h}_i, \ldots, \bar{x}^n) &= u^\nu(x^i, x^2, \ldots, x^i \ldots, x^n) \\ &+ \sum_{k=1}^{\infty} \frac{h_i^k}{k!}\frac{\partial^k u^\nu}{\partial (x^i)^k} + \delta a\Bigg\{ \eta^\nu + \sum_{k=1}^{\infty} \frac{h_i^k}{k!}\hat{D}_i^k \eta^\nu \\ &+ \frac{\delta h_i}{\delta a}\sum_{k=1}^{\infty} \frac{h_i^{k-1}}{(k-1)!}\frac{\partial^k u^\nu}{\partial (x^i)^k} - \sum_{k=1}^{\infty} \frac{h_i^k}{k!}\hat{D}_i^k \sum_{j=1}^{n} u_j^\nu \xi^j \\ &+ \sum_{j=1}^{n} \xi^j \sum_{k=1}^{\infty} \frac{h_i^k}{k!}\frac{\partial^k u_j^\nu}{\partial (x^i)^k} \Bigg\} \quad ,\end{aligned} \tag{2.147}$$

to first order terms in δa. The summations in this equation can be simplified as seen in the following identities:

$$u^\nu(x^i, x^2, \ldots, x^i + h_i, \ldots, x^n) = u^\nu(x^i, x^2, \ldots, x^i \ldots, x^n) + \sum_{k=1}^{\infty} \frac{h_i^k}{k!}\frac{\partial^k u^\nu}{\partial (x^i)^k} \quad , \tag{2.148}$$

$$\sum_{k=1}^{\infty} \frac{h_i^{k-1}}{(k-1)!} \frac{\partial^k u^\nu}{\partial(x^i)^k} = \sum_{n=0}^{\infty} \frac{h_i^n}{n!} \frac{\partial^n u_i^\nu}{\partial(x^i)^n} = \hat{S}_i^+(u_i^\nu) \quad . \tag{2.149}$$

$$\sum_{k=1}^{\infty} \frac{h_i^k}{k!} \hat{D}_i^k \, \eta^\nu = -\eta^\nu + \hat{S}_i^+(\eta^\nu) \quad . \tag{2.150}$$

$$\sum_{k=1}^{\infty} \frac{h_i^k}{k!} \hat{D}_i^k \sum_{j=1}^{n} u_j^\nu \xi^j = \sum_{j=1}^{n} \left[-u_j^\nu \xi^j + \hat{S}_i^+(u_j^\nu \xi^j) \right] \quad . \tag{2.151}$$

$$\sum_{j=1}^{n} \xi^j \sum_{k=1}^{\infty} \frac{h_i^k}{k!} \frac{\partial^k u_j^\nu}{\partial(x^i)^k} = \sum_{j=1}^{n} \left[-\xi^j u_j^\nu + \xi^j \hat{S}_i^+(u_j^\nu) \right] \quad . \tag{2.152}$$

Substituting (2.145), (2.148), (2.149), (2.150), (2.151), and (2.152) into (2.147) produces

$$\begin{aligned} \bar{u}^\nu(\bar{x}^1, \bar{x}^2, \ldots, \bar{x}^i + \bar{h}_i, \ldots, \bar{x}^n) &= u^\nu(x^1, x^2, \ldots, x^i + h_i, \ldots, x^n) \\ &+ \delta a \Big\{ \eta^\nu + \left[\hat{S}_i^+(\xi^i) - \xi^i \right] \hat{S}_i^+(u_i^\nu) - \eta^\nu + \hat{S}_i^+(\eta^\nu) \\ &+ \sum_{j=1}^{n} \left[-\xi^j u_j^\nu + \xi^j \hat{S}_i^+(u_j^\nu) + \xi^j u_j^\nu - \hat{S}_i^+(u_j^\nu \xi^j) \right] \Big\} \quad . \end{aligned} \tag{2.153}$$

Since

$$\hat{S}_i^+(u_j^\nu \xi^j) = \hat{S}_i^+(u_j^\nu) \hat{S}_i^+(\xi^j) \quad , \tag{2.154}$$

splitting off the $j = i$ term in (2.153) produces the following result for the infinitesimal transformation of the forward grid point value of the ith independent variable:

$$\begin{aligned} \bar{u}^\nu(\bar{x}^1, \bar{x}^2, \ldots, \bar{x}^i + \bar{h}_i, \ldots, \bar{x}^n) &= u^\nu(x^1, x^2, \ldots, x^i + h_i, \ldots, x^n) \\ &+ \delta a \left\{ \hat{S}_i^+(\eta^\nu) - \sum_{\substack{j=1 \\ j \neq i}}^{n} \hat{S}_i^+(u_j^\nu) \left[\hat{S}_i^+(\xi^j) - \xi^j \right] \right\} \quad , \end{aligned} \tag{2.155}$$

which holds for $1 \le i \le n$ and $1 \le \nu \le m$. The curly bracket in (2.155) is the Lie derivative of the forward grid point value, which can be written in the alternative form,

$$R_i^\nu = \frac{\delta u^\nu}{\delta a}(x^1, x^2, \ldots, x^i + h_i, \ldots, x^n) = \hat{S}_i^+(\eta^\nu) - \sum_{\substack{j=1 \\ j \neq i}}^{n} h_i \hat{\Delta}_i^+(\xi^j) \hat{S}_i^+(u_j^\nu) \quad , \tag{2.156}$$

in which the forward difference derivative $\hat{\Delta}_i^+(\xi^j)$ with respect to the ith independent variable is defined by

$$h_i\hat{\Delta}_i^+(\xi^j)=\hat{S}_i^+(\xi^j)-\xi^j \quad . \tag{2.157}$$

A similar derivation to that above shows that the Lie derivative of the backward grid point value of the ith independent variable is

$$L_i^\nu=\frac{\delta u^\nu}{\delta a}(x^1,x^2,\dots,x^i-h_i,\dots,x^n)=\hat{S}_i^-(\eta^\nu)+\sum_{\substack{j=1\\ j\neq i}}^{n}\hat{S}_i^-(u_j^\nu)\left[\xi^j-\hat{S}_i^-(\xi^j)\right] \quad , \tag{2.158}$$

or in terms of the backward difference derivative $\hat{\Delta}_i^-(\xi^j)$ defined by

$$h_i\hat{\Delta}_i^-(\xi^j)=\xi^j-\hat{S}_i^-(\xi^j) \quad , \tag{2.159}$$

we have

$$L_i^\nu=\frac{\delta u^\nu}{\delta a}(x^1,x^2,\dots,x^i-h_i,\dots,x^n)=\hat{S}_i^-(\eta^\nu)+\sum_{\substack{j=1\\ j\neq i}}^{n}h_i\hat{\Delta}_i^-(\xi^j)\hat{S}_i^-(u_j^\nu) \quad . \tag{2.160}$$

With the results contained in (2.145), (2.156), and (2.160) the discretized prolongation of the group generator (2.121) to grid spacings and neighboring grid point values is found to be

$$\hat{U}^{(G)}=\sum_{i=1}^{n}\xi^i\frac{\partial}{\partial x^i}+\sum_{\nu=1}^{m}\eta^\nu\frac{\partial}{\partial u^\nu}+\sum_{i=1}^{n}\left[\hat{S}_i^+(\xi^i)-\xi^i\right]\frac{\partial}{\partial h_i}$$
$$+\sum_{i=1}^{n}\sum_{\nu=1}^{m}R_i^\nu\frac{\partial}{\partial u^\nu(x^i+h_i)}+\sum_{i=1}^{n}\sum_{\nu=1}^{m}L_i^\nu\frac{\partial}{\partial u^\nu(x^i-h_i)} \quad , \tag{2.161}$$

where

$$u^\nu(x^1,x^2,\dots,x^i\pm h_i,\dots,x^n)=u^\nu(x^i\pm h_i) \quad . \tag{2.162}$$

This result for the discretized prolongation holds for uniform grids and is easily extended to the case of nonuniform grids.

2.2 LIE DERIVATIVES OF GRID POINT VALUES WITH MULTIPLE INCREMENTS

Implicit numerical schemes entail grid point values of dependent variables obtained by simultaneously incrementing no less than two independent variables. Extensions of group generators to grid point values with multiple incrementing of independent variables are derived in this section.

We want to find the discretized prolongation of the group generator,

$$\hat{U} = \xi^1 \frac{\partial}{\partial x^1} + \xi^2 \frac{\partial}{\partial x^2} + \eta \frac{\partial}{\partial u} \quad , \tag{2.163}$$

to the grid point values $u(x^1 \pm h_1, x^2 \pm h_2)$ and the grid spacings h_1 and h_2. For the case of uniform grids the grid spacing Lie derivatives are

$$\frac{\delta h_1}{\delta a} = \hat{S}_1^+(\xi^1) - \xi^1 \tag{2.164}$$

or

$$\frac{\delta h_1}{\delta a} = \xi^1 - \hat{S}_1^-(\xi^1) \quad , \tag{2.165}$$

and

$$\frac{\delta h_2}{\delta a} = \hat{S}_2^+(\xi^2) - \xi^2 \quad , \tag{2.166}$$

or

$$\frac{\delta h_2}{\delta a} = \xi^2 - \hat{S}_2^-(\xi^2) \quad , \tag{2.167}$$

in terms of the shift operators,

$$\hat{S}_1^\pm = e^{\pm h_1 \hat{D}_1} \quad , \tag{2.168}$$

$$\hat{S}_2^\pm = e^{\pm h_2 \hat{D}_2} \quad , \tag{2.169}$$

and total derivative operators,

$$\hat{D}_1 = \frac{\partial}{\partial x^1} + u_1 \frac{\partial}{\partial u} + u_{1,1} \frac{\partial}{\partial u_1} + u_{2,1} \frac{\partial}{\partial u_2} + \ldots \tag{2.170}$$

$$\hat{D}_2 = \frac{\partial}{\partial x^2} + u_2 \frac{\partial}{\partial u} + u_{2,1} \frac{\partial}{\partial u_1} + u_{2,2} \frac{\partial}{\partial u_2} + \ldots \quad . \tag{2.171}$$

Here, subscripts are used to denote partial derivatives, that is

$$\frac{\partial^{m+n} u(x^1, x^2)}{\partial (x^1)^m \partial (x^2)^n} = u_{m,n}(x^1, x^2) \quad . \tag{2.172}$$

The grid point value of the dependent variable at the point $\left(x^1+h_1,x^2+h_2\right)$ is given by

$$u\left(x^1+h_1,x^2+h_2\right)=\sum_{m=0}^{\infty}\sum_{n=0}^{\infty}\frac{h_1^m h_2^n}{m!n!}u_{m,n}\left(x^1,x^2\right) \quad . \tag{2.173}$$

Splitting off the $m=0$ and $n=0$ terms yields

$$u\left(x^1+h_1,x^2+h_2\right)=u\left(x^1,x^2\right)+\sum_{m=1}^{\infty}\frac{h_1^m}{m!}u_{m,o}\left(x^1,x^2\right)$$

$$+\sum_{n=1}^{\infty}\frac{h_2^n}{n!}u_{o,n}\left(x^1,x^2\right)+\sum_{m=1}^{\infty}\sum_{n=1}^{\infty}\frac{h_1^m h_2^n}{m!n!}u_{m,n}\left(x^1,x^2\right) \quad . \tag{2.174}$$

The Lie derivative of this grid point value is

$$\frac{\delta u}{\delta a}\left(x^1+h_1,x^2+h_2\right)=\frac{\delta u}{\delta a}+\sum_{m=1}^{\infty}\frac{h_1^m}{m!}\frac{\delta}{\delta a}u_{m,o}$$

$$+\sum_{n=1}^{\infty}\frac{h_2^n}{n!}\frac{\delta}{\delta a}u_{o,n}+\sum_{m=1}^{\infty}\sum_{n=1}^{\infty}\frac{h_1^m h_2^n}{m!n!}\frac{\delta}{\delta a}u_{m,o}$$

$$+\frac{\delta h_1}{\delta a}\left[\sum_{m=0}^{\infty}\frac{h_1^m}{m!}u_{m+1,0}+\sum_{m=0}^{\infty}\sum_{n=1}^{\infty}\frac{h_1^m h_2^n}{m!n!}u_{m+1,n}\right]$$

$$+\frac{\delta h_2}{\delta a}\left[\sum_{n=0}^{\infty}\frac{h_2^n}{n!}u_{0,n+1}+\sum_{m=1}^{\infty}\sum_{n=0}^{\infty}\frac{h_1^m h_2^n}{m!n!}u_{m,n+1}\right] \quad . \tag{2.175}$$

The Lie derivatives of the partial derivatives that appear in (2.175) are

$$\frac{\delta u_{m,o}}{\delta a}=\hat{D}_1^m\left(\frac{\delta u}{\delta a}-u_{1,0}\xi^1-u_{0,1}\xi^2\right)+u_{m+1,o}\xi^1+u_{m,1}\xi^2 \quad , \tag{2.176}$$

$$\frac{\delta u_{o,n}}{\delta a}=\hat{D}_2^n\left(\frac{\delta u}{\delta a}-u_{1,0}\xi^1-u_{0,1}\xi^2\right)+u_{1,n}\xi^1+u_{0,n+1}\xi^2 \quad , \tag{2.177}$$

and

$$\frac{\delta u_{m,n}}{\delta a}=\hat{D}_1^m\hat{D}_2^n\left(\frac{\delta u}{\delta a}-u_{1,0}\xi^1-u_{0,1}\xi^2\right)+u_{m+1,n}\xi^1+u_{m,n+1}\xi^2 \quad . \tag{2.178}$$

Substituting (2.176), (2.177), and (2.178) into (2.175) gives

$$\frac{\delta u}{\delta a}\left(x^1+h_1,x^2+h_2\right)=\frac{\delta u}{\delta a}+\sum_{m=1}^{\infty}\frac{h_1^m}{m!}\hat{D}_1^m\left(\frac{\delta u}{\delta a}\right)$$

$$+\sum_{n=1}^{\infty}\frac{h_2^n}{n!}\hat{D}_2^n\left(\frac{\delta u}{\delta a}\right)+\sum_{m=1}^{\infty}\sum_{n=1}^{\infty}\frac{h_1^m h_2^n}{m!n!}\hat{D}_1^m\hat{D}_2^n\left(\frac{\delta u}{\delta a}\right)$$

$$-\sum_{m=1}^{\infty}\frac{h_1^m}{m!}\hat{D}_1^m\left(u_{1,0}\xi^1+u_{0,1}\xi^2\right)-\sum_{n=1}^{\infty}\frac{h_2^n}{n!}\hat{D}_2^n\left(u_{1,0}\xi^1+u_{0,1}\xi^2\right)$$

$$-\sum_{m=1}^{\infty}\sum_{n=1}^{\infty}\frac{h_1^m h_2^n}{m!n!}\hat{D}_1^m\hat{D}_2^n\left(u_{1,0}\xi^1+u_{0,1}\xi^2\right)$$

$$+\sum_{m=1}^{\infty}\frac{h_1^m}{m!}\left(u_{m+1,0}\xi^1+u_{m,1}\xi^2\right)+\sum_{n=1}^{\infty}\frac{h_2^n}{n!}\left(u_{1,n}\xi^1+u_{0,n+1}\xi^2\right)$$

$$+\sum_{m=1}^{\infty}\sum_{n=1}^{\infty}\frac{h_1^m h_2^n}{m!n!}\left(u_{m+1,n}\xi^1+u_{m,n+1}\xi^2\right)$$

$$+\frac{\delta h_1}{\delta a}\left[\sum_{m=0}^{\infty}\frac{h_1^m}{m!}u_{m+1,0}+\sum_{m=0}^{\infty}\sum_{n=1}^{\infty}\frac{h_1^m h_2^n}{m!n!}u_{m+1,n}\right]$$

$$+\frac{\delta h_2}{\delta a}\left[\sum_{n=0}^{\infty}\frac{h_2^n}{n!}u_{0,n+1}+\sum_{m=1}^{\infty}\sum_{n=0}^{\infty}\frac{h_1^m h_2^n}{m!n!}u_{m,n+1}\right]=0 \quad . \tag{2.179}$$

The first four terms on the right hand side of (2.179) are

$$\hat{S}_2^+\hat{S}_1^+(\eta) \quad .$$

The fifth, sixth, and seventh terms on the right hand side of (2.179) are

$$u_{1,0}\xi^1+u_{0,1}\xi^2-\hat{S}_2^+\hat{S}_1^+\left(u_{1,0}\xi^1+u_{0,1}\xi^2\right) \quad .$$

The eighth, ninth, and tenth terms on the right hand side of (2.179) are

$$-u_{1,0}\xi^1-u_{0,1}\xi^2+\xi^1 u_{1,0}\left(x^1+h_1,x^2+h_2\right)+\xi^2 u_{0,1}\left(x^1+h_1,x^2+h_2\right) \quad .$$

The bracket in the eleventh term on the right hand side of (2.179) is

$$u_{1,0}\left(x^1+h_1,x^2+h_2\right)=\sum_{m=0}^{\infty}\sum_{n=0}^{\infty}\frac{h_1^m h_2^n}{m!n!}u_{m+1,n} \quad , \tag{2.180}$$

and the bracket in the twelfth term on the right hand side of (2.179)

$$u_{0,1}\left(x^1+h_1,x^2+h_2\right)=\sum_{m=0}^{\infty}\sum_{n=0}^{\infty}\frac{h_1^m h_2^n}{m!n!}u_{m,n+1} \quad . \tag{2.181}$$

Accordingly, equation (2.179) becomes

$$\frac{\delta u}{\delta a}\left(x^1+h_1,x^2+h_2\right)=\hat{S}_2^+\hat{S}_1^+(\eta)-\hat{S}_2^+\hat{S}_1^+\left(u_{1,0}\xi^1+u_{0,1}\xi^2\right)$$

$$+\xi^1 u_{1,0}\left(x^1+h_1,x^2+h_2\right)+\xi^2 u_{0,1}\left(x^1+h_1,x^2+h_2\right)$$

$$+\left[\hat{S}_1^+\left(\xi^1\right)-\xi^1\right]u_{1,0}\left(x^1+h_1,x^2+h_2\right)$$

$$+\left[\hat{S}_2^+\left(\xi^2\right)-\xi^2\right]u_{0,1}\left(x^1+h_1,x^2+h_2\right) \quad , \tag{2.182}$$

which simplifies to

$$\frac{\delta u}{\delta a}\left(x^1+h_1,x^2+h_2\right)=\hat{S}_2^+\hat{S}_1^+(\eta)-\hat{S}_2^+\hat{S}_1^+\left(u_{1,0}\xi^1+u_{0,1}\xi^2\right)$$

$$+\hat{S}_1^+\left(\xi^1\right)u_{1,0}\left(x^1+h_1,x^2+h_2\right)$$

$$+\hat{S}_2^+\left(\xi^2\right)u_{0,1}\left(x^1+h_1,x^2+h_2\right) \quad . \tag{2.183}$$

By a similar calculation the Lie derivative of the grid point value $u\left(x^1-h_1,x^2+h_2\right)$ is

$$\frac{\delta u}{\delta a}\left(x^1-h_1,x^2+h_2\right)=\hat{S}_2^+\hat{S}_1^-(\eta)-\hat{S}_2^+\hat{S}_1^-\left(u_{1,0}\xi^1+u_{0,1}\xi^2\right)$$

$$+\hat{S}_1^-\left(\xi^1\right)u_{1,0}\left(x^1-h_1,x^2+h_2\right)$$

$$+\hat{S}_2^+\left(\xi^2\right)u_{0,1}\left(x^1-h_1,x^2+h_2\right) \quad . \tag{2.184}$$

We also find that

$$\frac{\delta u}{\delta a}\left(x^1+h_1,x^2-h_2\right)=\hat{S}_2^-\hat{S}_1^+(\eta)-\hat{S}_2^-\hat{S}_1^+\left(u_{1,0}\xi^1+u_{0,1}\xi^2\right)$$

$$+\hat{S}_1^+\left(\xi^1\right)u_{1,0}\left(x^1+h_1,x^2-h_2\right)$$

$$+\hat{S}_2^-\left(\xi^2\right)u_{0,1}\left(x^1+h_1,x^2-h_2\right) \quad , \tag{2.185}$$

and

$$\frac{\delta u}{\delta a}\left(x^1-h_1,x^2-h_2\right)=\hat{S}_2^-\hat{S}_1^-(\eta)-\hat{S}_2^-\hat{S}_1^-\left(u_{1,0}\xi^1+u_{0,1}\xi^2\right)$$

$$+\hat{S}_1^-\left(\xi^1\right)u_{1,0}\left(x^1-h_1,x^2-h_2\right)$$

$$+\hat{S}_2^-(\xi^2)u_{0,1}(x^1-h_1, x^2-h_2) \quad , \tag{2.186}$$

for the indicated grid point values of the dependent variable.

3. INVARIANT DIFFERENCE OPERATORS

Invariant difference schemes for second order inhomogeneous linear ordinary differential equations and for linear systems of first and second order inhomogeneous ordinary differential equations can be constructed by using the concept of invariant difference operators. An invariant difference operator is a difference operator that inherits symmetry properties of the system of differential equations being discretized. To construct such operators requires a knowledge of how group generators are prolonged to grid point values of dependent variables.

3.1 CONSTRUCTION OF INVARIANT DIFFERENCE OPERATORS

3.1.1 INVARIANT DISCRETIZATION OF SECOND ORDER ORDINARY DIFFERENTIAL EQUATIONS

The methods for constructing invariant difference operators will be developed first for the diffusion equation,

$$\phi''(x) - \alpha^2\phi(x) + \frac{S(x)}{D} = 0 \quad , \tag{3.1}$$

for $0 \le x \le a$. Let

$$\hat{U} = \eta(x)\frac{\partial}{\partial\phi} \tag{3.2}$$

be the generator of a group of point transformations admitted by the diffusion equation. The second extension of this generator is

$$\hat{U}^{(2)} = \eta(x)\frac{\partial}{\partial\phi} + \eta'(x)\frac{\partial}{\partial\phi'} + \eta''(x)\frac{\partial}{\partial\phi''} \quad . \tag{3.3}$$

By operating on (3.1) with the second extension we see that the Lie derivative

$$\frac{\delta\phi}{\delta a}(x) = \eta(x) \tag{3.4}$$

is a solution of the homogeneous diffusion equation

$$\eta''(x) - \alpha^2\eta(x) = 0 \quad . \tag{3.5}$$

Also, from (2.39) and (2.40) the Lie derivatives of neighboring grid point values of the dependent variable are

$$\frac{\delta\phi}{\delta a}(x+h)=\hat{S}^{+}(\eta)=\eta(x+h) \quad , \tag{3.6}$$

and

$$\frac{\delta\phi}{\delta a}(x-h)=\hat{S}^{-}(\eta)=\eta(x-h) \quad . \tag{3.7}$$

Accordingly, the discretized prolongation of the group generator (3.2) is

$$\hat{U}^{(G)}=\eta(x)\frac{\partial}{\partial\phi(x)}+\eta(x+h)\frac{\partial}{\partial\phi(x+h)}+\eta(x-h)\frac{\partial}{\partial\phi(x-h)} \quad . \tag{3.8}$$

Let the discretized diffusion equation be

$$\hat{\Omega}\phi(x)+Q(x)=0 \quad , \tag{3.9}$$

in which the difference operator $\hat{\Omega}$ is to be determined such that (3.9) admits the group of point transformations that is generated by the discretized prolongation (3.8). The solution of the diffusion equation (3.1) can be written as the sum of the general solution of the homogeneous equation and a particular integral, that is,

$$\phi(x)=\phi_H(x)+\phi_P(x) \quad , \tag{3.10}$$

where $\phi_P(x)$ is the particular integral. Substituting (3.10) into the difference equation (3.9) gives

$$\hat{\Omega}\phi_H(x)+\hat{\Omega}\phi_P(x)+Q(x)=0 \quad . \tag{3.11}$$

The difference operator $\hat{\Omega}$ is determined such that the difference equation,

$$\hat{\Omega}\phi_H(x)=0 \quad , \tag{3.12}$$

is invariant under the extended group generated by (3.8). When this is done, the difference operator $\hat{\Omega}$ is said to be an invariant difference operator. Then the generalized discrete source term in the discretized diffusion equation takes the form,

$$Q(x)=-\hat{\Omega}\phi_P(x) \quad , \tag{3.13}$$

which is not necessarily the same as evaluating the source term in the diffusion equation itself at a single grid point, as will be seen below.

Invariant difference operators are not unique. A possible form is

$$\hat{\Omega}=E\left(\hat{S}^{+}+\hat{S}^{-}-2\right)-\alpha^2 \tag{3.14}$$

in terms of the shift operators, $\hat{S}^{\pm}$. The quantity E is found such that

$$\hat{\Omega}\phi(x) = E\left[\hat{S}^{+}(\phi) + \hat{S}^{-}(\phi) - 2\phi\right] - \alpha^2\phi$$

$$= E[\phi(x+h) + \phi(x-h) - 2\phi(x)] - \alpha^2\phi(x) = 0 \qquad (3.15)$$

is invariant under the group generated by (3.8). For this to be true it is necessary that

$$\hat{U}^{(G)}\left[\hat{\Omega}\phi(x)\right] = 0 \quad , \qquad (\text{mod } \hat{\Omega}\phi(x) = 0) \quad . \qquad (3.16)$$

This reduces to

$$E[\eta(x+h) + \eta(x-h) - 2\eta(x)] - \alpha^2\eta(x) = 0 \quad . \qquad (3.17)$$

If we take as a solution of (3.5)

$$\eta(x) = \cosh(\alpha x) \quad , \qquad (3.18)$$

then from (3.17) we obtain

$$E = \frac{\alpha^2}{4\sinh^2\left(\frac{\alpha h}{2}\right)} \quad , \qquad (3.19)$$

and the invariant difference operator (3.14) is

$$\hat{\Omega} = \frac{\alpha^2\left(\hat{S}^{+} + \hat{S}^{-} - 2\right)}{4\sinh^2\left(\frac{\alpha h}{2}\right)} - \alpha^2 \quad . \qquad (3.20)$$

Combining (3.20) and (3.13) produces the generalized discrete source term for the discretized diffusion equation, namely,

$$Q(x) = \alpha^2\phi_p(x) - \frac{\alpha^2\left[\phi_p(x+h) + \phi_p(x-h) - 2\phi_p(x)\right]}{4\sinh^2\left(\frac{\alpha h}{2}\right)} \quad . \qquad (3.21)$$

With the invariant difference operator (3.20) and the discretized source term (3.21) the invariant discretized diffusion equation is

$$\frac{\alpha^2\left[\phi(x+h) + \phi\,(x-h) - 2\phi(x)\right]}{4\sinh^2\left(\frac{\alpha h}{2}\right)} - \alpha^2\phi(x) + Q(x) = 0 \quad . \qquad (3.22)$$

Examples of the discretized source follow. If the source term in the diffusion equation is spatially uniform, a particular integral is

$$\phi_p(x) = \frac{S}{\alpha^2 D} \quad , \tag{3.23}$$

and the discretized source (3.21) becomes

$$Q(x) = \frac{S}{D} \quad . \tag{3.24}$$

Hence, for a spatially uniform source term the invariant discretized diffusion equation is

$$\frac{\alpha^2[\phi(x+h)+\phi(x-h)-2\phi(x)]}{4\sinh^2\left(\frac{\alpha h}{2}\right)} - \alpha^2\phi(x) + \frac{S}{D} = 0 \quad . \tag{3.25}$$

In the small mesh limit,

$$\sinh\left(\frac{\alpha h}{2}\right) = \frac{\alpha h}{2} + \ldots \tag{3.26}$$

and the invariant difference equation (3.9) becomes

$$\frac{1}{h^2}[\phi(x+h)+\phi(x-h)-2\phi(x)] - \alpha^2\phi(x) + \frac{S}{D} = 0 \quad , \tag{3.27}$$

which is recognized as the difference equation obtained for the diffusion equation (3.1) when a standard three-point central difference formula is used to approximate the second order derivative. The invariant difference equation (3.25) differs from the noninvariant difference equation (3.27) in that it is exact, while (3.27) is not exact. The invariant difference equation (3.25) is exact because its exact solutions for various boundary conditions agree with the exact solution of the diffusion equation for the same boundary conditions. Also, the invariant difference equation (3.25) is able to produce exact solutions for any grid spacing, but solutions obtained from the non-invariant difference equation become less precise as the grid spacing is increased.

If the source term in the diffusion equation is parabolic, that is,

$$S(x) = S\left[1 - \left(\frac{x}{a}\right)^2\right] \quad , \tag{3.28}$$

a particular integral is

$$\phi_p(x) = \frac{S}{\alpha^2 D}\left[1 - \frac{2}{(\alpha a)^2} - \left(\frac{x}{a}\right)^2\right] \quad . \tag{3.29}$$

The discretized source for the parabolic source from (3.21) is

$$Q(x)=\frac{S}{D}\left\{1-\frac{x^2}{a^2}-\frac{2}{(\alpha a)^2}\left[1-\frac{(\alpha h)^2}{4\sinh^2\left(\frac{\alpha h}{2}\right)}\right]\right\} \quad , \tag{3.30}$$

and the corresponding invariant difference equation is

$$\frac{\alpha^2[\phi(x+h)+\phi(x-h)-2\phi(x)]}{4\sinh^2\left(\frac{\alpha h}{2}\right)}-\alpha^2\phi(x)$$

$$+\frac{S}{D}\left\{1-\frac{x^2}{a^2}-\frac{2}{(\alpha a)^2}\left[1-\frac{(\alpha h)^2}{4\sinh^2\left(\frac{\alpha h}{2}\right)}\right]\right\}=0 \quad . \tag{3.31}$$

The small mesh limit of this invariant difference equation yields the standard difference equation,

$$\frac{1}{h^2}[\phi(x+h)+\phi(x-h)-2\phi(x)]-\alpha^2\phi(x)+\frac{S}{D}\left[1-\left(\frac{x}{a}\right)^2\right]=0 \quad , \tag{3.32}$$

which is not invariant or exact. The invariant difference equation (3.31) is exact, and its exact solutions coincide with the exact solutions of the diffusion equation for various boundary conditions and for arbitrary grid spacing.

An invariant difference equation to discretize the diffusion equation in spherical geometry, namely,

$$\phi''(r)+\frac{2}{r}\phi'(r)-\alpha^2\phi(r)+\frac{S(r)}{D}=0 \quad , \tag{3.33}$$

can be derived by a method similar to that used to obtain the invariant difference equation (3.25) in slab geometry. The diffusion equation is invariant under the group generated by

$$\hat{U}=\eta(r)\frac{\partial}{\partial\phi(r)} \quad , \tag{3.34}$$

in which the Lie derivative of the dependent variable, namely,

$$\frac{\delta\phi(r)}{\delta a}=\eta(r) \tag{3.35}$$

is a solution of the homogeneous diffusion equation,

$$\eta''(r)+\frac{2}{r}\eta'(r)-\alpha^2\eta(r)=0 \quad . \tag{3.36}$$

The discretized prolongation of the group generator is

$$\hat{U}^{(G)} = \eta(r)\frac{\partial}{\partial\phi(r)} + \eta(r+h)\frac{\partial}{\partial\phi(r+h)} + \eta(r-h)\frac{\partial}{\partial\phi(r-h)} \tag{3.37}$$

to the neighboring grid point values $\phi(r \pm h)$. The invariant difference equation is

$$\hat{\Omega}\phi(r) + Q(r) = 0 \quad , \tag{3.38}$$

where the invariant difference operator $\hat{\Omega}$ is determined to satisfy

$$\hat{U}^{(G)}\left[\hat{\Omega}\phi(r)\right] = 0 \quad , \quad \left(\text{mod}\ \hat{\Omega}\phi(r) = 0\right) \quad , \tag{3.39}$$

and the discretized source term is

$$Q(r) = -\hat{\Omega}\phi_p(r) \tag{3.40}$$

with a particular integral $\phi_p(r)$ of the diffusion equation (3.33) for a specified source term. The invariant difference operator $\hat{\Omega}$ is not unique and can be taken in the form,

$$\hat{\Omega} = E\left(\hat{S}^{+} + \hat{S}^{-} - 2\right) + F\left(\hat{S}^{+} - \hat{S}^{-}\right) - \alpha^2 \quad , \tag{3.41}$$

where the shift operators are $\hat{S}^{\pm}$, and the quantities E and F are determined so that (3.39) is satisfied. This condition becomes

$$E[\eta(r+h) + \eta(r-h) - 2\eta(r)] + F[\eta(r+h) - \eta(r-h)] - \alpha^2\eta(r) = 0 \quad . \tag{3.42}$$

This equation has the solution

$$\frac{\alpha^2 w\eta(r)}{\eta(r+h) + \eta(r-h) - 2\eta(r)} \quad , \tag{3.43}$$

and

$$F = \frac{\alpha^2(1-w)\eta(r)}{\eta(r+h) - \eta(r-h)} \quad , \tag{3.44}$$

where w is a weight factor. By taking the small mesh limit, it is found that

$$w = \frac{1}{3} \quad , \tag{3.45}$$

so that

$$\lim_{h\to 0}\hat{\Omega} = \frac{1}{h^2}\left(\hat{S}^{+} + \hat{S}^{-} - 2\right) + \frac{1}{rh}\left(\hat{S}^{+} - \hat{S}^{-}\right) - \alpha^2 \quad . \tag{3.46}$$

That is, when the weight factor is a third, the invariant difference operator reduces in the small mesh limit to the non-invariant difference operator formed by approximating the second order derivative with a three-point central difference formula and the first order derivative with a two-point central difference formula. Since a solution of (3.36) is

$$\eta(r)=\frac{\sinh(\alpha r)}{r} \quad , \tag{3.47}$$

the invariant difference equation (3.38) becomes

$$E[\phi(r+h)+\phi(r-h)-2\phi(r)]+F[\phi(r+h)-\phi(r-h)]-\alpha^2\phi(r)+Q(r)=0 \quad , \tag{3.48}$$

where the discretized source is given by (3.40), and

$$E=\frac{1}{3}\frac{\alpha^2\left(r^2-h^2\right)\sinh\left(\alpha r\right)}{\left\{r(r-h)\sinh\left[\alpha\left(r+h\right)\right]+r\left(r+h\right)\sinh\left[\alpha\left(r-h\right)\right]-\left(r^2-h^2\right)\sinh(\alpha r)\right\}} \quad , \tag{3.49}$$

and

$$F=\frac{2}{3}\frac{\alpha^2\left(r^2-h^2\right)\sinh\left(\alpha r\right)}{\left\{(r-h)\sinh\left[\alpha\left(r+h\right)\right]-(r+h)\sinh\left[\alpha\left(r-h\right)\right]\right\}} \quad . \tag{3.50}$$

The standard noninvariant difference equation for the diffusion equation (3.33) is

$$\frac{1}{h^2}[\phi(r+h)+\phi(r-h)-2\phi(r)]+\frac{1}{rh}[\phi(r+h)-\phi(r-h)]-\alpha^2\phi(r)+\frac{S(r)}{D}=0 \quad . \tag{3.51}$$

The invariant difference equation (3.48) is exact and holds for arbitrary grid spacings h. The non-invariant difference equation (3.51) is not exact.

For the case of a spatially uniform source a particular integral of the diffusion equation (3.33) is

$$\phi_p(r)=\frac{S}{\alpha^2 D} \quad , \tag{3.52}$$

and the corresponding discrete source in the invariant difference equation (3.48) is

$$Q(r)=\frac{S}{D} \quad . \tag{3.53}$$

If the source term is parabolic, that is, if

$$S(r)=S\left[1-\left(\frac{r}{a}\right)^2\right] \tag{3.54}$$

for $o\le r\le a$, then a particular integral of the diffusion equation is

$$\phi_P(r) = \frac{S}{\alpha^2 D}\left[1 - \frac{6}{(\alpha a)^2} - \left(\frac{r}{a}\right)^2\right] \quad , \tag{3.55}$$

and the discretized source for the invariant difference equation (3.48) is found to be

$$\begin{aligned} Q(r) &= -\hat{\Omega}\phi_P(r) \\ &= \frac{S}{D}\left[1 - \left(\frac{r}{a}\right)^2 - \frac{6}{(\alpha a)^2}\right] + \frac{SE}{(\alpha a)^2 D}\left(\hat{S}^+ - \hat{S}^- - 2\right)\left(r^2\right) \\ &+ \frac{SF}{(\alpha a)^2 D}\left(\hat{S}^+ - \hat{S}^-\right)\left(r^2\right) \quad , \end{aligned} \tag{3.56}$$

or

$$Q(r) = \frac{S}{D}\left[1 - \left(\frac{r}{a}\right)^2 + \frac{1}{(\alpha a)^2}\left(2h^2 E + 4rhF - 6\right)\right] \quad , \tag{3.57}$$

where E and F are given by (3.49) and (3.50), respectively. The small mesh limit of (3.57) is

$$\lim_{h \to 0} Q(r) = \frac{S}{D}\left[1 - \left(\frac{r}{a}\right)^2\right] \quad , \tag{3.58}$$

as occurs in the non-invariant standard difference equation (3.51) for the parabolic source.

3.1.2 INVARIANT DISCRETIZATION OF SYSTEMS OF FIRST ORDER ORDINARY DIFFERENTIAL EQUATIONS

The first order system equivalent of the diffusion equation (3.1), namely,

$$\frac{dJ}{dx}(x) + \sigma_a \phi(x) - S(x) = 0 \quad , \tag{3.59}$$

and

$$\frac{d\phi}{dx}(x) + \frac{1}{D}J(x) = 0 \quad , \tag{3.60}$$

will be used to illustrate the construction of invariant difference operators for linear first order systems. The discretized form of the system is first written as

$$\hat{\Omega}_1 J(x) + \hat{\Omega}_2 \phi(x) - Q_1(x) = 0 \quad , \tag{3.61}$$

and

$$\hat{\Omega}_3 \phi(x) + \hat{\Omega}_4 J(x) + Q_2(x) = 0 \quad . \tag{3.62}$$

The four difference operators, $\hat{\Omega}_1$, $\hat{\Omega}_2$, $\hat{\Omega}_3$ and $\hat{\Omega}_4$, in these last two equations and the discrete sources Q_1 and Q_2 are to be found so that the resulting difference scheme will be invariant under a group of point transformation admitted by the differential equations. The generator of this group can be taken in the form,

$$\hat{U} = \eta_1(x)\frac{\partial}{\partial\phi(x)} + \eta_2(x)\frac{\partial}{\partial J(x)} \quad . \tag{3.63}$$

The extension of this group to first order derivatives is

$$\hat{U}^{(1)} = \eta_1(x)\frac{\partial}{\partial\phi} + \eta_2(x)\frac{\partial}{\partial J} + \eta_1'(x)\frac{\partial}{\partial\phi'} + \eta_2'(x)\frac{\partial}{\partial J'} \quad , \tag{3.64}$$

and the extension to neighboring grid point values of the dependent variables is

$$\hat{U}^{(G)} = \eta_1(x)\frac{\partial}{\partial\phi(x)} + \eta_2(x)\frac{\partial}{\partial J(x)} + \eta_1(x+h)\frac{\partial}{\partial\phi(x+h)}$$

$$+\eta_2(x+h)\frac{\partial}{\partial J(x+h)} + \eta_1(x-h)\frac{\partial}{\partial\phi(x-h)} + \eta_2(x-h)\frac{\partial}{\partial J(x-h)} \quad . \tag{3.65}$$

Operating on the system (3.59) and (3.60) with the first extension of the group generator shows that the Lie derivatives of the two dependent variables, $\eta_1(x)$ and $\eta_2(x)$, are solutions of the homogeneous system,

$$\eta_2'(x) + \sigma_a\eta_1(x) = 0 \quad , \tag{3.66}$$

and

$$\eta_1'(x) + \frac{1}{D}\eta_2(x) = 0 \quad . \tag{3.67}$$

With $\alpha^2 = \sigma_a / D$ a solution of this system is

$$\eta_1(x) = \cosh(\alpha x) \quad , \tag{3.68}$$

and

$$-\eta_2(x) = \alpha D\sinh(\alpha x) \quad . \tag{3.69}$$

This group will be used to determine an invariant form of the difference equations (3.61) and (3.62).

The general solution of the system (3.59) and (3.60) is the sum of the general solution of the homegeneous system and a particular integral, that is,

$$\phi(x) = \phi_H(x) + \phi_P(x) \quad , \tag{3.70}$$

and

$$J(x) = J_H(x) + J_P(x) \quad , \tag{3.71}$$

where the particular integral is denoted by the subscript P. Substituting (3.70) and (3.71) into the difference equations (3.61) and (3.62) gives

$$\hat{\Omega}_1 J_H(x) + \hat{\Omega}_1 J_P(x) + \hat{\Omega}_2 \phi_H(x) + \hat{\Omega}_2 \phi_P(x) - Q_1(x) = 0 \quad , \tag{3.72}$$

and

$$\hat{\Omega}_3 \phi_H(x) + \hat{\Omega}_3 \phi_P(x) + \hat{\Omega}_4 J_H(x) + \hat{\Omega}_4 J_P(x) + Q_2(x) = 0 \quad . \tag{3.73}$$

The difference opérators are determined so that

$$\hat{\Omega}_1 J_H(x) + \hat{\Omega}_2 \phi_H(x) = 0 \quad , \tag{3.74}$$

and

$$\hat{\Omega}_3 \phi_H(x) + \hat{\Omega}_4 J_H(x) = 0 \quad , \tag{3.75}$$

are invariant under the discretized prolongation (3.65) to grid point values. Where this is done, the generalized discretized sources are given by

$$Q_1(x) = \hat{\Omega}_1 J_P(x) + \hat{\Omega}_2 \phi_P(x) \tag{3.76}$$

and

$$Q_2(x) = -\left[\hat{\Omega}_3 \phi_P(x) + \hat{\Omega}_4 J_P(x)\right] \quad . \tag{3.77}$$

The generalized discretized source $Q_2(x)$ appears in the second difference equation of the set (3.61) - (3.62), even though there is no source in the second differential equation of the system (3.59) - (3.60), in order to be able to construct invariant difference equations when the source in the differential system is spatially dependent.

The difference operators in the difference equations are not unique. The following operators will be developed:

$$\hat{\Omega}_1 = A\left(\hat{S}^+ - \hat{S}^-\right) \quad , \tag{3.78}$$

$$\hat{\Omega}_2 = \sigma_a \quad , \tag{3.79}$$

$$\hat{\Omega}_3 = B\left(\hat{S}^+ - \hat{S}^-\right) \quad , \tag{3.80}$$

$$\hat{\Omega}_4 = \frac{1}{D} \quad , \tag{3.81}$$

where the quantities A and B are found so that the difference equations (3.74) and (3.75) admit the discretized prolongation (3.65). With these four operators, the difference equation (3.74) and (3.75) become

$$A[J(x+h)-J(x-h)]+\sigma_a\phi(x)=0 \quad , \tag{3.82}$$

and

$$B[\phi(x+h)-\phi(x-h)]+\frac{J(x)}{D}=0 \quad . \tag{3.83}$$

By operating on (3.82) and (3.83) with the discretized prolongation (3.65) and solving the results for the quantities A and B, it is found that

$$A=\frac{-\sigma_a\eta_1(x)}{\eta_2(x+h)-\eta_2(x-h)} \tag{3.84}$$

and

$$B=\frac{-\eta_2(x)}{D[\eta_1(x+h)-\eta_1(x-h)]} \quad . \tag{3.85}$$

With the Lie derivatives in (3.68) and (3.69), these last two equations reduce to

$$A=\frac{\alpha}{2\sinh(\alpha h)}=B \quad . \tag{3.86}$$

and the difference operators $\hat{\Omega}_1$ and $\hat{\Omega}_3$ become

$$\hat{\Omega}_1=\hat{\Omega}_3=\frac{\alpha\left(\hat{S}^+-\hat{S}^-\right)}{2\sinh(\alpha h)} \quad . \tag{3.87}$$

Consequently, an invariant form of the difference equations (3.61) and (3.62) is given by

$$\frac{\alpha[J(x+h)-J(x-h)]}{2\sinh(\alpha h)}+\sigma_a\phi(x)-Q_1(x)=0 \quad , \tag{3.88}$$

and

$$\frac{\alpha[\phi(x+h)-\phi(x-h)]}{2\sinh(\alpha h)}+\frac{J(x)}{D}+Q_2(x)=0 \quad , \tag{3.89}$$

where the discretized sources are (3.76) and (3.77), respectively. The small grid spacing limit of (3.88) and (3.89) recovers standard difference equations constructed with two-point central difference approximations for the first order derivatives. That is, in the limit as $h \to 0$, equations (3.88) and (3.89) become

$$\frac{1}{2h}[J(x+h)-J(x-h)]+\sigma_a\phi(x)-S(x)=0 \quad , \tag{3.90}$$

and

$$\frac{1}{2h}[\phi(x+h)-\phi(x-h)]+\frac{J(x)}{D}=0 \quad . \tag{3.91}$$

For the case of a spatially uniform source, a particular integral of the differential system (3.59) and (3.60) is

$$\phi_p(x)=\frac{S}{\sigma_a} \quad , \tag{3.92}$$

and

$$J_p(x)=0 \quad . \tag{3.93}$$

The corresponding discretized sources are

$$Q_1(x)=S \quad , \tag{3.94}$$

and

$$Q_2(x)=0 \quad , \tag{3.95}$$

so that for this case the invariant difference equations are

$$\frac{\alpha[J(x+h)-J(x-h)]}{2\sinh(\alpha h)}+\sigma_a\phi(x)-S=0 \quad , \tag{3.96}$$

and

$$\frac{\alpha[\phi(x+h)-\phi(x-h)]}{2\sinh(\alpha h)}+\frac{J(x)}{D}=0 \quad . \tag{3.97}$$

These difference equations are exact because their exact solutions coincide with the exact solutions of the differential equations (3.59) and (3.60). By building a symmetry property of the differential equations into the discretized formulation, the resulting invariant difference equations are also found to be exact.

For the case of a parabolic source distribution for $0 \le x \le a$, namely,

$$S(x)=S\left[1-\left(\frac{x}{a}\right)^2\right] \quad , \tag{3.98}$$

a particular integral of the differential system (3.59) and (3.60) is

$$\phi_P(x)=\frac{S}{\sigma_a}\left[1-\frac{2}{(\alpha a)^2}-\left(\frac{x}{a}\right)^2\right] \quad , \tag{3.99}$$

and

$$J_p(x)=\frac{2xS}{(\alpha a)^2} \quad . \tag{3.100}$$

The discretized sources for the parabolic source are

$$Q_1(x)=S\left\{1-\left(\frac{x}{a}\right)^2+\frac{2}{(\alpha a)^2}\left[\frac{\alpha h}{\sinh(\alpha h)}-1\right]\right\} \quad , \tag{3.101}$$

and

$$Q_2(x)=\frac{2xS}{D(\alpha a)^2}\left[\frac{\alpha h}{\sinh(\alpha h)}-1\right] \quad . \tag{3.102}$$

The invariant difference equations (3.88) and (3.89) become for this case

$$\frac{\alpha[J(x+h)-J(x-h)]}{2\sinh(\alpha h)}+\sigma_a\phi(x)-S\left\{1-\left(\frac{x}{a}\right)^2+\frac{2}{(\alpha a)^2}\left[\frac{\alpha h}{\sinh(\alpha h)}-1\right]\right\}=0 \quad , \tag{3.103}$$

and

$$\frac{\alpha[\phi(x+h)-\phi(x-h)]}{2\sinh(\alpha h)}+\frac{J(x)}{D}+\frac{2xS}{D(\alpha a)^2}\left[\frac{\alpha h}{\sinh(\alpha h)}-1\right]=0 \quad . \tag{3.104}$$

Again by building in a symmetry property of the differential equations, exact invariant difference equations are obtained.

The invariant difference equations (3.88) and (3.89) are not unique. They were constructed in terms of shift operators such that the small grid spacing limit led to two-point central difference formulae for first order derivatives. It is also possible to construct invariant difference equations in terms of shift operators whose small grid spacing limit leads to two-point forward difference formula approximations for first order derivatives. Alternative forms for the operators $\hat{\Omega}_1$, and $\hat{\Omega}_3$ are

$$\hat{\Omega}_1=E\left(\hat{S}^+-1\right) \quad , \tag{3.105}$$

and

$$\hat{\Omega}_3=F\left(\hat{S}^+-1\right) \quad , \tag{3.106}$$

in which the quantities E and F are determined so that

$$E\left(\hat{S}^+-1\right)J(x)+\sigma_a\phi(x)=0 \tag{3.107}$$

and

$$F\left(\hat{S}^{+}-1\right)\phi(x)+\frac{J(x)}{D}=0 \qquad (3.108)$$

admit the group of point ransformations generated by the discretized prolongation (3.65). It is found that

$$E=\frac{-\sigma_a\eta_1(x)}{\eta_2(x+h)-\eta_2(x)} \quad , \qquad (3.109)$$

and

$$F=\frac{-\eta_2(x)}{D[\eta_1(x+h)-\eta_1(x)]} \quad . \qquad (3.110)$$

With the Lie derivatives (3.68) and (3.69) these last two equations become

$$E=\frac{\alpha\cosh(\alpha x)}{2\cosh\left[\alpha\left(x+\frac{h}{2}\right)\right]\sinh\left(\frac{\alpha h}{2}\right)} \quad , \qquad (3.111)$$

and

$$F=\frac{\alpha\sinh(\alpha x)}{2\sinh\left[\alpha\left(x+\frac{h}{2}\right)\right]\sinh\left(\frac{\alpha h}{2}\right)} \quad . \qquad (3.112)$$

For the case of a spatially uniform source an alternative form for the invariant difference equations (3.88) and (3.89) is given by

$$\frac{\alpha\cosh(\alpha x)[J(x+h)-J(x)]}{2\cosh\left[\alpha\left(x+\frac{h}{2}\right)\right]\sinh\left(\frac{\alpha h}{2}\right)}+\sigma_a\phi(x)-S=0 \quad , \qquad (3.113)$$

and

$$\frac{\alpha\sinh(\alpha x)[\phi(x+h)-\phi(x)]}{2\sinh\left[\alpha\left(x+\frac{h}{2}\right)\right]\sinh\left(\frac{\alpha h}{2}\right)}+\frac{J(x)}{D}=0 \quad . \qquad (3.114)$$

This set of difference equations is exact as is the case with the sets (3.96) and (3.97) and (3.103) and (3.104). The small grid spacing limit of (3.113) and (3.114) is

$$\frac{1}{h}[J(x+h)-J(x)]+\sigma_a\phi(x)-S=0 \quad , \qquad (3.115)$$

and

$$\frac{1}{h}[\phi(x+h)-\phi(x)]+\frac{J(x)}{D}=0 \quad , \tag{3.116}$$

which corresponds to a standard difference approximation in which the first order derivatives are approximated by two-point forward difference formulae. However, the set of difference equations (3.115) and (3.116) is not exact as the invariant set (3.113) and (3.114) is.

3.1.3 INVARIANT DISCRETIZATION OF SYSTEMS OF SECOND ORDER ORDINARY DIFFERENTIAL EQUATIONS

In this section an invariant discrete simulation of the two-group diffusion equations,

$$\phi_1''(x)-\alpha_1^2\phi_1(x)+\frac{S_1(x)}{D_1}=0 \quad , \tag{3.117}$$

and

$$\phi_2''(x)-\alpha_2^2\phi_2(x)+\frac{\sigma_S(1\rightarrow 2)\phi_1(x)+S_2(x)}{D_2}=0 \quad , \tag{3.118}$$

will be constructed. This simulation will be taken in the form,

$$\hat{\Omega}_{11}\phi_1(x)+Q_1(x)=0 \quad , \tag{3.119}$$

and

$$\hat{\Omega}_{22}\phi_2(x)+\hat{\Omega}_{21}\phi_1(x)+Q_2(x)=0 \quad , \tag{3.120}$$

in which the difference operators $\hat{\Omega}_{ij}$ and generalized discrete sources $Q_j(x)$ are to be determined so that these two difference equations will be invariant under a two-parameter group admitted by the differential equations (3.117) and (3.118).

The general solution of the above diffusion equations can be written as the sum of the general solution of the homogeneous equations and a particular integral, that is,

$$\phi_1(x)=\phi_{1,H}(x)+\phi_{1,P}(x) \quad , \tag{3.121}$$

and

$$\phi_2(x)=\phi_{2,H}(x)+\phi_{2,P}(x) \quad , \tag{3.122}$$

where the subscript H denotes the solution of the homegeneous system, and the subscipt P denotes the particular integral. By substituting (3.121) and (3.122) into the difference equations (3.119) and (3.120) and by calculating the difference operators $\hat{\Omega}_{ij}$ so that

$$\hat{\Omega}_{11}\phi_{1,H}=0 \tag{3.123}$$

and

$$\hat{\Omega}_{22}\phi_{2,H}(x)+\hat{\Omega}_{21}\phi_{1,H}(x)=0 \tag{3.124}$$

admit a two-parameter group that is also admitted by the two-group diffusion equations, it is found that the generalized discrete sources are given by

$$Q_1(x)=-\hat{\Omega}_{11}\phi_{1,P}(x) \quad , \tag{3.125}$$

and

$$Q_2(x)=-\hat{\Omega}_{22}\phi_{2,P}(x)-\hat{\Omega}_{21}\phi_{1,P}(x) \quad . \tag{3.126}$$

When the difference equations (3.119) and (3.120) are constructed by this method they are not only invariant but also exact.

Let the generator of the second extension of a group of point transformations to be admitted by the diffusion equations (3.117) and (3.118) be

$$\hat{U}^{(2)}=\eta_1(x)\frac{\partial}{\partial\phi_1}+\eta_2(x)\frac{\partial}{\partial\phi_2}+\eta_1'(x)\frac{\partial}{\partial\phi_1'}+\eta_2'(x)\frac{\partial}{\partial\phi_2'}+\eta_1''(x)\frac{\partial}{\partial\phi_1''}+\eta_2''(x)\frac{\partial}{\partial\phi_2''} \quad . \tag{3.127}$$

$$\eta_1''(x)-\alpha_1^2\eta_1(x)=0 \quad , \tag{3.128}$$

and

$$\eta_2''(x)-\alpha_2^2\eta_2(x)+\frac{\sigma_s(1\to 2)\eta_1(x)}{D_2}=0 \quad , \tag{3.129}$$

as may be shown by operating on the two-group diffusion equations with the generator of the second extension, namely, $\hat{U}^{(2)}$. The general solution of (3.128) and (3.129) is

$$\eta_1(x)=A_1\cosh(\alpha_1 x)+A_2\sinh(\alpha_1 x) \tag{3.130}$$

and

$$\eta_2(x)=A_3\cosh(\alpha_2 x)+A_4\sinh(\alpha_2 x)+\frac{\sigma_s(1\to 2)}{D_2(\alpha_2^2-\alpha_1^2)}\left[A_1\cosh(\alpha_1 x)+A_2\sinh(\alpha_1 x)\right] \quad , \tag{3.131}$$

where the four constants A_i , $1\le i\le 4$, may be interpreted as four group parameters. This means that equations (3.130) and (3.131) yield a four-parameter group that is admitted by the two-group diffusion equations with arbitrary source distributions in each energy group. The basis of the four-dimensional Lie algebra of this group may be taken in the form,

$$\hat{U}_1=\cosh(\alpha_1 x)\frac{\partial}{\partial\phi_1}+\frac{\sigma_s(1\to 2)}{D_2(\alpha_2^2-\alpha_1^2)}\cosh(\alpha_1 x)\frac{\partial}{\partial\phi_2} \quad , \tag{3.132}$$

$$\hat{U}_2 = \sinh(\alpha_1 x)\frac{\partial}{\partial\phi_1} + \frac{\sigma_s(1\to 2)}{D_2(\alpha_2^2 - \alpha_1^2)}\sinh(\alpha_1 x)\frac{\partial}{\partial\phi_2} \quad , \tag{3.133}$$

$$\hat{U}_3 = \cosh(\alpha_2 x)\frac{\partial}{\partial\phi_2} \quad , \tag{3.134}$$

and

$$\hat{U}_4 = \sinh(\alpha_2 x)\frac{\partial}{\partial\phi_2} \quad . \tag{3.135}$$

The two-parameter subgroup of point transformation generated by

$$\hat{U} = A_1 \cosh(\alpha_1 x)\frac{\partial}{\partial\phi_1} + \left[A_3\cosh(\alpha_2 x) + A_1\frac{\sigma_s(1\to 2)\cosh(\alpha_1 x)}{D_2(\alpha_2^2 - \alpha_1^2)}\right]\frac{\partial}{\partial\phi_2} \tag{3.136}$$

will be used to determine invariant forms for the difference operators Ω_{ij} in the difference equations (3.119) and (3.120) together with the corresponding discrete source terms.

The discretized prolongation of the group generator,

$$\hat{U} = \eta_1(x)\frac{\partial}{\partial\phi_1(x)} + \eta_2(x)\frac{\partial}{\partial\phi_2(x)} \tag{3.137}$$

to neighboring grid point values of the dependent variables is

$$\hat{U}^{(G)} = \eta_1(x)\frac{\partial}{\partial\phi_1(x)} + \eta_2(x)\frac{\partial}{\partial\phi_2(x)} + \eta_1(x+h)\frac{\partial}{\partial\phi_1(x+h)}$$

$$+\eta_2(x+h)\frac{\partial}{\partial\phi_2(x+h)} + \eta_1(x-h)\frac{\partial}{\partial\phi_1(x-h)} + \eta_2(x-h)\frac{\partial}{\partial\phi_2(x-h)} \quad . \tag{3.138}$$

The Lie derivatives of the dependent variables in this prolongation are interpreted as those of the two-parameter subgroup given in (3.136). Upon dropping the subscript H in (3.123) and (3.124), we determine the difference operators $\hat{\Omega}_{ij}$ by imposing the invariance conditions,

$$\hat{U}^{(G)}\left[\hat{\Omega}_{11}\phi_1(x)\right] = 0 \quad , \tag{3.139}$$

and

$$\hat{U}^{(G)}\left[\hat{\Omega}_{22}\phi_2(x) + \hat{\Omega}_{21}\phi_1(x)\right] = 0 \quad . \tag{3.140}$$

These difference operators are not necessarily unique. The forms that follow will be used:

$$\hat{\Omega}_{11} = H_1(x)\left[\hat{S}^+ + \hat{S}^- - 2\right] - \alpha_1^2 \quad , \tag{3.141}$$

$$\hat{\Omega}_{22} = H_2(x)\left[\hat{S}^+ + \hat{S}^- - 2\right] - \alpha_2^2 \quad , \tag{3.142}$$

and

$$\hat{\Omega}_{21} = G_2(x) \quad , \tag{3.143}$$

where the quantities $H_1(x)$, $H_2(x)$ and $G_2(x)$ are found with (3.139) and (3.140). The first invariance condition (3.139) reduces to

$$H_1(x)[\eta_1(x+h) + \eta_1(x-h) - 2\eta_1(x)] - \alpha_1^2\eta_1(x) = 0 \quad . \tag{3.144}$$

With the Lie derivative for the dependent variable $\phi_1(x)$ given in (3.136), we obtain

$$H_1(x) = \frac{\alpha_1^2}{4\sinh^2\left(\frac{\alpha_1 h}{2}\right)} \quad . \tag{3.145}$$

The second invariance condition (3.140) becomes, with (3.142) and (3.143),

$$H_2(x)[\eta_2(x+h) + \eta_2(x-h) - 2\eta_2(x)] - \alpha_2^2\eta_2(x) + G_2(x)\eta_1(x) = 0 \quad . \tag{3.146}$$

By using the two-parameter subgroup Lie derivatives that appear in the generator (3.136), this last equation reduces to

$$\begin{aligned} &H_2(x)\left\{A_3\left[\cosh(\alpha_2(x+h)) + \cosh(\alpha_2(x+h)) - 2\cosh(\alpha_2 x)\right]\right\} \\ &-\alpha_2^2 A_3 \cosh(\alpha_2 x) + H_2(x)\left\{\frac{\sigma_s(1\rightarrow 2)A_1}{D_2\left(\alpha_2^2 - \alpha_1^2\right)}\left[\cosh(\alpha_1(x+h))\right.\right. \\ &\left.\left.+\cosh(\alpha_1(x-h)) - 2\cosh(\alpha_1 x)\right]\right\} - \frac{\sigma_s(1\rightarrow 2)\alpha_2^2 A_1}{D_2\left(\alpha_2^2 - \alpha_1^2\right)}\cosh(\alpha_1 x) \\ &+G_2(x)A_1\cosh(\alpha_1 x) = 0 \quad . \end{aligned} \tag{3.147}$$

This equation must be an identity in the two group parameters A_1 and A_3. From the coefficient of A_3 set equal to zero, we obtain

$$H_2(x) = \frac{\alpha_2^2}{4\sinh^2\left(\frac{\alpha_2 h}{2}\right)} \quad . \tag{3.148}$$

By setting the coefficent of A_1 equal to zero we obtain

$$G_2(x)=\frac{\sigma_s(1\to 2)\alpha_2^2}{D_2\left(\alpha_2^2-\alpha_1^2\right)}\left[1-\frac{\sinh^2\left(\frac{\alpha_1 h}{2}\right)}{\sinh^2\left(\frac{\alpha_2 h}{2}\right)}\right] \quad . \tag{3.149}$$

Hence, invariant difference operators for the two-group diffusion equations are

$$\hat{\Omega}_{11}=\frac{\alpha_1^2}{4\sinh^2\left(\frac{\alpha_1 h}{2}\right)}\left[\hat{S}^+ +\hat{S}^- -2\right]-\alpha_1^2 \quad , \tag{3.150}$$

$$\hat{\Omega}_{22}=\frac{\alpha_2^2}{4\sinh^2\left(\frac{\alpha_2 h}{2}\right)}\left[\hat{S}^+ +\hat{S}^- -2\right]-\alpha_2^2 \quad , \tag{3.151}$$

and

$$\hat{\Omega}_{21}=\frac{\sigma_s(1\to 2)\alpha_2^2}{D_2\left(\alpha_2^2-\alpha_1^2\right)}\left[1-\frac{\sinh^2\left(\frac{\alpha_1 h}{2}\right)}{\sinh^2\left(\frac{\alpha_2 h}{2}\right)}\right] \quad . \tag{3.152}$$

These difference operators are valid for arbitrary grid spacings h. The corresponding invariant difference equatrions (3.119) and (3.120) with the invariant discrete sources (3.125) and (3.126) are also valid for arbitrary grid spacings. In the limit of very small grid spacings, the invariant difference operators become the following non-invariant difference operators:

$$\lim_{h\to 0}\hat{\Omega}_{11}=\frac{1}{h^2}\left[\hat{S}^+ +\hat{S}^- -2\right]-\alpha_1^2 \quad , \tag{3.153}$$

$$\lim_{h\to 0}\hat{\Omega}_{22}=\frac{1}{h^2}\left[\hat{S}^+ +\hat{S}^- -2\right]-\alpha_2^2 \quad , \tag{3.154}$$

and

$$\lim_{h\to 0}\hat{\Omega}_{21}=\frac{\sigma_s(1\to 2)}{D_2} \quad . \tag{3.155}$$

Hence, in the small grid spacing limit, the invariant difference equations reduce to noninvariant difference equations obtained with standard three-point central difference formulae approximations to second order derivatives.

The specific forms assumed by the invariant difference equations (3.119) and (3.120) for arbtirary grid spacings depend upon the source distributions in the two energy groups. For example, suppose the fast group source is spatially uniform and the slow group source is zero. For this case a particular integral is

$$\phi_{1,P}(x) = \frac{S_1}{\alpha_1^2 D_1} \tag{3.156}$$

and

$$\phi_{2,P}(x) = \frac{\sigma_s(1\rightarrow 2)}{\alpha_2^2 D_2}\frac{S_1}{\alpha_1^2 D_1} \quad . \tag{3.157}$$

Upon evaluating the discrete formulation sources given by (3.125) and (3.126), the invariant difference equations for this source case are found to be

$$\hat{\Omega}_{11}\phi_1(x) + \frac{S_1}{D_1} = 0 \quad , \tag{3.158}$$

and

$$\hat{\Omega}_{22}\phi_2(x) + \hat{\Omega}_{21}\phi_1(x) + \frac{\sigma_s(1\rightarrow 2)}{D_2}\frac{S_1}{\alpha_1^2 D_1}$$
$$-\frac{\sigma_s(1\rightarrow 2)}{D_2}\frac{\alpha_2^2}{\left(\alpha_2^2-\alpha_1^2\right)}\left[1-\frac{\sinh^2\left(\frac{\alpha_1 h}{2}\right)}{\sinh^2\left(\frac{\alpha_2 h}{2}\right)}\right]\frac{S_1}{\alpha_1^2 D_1} = 0 \quad , \tag{3.159}$$

where the invariant difference operators are given in (3.150), (3.151), and (3.152). Exact solutions of these invariant difference equations are the same as exact solutions of the two-group diffusion equations.

3.2 ALGORITHMS FOR SOLVING INVARIANT DIFFERENCE EQUATIONS

3.2.1 SOLUTION OF SECOND ORDER INVARIANT DIFFERENCE EQUATIONS

The invariant exact difference equation,

$$\frac{\phi(x+h)+\phi(x-h)-2\phi(x)}{4\sinh^2\left(\frac{\alpha h}{2}\right)} - \phi(x) + \frac{S}{\alpha^2 D} = 0 \quad , \tag{3.160}$$

obtained in (3.25) for the diffusion equation for $0 \le x \le a$ can be solved in a number of ways. By setting

$$x = x_m = mh \, , m = 0, 1, 2, 3, \ldots, N \tag{3.161}$$

a set of algetraic equations for $\phi_m = \phi(xm)$ is obtained. This set has a tridiagonal coefficient matrix and can be solved with a tridiagonal matrix algorithm. A simpler procedure that inverts the matrix is the following.

Since the difference equation (3.160) is exact, it is valid for any choice of the grid spacing h. First set $x=0$ and $h=a$ in this difference quation to find that

$$\frac{\phi(a)+\phi(-a)-2\phi(0)}{4\sinh^2\left(\frac{\alpha a}{2}\right)}-\phi(0)+\frac{S}{\alpha^2 D}=0 \quad . \tag{3.162}$$

If Dirichlet boundary conditions are imposed at $x=\pm a$, then $\phi(\pm a)=0$, and we obtain

$$\begin{aligned}\phi(0)&=\frac{S}{\alpha^2 D}\frac{2\sinh^2\left(\frac{\alpha a}{2}\right)}{1+2\sinh^2\left(\frac{\alpha a}{2}\right)}\\ &=\frac{S}{\alpha^2 D}\left[1-\frac{1}{\cosh(\alpha a)}\right]\end{aligned} \tag{3.163}$$

which is, in fact, the exact solution of the diffusion equation at the center with a spatially uniform source and for the case of Dirichlet boundary conditions.

Next set $x=a/2$ and $h=a/2$ in the difference equation (3.160) to find that

$$\frac{\phi(a)+\phi(0)-2\phi(a/2)}{4\sinh^2\left(\frac{\alpha a}{4}\right)}-\phi(a/2)+\frac{S}{\alpha^2 D}=0 \quad . \tag{3.164}$$

With $\phi(a)=0$ and $\phi \doteq (0)$ known from (3.163) we obtain

$$\left[1+2\sinh^2\left(\frac{\alpha a}{4}\right)\right]\phi\left(\frac{a}{2}\right)=\frac{S}{\alpha^2 D}\left[2\sinh^2\left(\frac{\alpha a}{4}\right)+\frac{2\sinh^2\left(\frac{\alpha a}{2}\right)}{1+2\sinh^2\left(\frac{\alpha a}{2}\right)}\right] , \tag{3.165}$$

which simplifies to

$$\phi\left(\frac{a}{2}\right)=\frac{S}{\alpha^2 D}\left[1-\frac{\cosh\left(\frac{\alpha a}{2}\right)}{\cosh(\alpha a)}\right] \quad . \tag{3.166}$$

This agrees with the exact solution of the diffusion equation at $x=a/2$ with Dirichlet boundary conditions and a uniform source.

Next set $x=a/4$ and $h=a/4$ in the difference equation (3.160) to find that

$$\frac{\phi\left(\frac{a}{2}\right)+\phi(0)-2\phi\left(\frac{a}{4}\right)}{4\sinh^2\left(\frac{\alpha a}{8}\right)}-\phi\left(\frac{a}{4}\right)+\frac{S}{\alpha^2 D}=0 \quad . \tag{3.167}$$

With $\phi(0)$ given in (3.163) and $\phi(a/2)$ given in (3.166), the solution of (3.167) is found to be

$$\phi\left(\frac{a}{4}\right)=\frac{S}{\alpha^2 D}\left[1-\frac{\cosh\left(\frac{\alpha a}{4}\right)}{\cosh(\alpha a)}\right] \quad , \tag{3.168}$$

which is the exact solution of the diffusion equation at $x=a/4$. Next set $x=3a/4$ and $h=a/4$ in the difference euqation (3.160) to find that

$$\frac{\phi(a)+\phi\left(\frac{a}{2}\right)-2\phi\left(\frac{3a}{4}\right)}{4\sinh^2\left(\frac{\alpha a}{8}\right)}-\phi\left(\frac{3a}{4}\right)+\frac{S}{\alpha^2 D}=0 \quad . \tag{3.169}$$

With $\phi(a)=0$ and $\phi(a/2)$ given in (3.166), solving (3.169) produces

$$\phi\left(\frac{3a}{4}\right)=\frac{S}{\alpha^2 D}\left[1-\frac{\cosh\left(\frac{3\alpha a}{4}\right)}{\cosh(\alpha a)}\right] \quad , \tag{3.170}$$

the exact solution of the diffusion equation at $x=3a/4$. By repeatedly halving the grid spacing h in the difference equation (3.160), the solution of this difference equation at as many grid points as desired may be obtained sequentially without using a tridiagonal matrix algorithm. If we set $h=a/8$ in the difference equation (3.160), then by letting $x=a/8$, $x=3a/8$, $x=5a/8$, and $x=7a/8$ and by using (3.163), (3.166), (3.168), and (3.170) we obtain the exact results for $\phi(a/8)$, $\phi(3a/8)$, $\phi(5a/8)$, and $\phi(7a/8)$.

Exact solutions of the invariant difference equation (3.160) have been calculated above for the case of homogeneous Dirichlet boundary conditions at $x=\pm a$. It is also possible to do this for the case of homogeneous boundary conditions of the third type at $x=\pm a$. For the diffusion equation, homogeneous boundary conditions of the third type correspond to vanishing inward partial currents and are consistent with the P_1. approximation to the transport equation. The flux does not vanish on the surface when homogeneous boundary conditions of the third type are used. On the surface at $x=a$, a vanishing inward partial current leads to the homogeneous boundary condition,

$$\phi(a)+2D\phi'(a)=0 \quad . \tag{3.171}$$

When the first order derivative is thought of as being approximated by a two-point central difference formula, the invariant discretization of the boundary condition (3.171) is given by

$$\phi_N + \frac{2\alpha D(\phi_{N+1} - \phi_{N-1})}{2\sinh(\alpha h)} = 0 \tag{3.172}$$

where $\phi_N = \phi(Nh) = \phi(a)$. Evaluating the invariant difference equation (3.160) at $x = a$ yields

$$\frac{\phi_{N+1} - \phi_{N-1} - 2\phi_N}{4\sinh^2\left(\frac{\alpha h}{2}\right)} - \phi_N + \frac{S}{\alpha^2 D} = 0 \quad . \tag{3.173}$$

The quantity ϕ_{N+1} is eliminated from (3.172) and (3.173) in order to apply the zero inward partial current boundary condition at $x = a$. Both equations (3.172) and (3.173) are valid for an arbitrary grid spacing h.

To evaluate the flux at the center and on the surface for the zero inward partial current case, we first set $x = 0$ and $h = a$ in the difference equation (3.160) to get

$$\frac{\phi(a) - \phi(-a) - 2\phi(0)}{4\sinh^2\left(\frac{\alpha a}{2}\right)} - \phi(0) + \frac{S}{\alpha^2 D} = 0 \quad . \tag{3.174}$$

Then set $x = a$ and $h = a$ in (3.160) to get

$$\frac{\phi(2a) - \phi(0) - 2\phi(a)}{4\sinh^2\left(\frac{\alpha a}{2}\right)} - \phi(a) + \frac{S}{\alpha^2 D} = 0 \quad . \tag{3.175}$$

Set $h = a$ in the invariant discretized boundary condition (3.172) to get

$$\phi(a) + \frac{2\alpha D[\phi(2a) - \phi(0)]}{2\sinh(\alpha a)} = 0 \quad . \tag{3.176}$$

By noting that

$$\phi(-a) = \phi(a) \tag{3.177}$$

in (3.174) because of symmetry and by eliminating $\phi(2a)$ from (3.175) with (3.176), the following two algebraic equations are found for $\phi(0)$ and $\phi(a)$:

$$-\cosh(\alpha a)\phi(0) + \phi(a) + [\cosh(\alpha a) - 1]\frac{S}{\alpha^2 D} = 0 \quad , \tag{3.178}$$

and

$$\phi(0) - \left[\cosh(\alpha a) + \frac{\sinh(\alpha a)}{2\alpha D}\right]\phi(a) + [\cosh(\alpha a) - 1]\frac{S}{\alpha^2 D} = 0 \quad . \tag{3.179}$$

Solving these last two equations yields

$$\phi(0)=\frac{S}{\alpha^2 D}\left[1-\frac{1}{\cosh(\alpha a)+2\alpha D\sinh(\alpha a)}\right] \tag{3.180}$$

and

$$\phi(a)=\frac{S}{\alpha^2 D}\left[\frac{2\alpha D\sinh(\alpha a)}{\cosh(\alpha a)+2\alpha D\sinh(\alpha a)}\right] \quad . \tag{3.181}$$

The results obtained in (3.180) and (3.181) from the invariant difference equation (3.160) and invariant discretized boundary condition of the third type (3.172) both agree with the analytical solution of the diffusion equation with a spatially uniform source and a zero inward partial current boundary condition on the surface. By systematically halving the grid spacing in the difference equation (3.160) results for $\phi(a/2)$, $\phi(a/4)$, $\phi(3a/4)$, $\phi(a/8)$, $\phi(3a/8)$, $\phi(5a/8)$, $\phi(7a/8)$, and so on can be calculated sequentially for the boundary condition of the third type.

3.2.2 SOLUTION OF SYSTEMS OF FIRST ORDER INVARIANT DIFFERENCE EQUATIONS

The system of invariant first order difference equations,

$$\frac{\alpha[J(x+h)-J(x-h)]}{2\sinh(\alpha h)}+\sigma_a\phi(x)-S=0 \quad , \tag{3.182}$$

and

$$\frac{\alpha[\phi(x+h)-\phi(x-h)]}{2\sinh(\alpha h)}+\frac{J(x)}{D}=0 \quad , \tag{3.183}$$

which discretize the differential system (3.59) and (3.60) with a spatially uniform source, is valid for an arbitrary grid spacing h. This fact leads to the following algorithm for their solution.

Set $h=a/2$ and $x=0$ in (3.182) to get

$$\frac{\alpha[J(a/2)-J(-a/2)]}{2\sinh\left(\frac{\alpha a}{2}\right)}+\sigma_a\phi(0)-S=0 \quad , \tag{3.184}$$

in which

$$-J(-a/2)=J(a/2) \tag{3.185}$$

due to symmetry. Set $h=a/2$ and $x=a/2$ in (3.183) to get

$$\frac{\alpha[\phi(a)-\phi(0)]}{2\sinh\left(\frac{\alpha a}{2}\right)}+\frac{J(a/2)}{D}=0 \quad . \tag{3.186}$$

Imposing the Dirichlet boundary condition $\phi(a)=0$ and solving (3.184) and (3.186) yield

$$\phi(0)=\frac{S}{\sigma_a}\frac{2\sinh^2\left(\frac{\alpha a}{2}\right)}{\cosh(\alpha a)} \tag{3.187}$$

and

$$J(a/2)=\frac{S\alpha D}{\sigma_a}\frac{\sinh\left(\frac{\alpha a}{2}\right)}{\cosh(\alpha a)} \quad . \tag{3.188}$$

These last two results agree with those obtained by solving the differential system analytically and evaluating the solutions for $\phi(x)$ at $x=0$ and $J(x)$ at $x=a/2$.

Set $h=a/4$ and $x=0$ in (3.182) to get

$$\frac{\alpha[J(a/4)-J(-a/4)]}{2\sinh\left(\frac{\alpha a}{4}\right)}+\sigma_a\,\phi(0)-S=0 \quad . \tag{3.189}$$

Because of symmetry

$$J(-a/4)=-J(a/4) \quad , \tag{3.190}$$

so solving (3.189) with $\phi(0)$ from (3.187) yields

$$J(a/4)=\frac{S\alpha D}{\sigma_a}\frac{\sinh\left(\frac{\alpha a}{4}\right)}{\cosh(\alpha a)} \quad , \tag{3.191}$$

which is an exact result for the net current at $x=a/4$. Set $h=a/4$ and $x=a/4$ in (3.182) to get

$$\frac{\alpha[J(a/2)-J(0)]}{2\sinh\left(\frac{\alpha a}{4}\right)}+\sigma_a\,\phi(a/4)-S=0 \quad . \tag{3.192}$$

Because of symmetry $J(o)=0$, and the solution of (3.192) with result for $J(a/2)$ in (3.188) is

$$\phi(a/4)=\frac{S}{\sigma_a}\left[1-\frac{\cosh\left(\frac{\alpha a}{4}\right)}{\cosh(\alpha a)}\right] \quad , \tag{3.193}$$

the exact result for the flux at $x = a/4$. Set $h = a/4$ and $x = h/4$ in (3.183) to get

$$\frac{\alpha[\phi(a/2) - \phi(0)]}{2\sinh\left(\frac{\alpha a}{4}\right)} + \frac{1}{D} J_1(a/4) = 0 \quad , \tag{3.194}$$

which with (3.187) and (3.191) yields the exact solution,

$$\phi(a/2) = \frac{S}{\sigma_a}\left[1 - \frac{\cosh\left(\frac{\alpha a}{2}\right)}{\cosh(\alpha a)}\right] \quad . \tag{3.195}$$

Set $h = a/4$ and $x = a/2$ in (3.182) to get

$$\frac{\alpha[J(3a/4) - J(a/4)]}{2\sinh\left(\frac{\alpha a}{4}\right)} + \sigma_a\, \phi(a/2) - S = 0 \quad . \tag{3.196}$$

Solving (3.196) with (3.191) and (3.195) produces

$$J(3a/4) = \frac{S\alpha D}{\sigma_a} \frac{\sinh\left(\frac{3\alpha a}{4}\right)}{\cosh(\alpha a)} \quad , \tag{3.197}$$

an exact result. Set $h = a/4$ and $x = a/2$ in (3.183) to get

$$\frac{\alpha[\phi(3a/4) - \phi(a/4)]}{2\sinh\left(\frac{\alpha a}{4}\right)} + \frac{1}{D} J(a/2) = 0 \quad , \tag{3.198}$$

which with (3.188) and (3.193) gives the exact result,

$$\phi(3a/4) = \frac{S}{\sigma_a}\left[1 - \frac{\cosh\left(\frac{3\alpha a}{4}\right)}{\cosh(\alpha a)}\right] \quad . \tag{3.199}$$

Set $h = a/4$ and $x = 3a/4$ in (3.182) to get

$$\frac{\alpha[J(a) - J(a/2)]}{4\sinh\left(\frac{\alpha a}{4}\right)} + \sigma_a \phi(3a/4) - S = 0 \quad . \tag{3.200}$$

Solving (3.200) with (3.188) and (3.199) yields the following exact result for the net current on the surface:

$$J(a)=\frac{S\alpha D}{\sigma_a}\tanh(\alpha a) \quad . \tag{3.201}$$

Further results for the flux and net current at additional grid points can be calculated from the exact invariant difference equations (3.182) and (3.183) by continuing to cut the grid spacing in half.

4. CONSTRUCTION OF INVARIANT DIFFERENCE SCHEMES IN CONSERVATION FORM

Difference schemes that are constructed by using group generators extended to grid point values of dependent variables and grid spacings for the case of two independent variables are worked out in this section. The starting point is the conservation form of a difference scheme written in terms of numerical flux functions thought of as functions of $p+q+1$ arguments which are grid point values of the dependent variables. The requirement that the difference scheme admit the same group of transformations as that admitted by the differential equation being simulated is determined by evaluating the Lie derivative of the conservation form itself. This produces a partial differential equation for the numerical flux function whose solution provides invariant flux functions that yield group invariant difference schemes.

4.1 LIE DERIVATIVES OF CONSERVATION FORMS OF DIFFERENCE SCHEMES

Invariant difference schemes are invariant functions of a transformation group. If a conservation law is given in the form,

$$\frac{\partial u}{\partial t}+\frac{\partial}{\partial x}f(u)=0 \quad , \tag{4.1}$$

the conservation form of an explicit difference scheme may be taken as

$$u_j^{n+1}-u_j^n+\frac{\tau}{h}\Big[F\big(u_{j-p}^n,u_{j-p+1}^n,\ldots,u_{j+q}^n;h,\tau\big)$$

$$-F\big(u_{j-1-p}^n,u_{j-p}^n,\ldots,u_{j-1+q}^n;h,\tau\big)\Big]=0 \quad , \tag{4.2}$$

where

$$u_j^n=u(jh,n\tau) \quad , \tag{4.3}$$

the spatial grid spacing is h, the time grid spacing is τ, and $F\big(u_{j-p}^n,u_{j-p+1}^n,\ldots,u_{j+q}^n;h,\tau\big)$ is the numerical flux function. The integers p and q in (4.2) define the number of support points $p+q+1$ for the numerical flux function. Let $W\big(u_j^{n+1},u_{j-p}^n,u_{j-p+1}^n,\ldots,u_{j+q}^n;h,\tau\big)$ denote the left hand side of the difference scheme (4.2). Then the condition that this difference scheme is an invariant equation of a transformation group is

$$\frac{\delta W}{\delta a} = \theta\left(u_j^{n+1}, u_{j-p}^n, u_{j-p+1}^n, \ldots, u_{j+q}^n; h, \tau\right) W \quad , \tag{4.4}$$

in which the left hand side is the Lie derivative of the function W, and the function θ is an arbitrary function of the indicated arguments. If the group action on a grid point value of the dependent variable is

$$\frac{\delta u_j^n}{\delta a} \quad ,$$

on the spatial grid spacing is

$$\frac{\delta h}{\delta a} \quad ,$$

and the time grid spacing is

$$\frac{\delta \tau}{\delta a} \quad ,$$

the explicit form of the conservative difference scheme invariance condition (4.4) is

$$\frac{\delta u_j^{n+1}}{\delta a} - \frac{\delta u_j^n}{\delta a} + \left(\frac{1}{h}\frac{\delta \tau}{\delta a} - \frac{\tau}{h^2}\frac{\delta h}{\delta a}\right)\left[F\left(u_{j-p}^n, \ldots, u_{j+q}^n; h_1\tau\right)\right.$$

$$\left. - F\left(u_{j-1-p}^n, \ldots, u_{j-1+q}^n; h_1\tau\right)\right] + \frac{\tau}{h}\left[\frac{\delta F}{\delta a}\left(u_{j-p}^n, \ldots, u_{j+q}^n; h_1\tau\right)\right.$$

$$\left. - \frac{\delta F}{\delta a}\left(u_{j-1-p}^n, \ldots, u_{j-1+q}^n; h_1\tau\right)\right] = \theta\left\{ u_j^{n+1} - u_j^n\right.$$

$$\left. + \frac{\tau}{h}\left[F\left(u_{j-p}^n, \ldots, u_{j+q}^n; h_1\tau\right) - F\left(u_{j-1-p}^n, \ldots, u_{j-1+q}^n; h_1\tau\right)\right] \right\} \quad . \tag{4.5}$$

The Lie derivative of the numerical flux function that appears in (4.5) is given by

$$\frac{\delta F}{\delta a}\left(u_{j-p}^n, \ldots, u_{j+q}^n; h_1\tau\right) = \frac{\delta u_{j-p}^n}{\delta a}\frac{\partial F}{\partial u_{j-p}^n} + \ldots + \frac{\delta u_{j+q}^n}{\delta a}\frac{\partial F}{\partial u_{j+q}^n} + \frac{\delta h}{\delta a}\frac{\partial F}{\partial h} + \frac{\delta \tau}{\delta a}\frac{\partial F}{\partial \tau} \quad , \tag{4.6}$$

that is,

$$\frac{\delta F}{\delta a}\left(u_{j-p}^n, \ldots, u_{j+q}^n; h_1\tau\right) = \hat{U}^{(G)} F\left(u_{j-p}^n, \ldots, u_{j+q}^n; h_1\tau\right) \quad , \tag{4.7}$$

where $\hat{U}^{(G)}$ is the prolongation of the group generator to grid point values of the dependent variable and the grid spacings. The invariance condition (4.5) is a linear first order partial differential equation whose solutions provide numerical flux functions that yield explicit difference schemes in the conservation form (4.2). These also admit the same transformation group as that under which the conservation law (4.1) is invariant.

4.2 INVARIANT NUMERICAL FLUX FUNCTIONS FOR THE ADVECTION EQUATION

The advection equation,

$$u_t + cu_x = 0 \quad , \tag{4.8}$$

is invariant under a four-parameter group with the Lie algebra of generators,

$$\hat{U}_1 = \frac{\partial}{\partial x} \quad , \tag{4.9}$$

$$\hat{U}_2 = \frac{\partial}{\partial t} \quad , \tag{4.10}$$

$$\hat{U}_3 = x\frac{\partial}{\partial x} + t\frac{\partial}{\partial t} \quad , \tag{4.11}$$

and

$$\hat{U}_4 = u\frac{\partial}{\partial u} \quad . \tag{4.12}$$

The prolongations of these group generators to the grid point values of the dependent variable and the grid spacings are

$$\hat{U}_1^{(G)} = \frac{\partial}{\partial x} \quad , \tag{4.13}$$

$$\hat{U}_2^{(G)} = \frac{\partial}{\partial t} \quad , \tag{4.14}$$

$$\hat{U}_3^{(G)} = x\frac{\partial}{\partial x} + t\frac{\partial}{\partial t} + h\frac{\partial}{\partial h} + \tau\frac{\partial}{\partial \tau} \quad , \tag{4.15}$$

and

$$\hat{U}_4^{(G)} = u\frac{\partial}{\partial u} + u_j^{n+1}\frac{\partial}{\partial u_j^{n+1}} + u_{j-p}^n\frac{\partial}{\partial u_{j-p}^n} + \ldots + u_j^n\frac{\partial}{\partial u_j^n} + \ldots +$$

$$u_{j+q}^n\frac{\partial}{\partial u_{j+q}^n} + u_{j-1-p}^n\frac{\partial}{\partial u_{j-1-p}^n} + \ldots + u_{j-1+q}^n\frac{\partial}{\partial u_{j-1+q}^n} \quad , \tag{4.16}$$

as computed from the prolongation formulae derived in Section 2. From (2.104) note that for the fourth group generator we have

$$\frac{\delta u_j^n}{\delta a} = u_j^n \quad , \tag{4.17}$$

and

$$\frac{\delta u_j^{n+1}}{\delta a} = u_j^{n+1} \quad . \tag{4.18}$$

For the case of the advection equation (4.8) the difference scheme invariance condition (4.5) is satisfied with $\theta = 0$ for each of the one-parameter subgroups generated by $\hat{U}_1^{(G)}$, $\hat{U}_2^{(G)}$, and $\hat{U}_3^{(G)}$ in (4.13), (4.14), and (4.15), respectively.. For the fourth one-parameter subgroup generated by $\hat{U}_4^{(G)}$ in (4.16), the invariance condition (4.5) reduces to

$$\frac{\delta F}{\delta a}\left(u_{j-p}^n, \ldots, u_{j+q}^n; h_1\tau\right) = F\left(u_{j-p}^n, \ldots, u_{j+q}^n; h_1\tau\right) \quad , \tag{4.19}$$

that is,

$$\hat{U}_4^{(G)} F\left(u_{j-p}^n, \ldots, u_{j+q}^n; h_1\tau\right) = F\left(u_{j-p}^n, \ldots, u_{j+q}^n; h_1\tau\right) \tag{4.20}$$

when $\theta = 1$ and in view of the Lie derivatives (4.17) and (4.18). This is a linear first order partial differential equation for the numerical flux function F which takes the explicit form,

$$u_{j-p}^n \frac{\partial F}{\partial u_{j-p}^n} + u_{j-p+1}^n \frac{\partial F}{\partial u_{j-p+1}^n} + \ldots + u_{j+q}^n \frac{\partial F}{\partial u_{j+q}^n} = F \quad . \tag{4.21}$$

Solutions of this partial differential equation yield numerical flux functions which result in invariant, conservative difference schemes for the advection equation.

The general solution of the numerical flux function partial differential equation (4.21) is an arbitrary function of the solutions of the characteristic equations, which are

$$\frac{dh}{0} = \frac{d\tau}{0} = \frac{du_{j-p}^n}{u_{j-p}^n} = \frac{du_{j-p+1}^n}{u_{j-p+1}^n} = \ldots = \frac{du_{j+q}^n}{u_{j+q}^n} = \frac{dF}{F} \quad , \tag{4.22}$$

with solutions

$$h = \text{const.} \quad , \tag{4.23}$$

$$\tau = \text{const.} \quad , \tag{4.24}$$

$$\frac{u_{j-p}^n}{u_j^n} = \text{const.} \quad , \tag{4.25}$$

$$\frac{u_{j-p+1}^n}{u_j^n} = \text{const.} \quad , \tag{4.26}$$

$$\frac{u_{j+q}^n}{u_j^n} = \text{const.} \quad , \tag{4.27}$$

and

$$\frac{F}{u_j^n} = \text{const.} \quad . \tag{4.28}$$

Hence, the general solution for the invariant numerical flux function is given by

$$F = u_j^n H_1\left(\frac{u_{j-p}^n}{u_j^n}, \frac{u_{j-p+1}^n}{u_j^n}, \ldots, \frac{u_{j+q}^n}{u_j^n}, \frac{\tau}{h}\right) \quad , \tag{4.29}$$

where H_1 is an arbitrary function of the indicated arguments. The fact that an arbitrary function appears in this result for the invariant numerical flux function shows that an infinite number of invariant conservative difference schemes of the form (4.2) can, in principle, be constructed for the advection equation.

Numerical flux functions that lead to difference schemes in conservation form and that have been reported in the literature can be obtained as special cases of the general result obtained in (4.29) with invariance arguments. If we set $p = 0$ and $q = 0$ and take $H_1 = c$, we get the numerical flux function for the upwind scheme, namely,

$$F\left(u_j^n\right) = c u_j^n \text{ , for c} > 0 \quad . \tag{4.30}$$

If we take $p = 0$ and $q = 1$ and

$$H_1 = c\frac{u_{j+1}^n}{u_j^n} \quad , \tag{4.31}$$

we obtain

$$F\left(u_{j+1}^n\right) = c\, u_{j+1}^n \text{ , for c} < 0 \quad , \tag{4.32}$$

the upwind scheme for negative values of c. With $p = 0$ and $q = 1$ and

$$H_1 = \frac{h}{2\tau}\left(1 - \frac{u_{j+1}^n}{u_j^n}\right) + \frac{c}{2}\left(1 + \frac{u_{j+1}^n}{u_j^n}\right) \quad , \tag{4.33}$$

equation (4.29) becomes the numerical flux function for the Lax-Friedrichs scheme [6], namely,

$$F\left(u_j^n, u_{j+1}^n\right) = \frac{h}{2\tau}\left(u_j^n - u_{j+1}^n\right) + \frac{c}{2}\left(u_j^n + u_{j+1}^n\right) \quad . \tag{4.34}$$

Also with $p = 0$ and $q = 1$ and

$$H_1 = \frac{c}{2}\left(1 + \frac{u_{j+1}^n}{u_j^n}\right) - \frac{\tau A^2}{2h}\left(\frac{u_{j+1}^n}{u_j^n} - 1\right) \quad , \tag{4.35}$$

equation (4.29) is the numerical flux function for the Lax-Wendroff scheme [6], namely,

$$F\left(u_j^n, u_{j+1}^n\right) = \frac{c}{2}\left(u_{j+1}^n + u_j^n\right) - \frac{\tau c^2}{2h}\left(u_{j+1}^n - u_j^n\right) \quad . \tag{4.36}$$

If $p = 1$ and $q = 2$, numerical flux functions for the Crowley, Rusanov, and Burstein and Mirin schemes come out of the general result (4.29). For the Crowley algorithm [7]

$$H_1 = \frac{c}{2}\left(1 + \frac{u_{j+1}^n}{u_j^n}\right) + \frac{\tau c^2}{8h}\left(\frac{u_{j+2}^n}{u_j^n} + \frac{u_{j+1}^n}{u_j^n} - 1 - \frac{u_{j-1}^n}{u_j^n}\right)$$

$$-\frac{\tau^2 c^3}{12h^2}\left(\frac{u_{j+2}^n}{u_j^n} - \frac{u_{j+1}^n}{u_j^n} - 1 + \frac{u_{j-1}^n}{u_j^n}\right) \quad , \tag{4.37}$$

and the corresponding numerical flux function is

$$F\left(u_{j-1}^n, u_j^n, u_{j+1}^n, u_{j+2}^n\right) = \frac{c}{2}\left(u_j^n + u_{j+1}^n\right)$$

$$+\frac{\tau c^2}{8h}\left(u_{j+2}^n + u_{j+1}^n - u_j^n - u_{j-1}^n\right)$$

$$-\frac{\tau^2 c^3}{12h^2}\left(u_{j+2}^n - u_{j+1}^n - u_j^n + u_{j-1}^n\right) \quad . \tag{4.38}$$

For the Rusanov [8], and Burstein and Misin [9], algorithm we take

$$H_1 = \frac{F}{h}\left(u_{j-1}^n, u_j^n, u_{j+1}^n, u_{j+2}^n\right) \quad , \tag{4.39}$$

where the numerical flux function is given by

$$F\left(u_{j-1}^n, u_j^n, u_{j+1}^n, u_{j+2}^n\right) = \frac{c}{2}\left(u_{j+1}^n + u_j^n\right)$$

$$+\frac{c}{12}\left(u_{j+2}^n - u_{j+1}^n - u_j^n + u_{j-1}^n\right) + \frac{\tau c^2}{2h}\left(u_{j+1}^n - u_j^n\right)$$

$$+\frac{\tau c^2}{8h}\left(u_{j+2}^n - 3\,u_{j+1}^n + 3\,u_j^n - u_{j-1}^n\right) - \frac{\tau^2 c^3}{12h^2}\left(u_{j+2}^n - u_{j+1}^n - u_j^n + u_{j-1}^n\right)$$

$$-\frac{h\omega}{24\tau}\left(u_{j+2}^n - 3\,u_{j+1}^n + 3\,u_j^n - u_{j-1}^n\right) \quad . \tag{4.40}$$

With $p = 1$ and $q = 0$ and

$$H_1 = \frac{c}{2}\left(3\,u_j^n - u_{j-1}^n\right) - \frac{\tau c^2}{2h}\left(u_j^n - u_{j-1}^n\right) \quad , \tag{4.41}$$

we obtain the numerical flux function for the Beam-Warming upwind scheme [10], namely,

$$F\left(u_{j-1}^n, u_j^n\right) = \frac{c}{2}\left(3u_j^n - u_{j-1}^n\right) - \frac{\tau c^2}{2h}\left(u_j^n - u_{j-1}^n\right) \quad . \tag{4.42}$$

It should be noted that the numerical flux functions for the upwind scheme with $c > 0$ in (4.30), for the upwind scheme with $c < 0$ in (4.32), for the Lax-Friedrichs scheme (4.34), for the Lax-Wendroff scheme (4.36), for the Crowley scheme (4.38), for the Rusanov, and Burstein and Misin scheme (4.40), and for the Beam-Warming scheme (4.42) are all invariant under the four-parameter group with the generators (4.9), (4.10), (4.11), and (4.12) that is admitted by the advection equation.

The numerical flux function for the Fromm algorithm [11], is also a special case of the general result (4.29). The Fromm algorithm is intended to reduce dispersion by constructing a numerical flux function as a linear combination of numerical flux functions which have opposite phase errors. Let $F_{LW}\left(j_j^n, j_{j+1}^n\right)$ denote the numerical flux function for the Lax-Wendroff method given by (4.36). Let $F_{BW}\left(j_{j-1}^n, j_j^n\right)$ denote the numerical flux function for the Beam-Warming method given by (4.42). Then the numerical flux function for the Fromm algorithm is

$$F\left(u_{j-1}^n, u_j^n, u_{j+1}^n\right) = \frac{1}{2}\left[F_{BW}\left(u_{j-1}^n, u_j^n\right) + F_{LW}\left(u_j^n, u_{j+1}^n,\right)\right] \quad . \tag{4.43}$$

The Fromm scheme has a reduced phase error due to the cancelling of the lagging phase error of the Lax-Wendroff scheme and the leading phase error of the Beam-Warming scheme. The numerical flux function for the Fromm algorithm is also invariant under the four-parameter group admitted by the advection equation and, therefore, is not symmetry breaking.

If we set $p = 1$ and $q = 2$ and specialize the general invariant result (4.29) to the consistent numerical flux function,

$$F\left(u_{j-1}^n, u_j^n, u_{j+1}^n, u_{j+2}^n\right) = -\frac{c}{12}\left(u_{j+2}^n - 7u_{j+1}^n - 7u_j^n + u_{j-1}^n\right)$$

$$\frac{c^2\tau}{24h}\left(u_{j+2}^n - 15u_{j+1}^n + 15u_j^n - u_{j-1}^n\right) \quad , \tag{4.44}$$

the corresponding difference scheme in conservation form is

$$u_j^{n+1} = u_j^n - \frac{\tau}{h}\left[F\left(u_{j-1}^n, u_j^n, u_{j+1}^n, u_{j+2}^n\right) - F\left(u_{j-2}^n, u_{j-1}^n, u_j^n, u_{j+1}^n\right)\right] \quad , \tag{4.45}$$

that is,

$$u_j^{n+1} = u_j^n + \frac{c\tau}{12h}\left(u_{j+2}^n, -8\, u_{j+1}^n + 8\, u_{j-1}^n - u_{j-2}^n\right)$$

$$-\frac{c^2\tau^2}{24h^2}\left(u_{j+2}^n - 16u_{j+1}^n + 30u_j^n - 16u_j^n + u_{j-2}^n\right) \quad . \tag{4.46}$$

This invariant conservative difference scheme also follows from

$$u(x,t+\tau) = u(x,t) - c\tau u_x(x,t) + \frac{\tau^2 c^2}{2} u_{xx}(x,t) \tag{4.47}$$

with

$$u_x(x,t) = \frac{1}{12h}\left(-u_{j+2}^n + 8u_{j+1}^n - 8u_{j-1}^n + u_{j-2}^n\right) \quad , \tag{4.48}$$

and

$$u_{xx}(x,t) = \frac{-1}{12h^2}\left(u_{j+2}^n - 16u_{j+1}^n + 30u_j^n - 16u_{j-1}^n + u_{j-2}^n\right) \quad , \tag{4.49}$$

which are fourth order accurate approximations to the first and second order derivatives.

4.3 INVARIANT NUMERICAL FLUX FUNCTIONS FOR THE INVISCID BURGERS EQUATION

If $f(u) = u^2/2$, the conservation law (4.1) becomes the inviscid Burgers equation,

$$u_t + u\, u_x = 0 \quad , \tag{4.50}$$

which admits the four-parameter group with the Lie algebra of generators,

$$\hat{U}_1 = \frac{\partial}{\partial x} \quad , \tag{4.51}$$

$$\hat{U}_2 = \frac{\partial}{\partial t} \quad , \tag{4.52}$$

$$\hat{U}_3 = x\frac{\partial}{\partial x} + t\frac{\partial}{\partial t} \ , \tag{4.53}$$

and

$$\hat{U}_4 = x\frac{\partial}{\partial x} + u\frac{\partial}{\partial u} \quad . \tag{4.54}$$

When this group is extended to grid point values of the dependent variable and the grid spacings, the group generators are

$$\hat{U}_1^{(G)} = \frac{\partial}{\partial x} \quad , \tag{4.55}$$

$$\hat{U}_2^{(G)} = \frac{\partial}{\partial t} \quad , \tag{4.56}$$

$$\hat{U}_3^{(G)} = x\frac{\partial}{\partial x} + t\frac{\partial}{\partial t} + h\frac{\partial}{\partial h} + \tau\frac{\partial}{\partial \tau} \quad , \tag{4.57}$$

and

$$\hat{U}_4^{(G)} = x\frac{\partial}{\partial x} + u\frac{\partial}{\partial u} + h\frac{\partial}{\partial h} + u_j^n\frac{\partial}{\partial u_j^n} + u_j^{n+1}\frac{\partial}{\partial u_j^{n+1}}$$

$$+ u_{j-p}^n\frac{\partial}{\partial u_{j-p}^n} + \ldots + u_{j+q}^n\frac{\partial}{\partial u_{j+q}^n} + u_{j-1-p}^n\frac{\partial}{\partial u_{j-1-p}^n}$$

$$+ \ldots + u_{j-1+q}^n\frac{\partial}{\partial u_{j-1+q}^n} \quad . \tag{4.58}$$

For the case of the inviscid Burgers equation the invariance condition (4.5) is satisfied for the one-parameter subgroups with generators (4.55), (4.56) and (4.57) with $\theta = 0$. The fourth one-parameter subgroup with the generator $\hat{U}_4^{(G)}$ is admitted by the difference scheme provided that the numerical flux function satisfies the linear first order partial differential equation,

$$\frac{\delta F}{\delta a}\left(u_{j-p}^n, \ldots, u_{j+q}^n; h_1\tau\right) = 2F\left(u_{j-p}^n, \ldots, u_{j+q}^n; h_1\tau\right) \quad , \tag{4.59}$$

that is,

$$\hat{U}_4^{(G)} F\left(u_{j-p}^n, \ldots, u_{j+q}^n; h_1\tau\right) = 2F\left(u_{j-p}^n, \ldots, u_{j+q}^n; h_1\tau\right) \quad , \tag{4.60}$$

as follows from the Lie derivative (4.5). The detailed explicit form of (4.60) is

$$h\frac{\partial F}{\partial h}+u_{j-p}^{n}\frac{\partial F}{\partial u_{j-p}^{n}}+\ldots+u_{j+q}^{n}\frac{\partial F}{\partial u_{j+q}^{n}}+u_{j-1-p}^{n}\frac{\partial F}{\partial u_{j-1-p}^{n}}+\ldots+u_{j-1+q}^{n}\frac{\partial F}{\partial u_{j-1+q}^{n}}=2F \quad , \qquad (4.61)$$

for invariant numerical flux functions for the inviscid Burgers equation. The characteristic equations of (4.61) are

$$\frac{d\tau}{0}=\frac{dh}{h}=\frac{du_{j-p}^{n}}{u_{j-p}^{n}}=\frac{du_{j+q}^{n}}{u_{j+q}^{n}}=\frac{du_{j-1-p}^{n}}{u_{j-1-p}^{n}}=\frac{du_{j-1+q}^{n}}{u_{j-1+q}^{n}}=\frac{dF}{2F} \qquad (4.62)$$

with solutions

$$\frac{F}{h^2}=\text{const.} \quad , \qquad (4.63)$$

$$\tau=\text{const.} \quad , \qquad (4.64)$$

$$\frac{u_{j-p}^{n}}{h}=\text{const.} \quad , \qquad (4.65)$$

$$\frac{u_{j+q}^{n}}{h}=\text{const.} \quad , \qquad (4.66)$$

$$\frac{u_{j-1-p}^{n}}{h}=\text{const.} \quad , \qquad (4.67)$$

and

$$\frac{u_{j-1+q}^{n}}{h}=\text{const.} \qquad (4.68)$$

Therefore, the general solution for the invariant numerical flux function for the inviscid Burgers equation can be written as

$$F=h^2H_2\left(\frac{u_{j-p}^{n}}{h},\ldots,\frac{u_{j+q}^{n}}{h},\frac{u_{j-1-p}^{n}}{h},\ldots,\frac{u_{j-1+q}^{n}}{h};\tau\right) \quad , \qquad (4.69)$$

in which H_2 is an arbitrary function of the indicated arguments. As was the case for the advection equation, it is possible, in principle, to construct an infinite number of invariant conservative difference schemes for the inviscid Burgers equation because of the arbitrary function in (4.69).

Examples of difference schemes whose numerical flux functions for the inviscid Burgers equation are special cases of the invariant result (4.69) include (1) Lax-Friedrichs, (2) Lax-Wendroff, (3) forward-backward MacCormack, (4) backward-forward MacCormack, (5) Richtmyer two-step Lax-Wendroff, and (6) Beam-Warming. The first five of these difference schemes are included in the $p=0$ and $q=1$ case of the conservation form (4.2), namely

$$u_j^{n+1}=u_j^n-\frac{\tau}{h}\left[F\left(u_j^n,u_{j+1}^n\right)-F\left(u_{j-1}^n,u_j^n\right)\right] \quad . \qquad (4.70)$$

The corresponding invariant numerical flux functions for the inviscid Burgers equation that come out of the choice of the function H_2 in (4.69) are as follows:

(1) For the Lax-Friedrichs scheme, we obtain

$$F\left(u_j^n, u_{j+1}^n\right) = \frac{h}{2\tau}\left(u_j^n - u_{j+1}^n\right) + \frac{1}{4}\left[\left(u_j^n\right)^2 + \left(u_{j+1}^n\right)^2\right] \quad . \tag{4.71}$$

(2) For Lax-Wendroff,

$$F\left(u_j^n, u_{j+1}^n\right) = \frac{1}{4}\left[\left(u_j^n\right)^2 + \left(u_{j+1}^n\right)^2\right] - \frac{\tau}{8h}\left(u_j^n + u_{j+1}^n\right)\left[\left(u_{j+1}^n\right)^2 - \left(u_j^n\right)^2\right] \quad . \tag{4.72}$$

(3) For forward-backward MacCormack,

$$F\left(u_j^n, u_{j+1}^n\right) = \frac{\left(u_{j+1}^n\right)^2}{4} + \frac{1}{4}\left\{u_j^n - \frac{\tau}{2h}\left[\left(u_{j+1}^n\right)^2 - \left(u_j^n\right)^2\right]\right\}^2 \quad . \tag{4.73}$$

(4) For backward-forward MacCormack,

$$F\left(u_j^n, u_{j+1}^n\right) = \frac{\left(u_j^n\right)^2}{4} + \frac{1}{4}\left\{u_{j+1}^n - \frac{\tau}{2h}\left[\left(u_{j+1}^n\right)^2 - \left(u_j^n\right)^2\right]\right\}^2 \quad . \tag{4.74}$$

(5) For Richtmyer two-step Lax-Wendroff,

$$F\left(u_j^n, u_{j+1}^n\right) = \frac{1}{2}\left(u_{j+\frac{1}{2}}^{n+\frac{1}{2}}\right)^2 \quad , \tag{4.75}$$

where

$$u_{j+\frac{1}{2}}^{n+\frac{1}{2}} = \frac{1}{2}\left(u_j^n + u_{j+1}^n\right) - \frac{\tau}{4h}\left[\left(u_{j+1}^n\right)^2 - \left(u_j^n\right)^2\right] \quad . \tag{4.76}$$

The Beam-Warming scheme is a $p = 1$ and $q = 0$ case of the conservation form (4.2), that is,

$$u_j^{n+1} = u_j^n - \frac{\tau}{h}\left[F\left(u_{j-1}^n,\ u_j^n\right) - F\left(u_{j-2}^n,\ u_{j-1}^n\right)\right] \quad , \tag{4.77}$$

and the corresponding invariant numerical flux function for the inviscid Burgers equation is

$$F\left(u_{j-1}^n, u_j^n\right) = \frac{1}{4}\left[3\left(u_j^n\right)^2 - \left(u_{j-1}^n\right)^2\right] - \frac{\tau}{8h}\left(u_j^n + u_{j-1}^n\right)\left[\left(u_j^n\right)^2 - \left(u_{j-1}^n\right)^2\right] \quad . \tag{4.78}$$

It will be noted that all of the invariant numerical flux functions that have been found in equations (4.71)-(4.75), and (4.78) for the inviscid Burgers equation are all consistent, that is,

$$F(u,u)=\frac{u^2}{2} \quad . \tag{4.79}$$

Also, if each of these results is divided by h^2, they are seen to be a special case of the general result (4.69).

4.4 INVARIANT FLUX LIMITERS

The method of flux limiters combines low and high order numerical flux functions in such a way that the resulting numerical flux function reduces to high order in smooth regions and to low order near discontinuities. Let F_H be the numerical flux function of a high order scheme, such as Lax-Wendroff or Beam-Warming, and let F_L be the numerical flux function of a lower order scheme, such as upwind or Lax-Friedrichs. Then

$$F_H = F_L + (F_H - F_L) \quad , \tag{4.80}$$

in which the term $F_H - F_L$ is called the antidiffusive flux. In a numerical flux function with a flux limiter denoted by Φ, the antidiffusive term is weighted with the limiter to obtain the numerical flux function with a flux limiter, namely, F_{FL} given by

$$F_{FL} = F_L + \Phi(F_H - F_L) \quad . \tag{4.81}$$

Flux limiters tend to be near unity in smooth regions and near zero around discontinuites. If both the low and high order flux functions used in a flux limited numerical flux function are group invariant, the introduction of the flux limiter can conceivably lead to a breaking of the symmetry of the flux. A proof follows that shows the argument of the flux limiter can be constructed so as to maintain the invariance properties of a flux limited numerical flux function.

A measure of data smoothness used is the ratio of consecutive gradients given by

$$r_j = \frac{u_j - u_{j-1}}{u_{j+1} - u_j} \quad . \tag{4.82}$$

If this ratio is near unity, the data is presumably smooth near u_j, but if it is far from unity, then the data is not smooth. If the limiter is taken as a function of the ratio of consecutive gradients, the resulting numerical flux function is, in fact, also invariant if the low and high order components are. To illustrate this let the low order component be the numerical flux function,

$$F_L = c\, u_j^n \,, \quad \text{if } c > 0 \quad , \tag{4.83}$$

of the upwind scheme,

$$u_j^{n+1} = u_j^n - \frac{c\tau}{h}\left(u_j^n - u_{j-1}^n\right) \quad , \tag{4.84}$$

for the advection equation. Also, let the high order component be the numerical flux function,

$$F_H = \frac{c}{2}\left(u_j^n + u_{j+1}^n\right) - \frac{\tau c^2}{2h}\left(u_{j+1}^n - u_j^n\right) \quad , \tag{4.85}$$

of the Lax-Wendroff scheme,

$$u_j^{n+1} = u_j^n - \frac{\tau c}{2h}\left(u_{j+1}^n - u_{j-1}^n\right) + \frac{1}{2}\left(\frac{\tau c}{h}\right)^2\left(u_{j+1}^n + u_{j-1}^n - 2u_j^n\right) \quad , \tag{4.86}$$

for the advection equation. With

$$\Phi_j = \Phi\left(r_j\right) \quad , \tag{4.87}$$

the flux limited numerical flux function is

$$F_L = c\,u_j^n + \Phi_j \frac{c}{2}\left(1 - \frac{c\tau}{h}\right)\left(u_{j+1}^n - u_j^n\right) \quad . \tag{4.88}$$

By rewriting this as

$$\frac{F_{FL}}{u_j^n} = c + \Phi_j \frac{c}{2}\left(1 - \frac{c\tau}{h}\right)\left(\frac{u_{j+1}^n}{u_j^n} - 1\right) \quad , \tag{4.89}$$

and noting that

$$r_j = \frac{1 - \dfrac{u_{j-1}^n}{u_j^n}}{\dfrac{u_{j+1}^n}{u_j^n} - 1} \quad , \tag{4.90}$$

we see that the flux function (4.8) with the limiter (4.87) is a special case of the general invariant result given in (4.29) for the advection equation. The high resolution difference scheme that is obtained with the flux limited flux (4.88) is

$$u_j^{n+1} = u_j^n - \frac{c\tau}{h}\left(u_j^n - u_{j-1}^n\right) - \frac{1}{2}\frac{c\tau}{h}\left(1 - \frac{c\tau}{h}\right)\left[\Phi_j\left(u_{j+1}^n - u_j^n\right) - \Phi_{j-1}\left(u_j^n - u_{j-1}^n\right)\right] \quad . \tag{4.91}$$

This scheme is conservative and admits the same four-parameter group as that admitted by the advection equation. The flux limiter (4.87) does not break symmetry.

Limiters that yield TVD methods are discussed by Sweby [12]. These include Roe's "superbee limiter"

$$\Phi\left(r_j\right) = \max\left[0, \min\left(1, 2r_j\right), \min\left(r_j, 2\right)\right] \quad , \tag{4.92}$$

and the von Leer limiter,

$$\Phi(r_j)=\frac{|r_j|+r_j}{1+|r_j|} \quad , \tag{4.93}$$

both of which are non-symmetry breaking.

In the case of the advection equation flux limiters and slope limiters σ_j^n discussed in Section 4.5 are related by

$$\Phi_j=\frac{h\sigma_j^n}{u_{j+1}^n-u_j^n} \quad . \tag{4.94}$$

Hence, the minmod function slope limiter,

$$h\sigma_j^n=\min\operatorname{mod}\left(u_{j+1}^n-u_j^n,\, u_j^n-u_{j-1}^n\right) \quad , \tag{4.95}$$

corresponds to the flux limiter,

$$\Phi_j=\begin{cases}0 & \text{if} \quad r_j\le 0\\ r_j & \text{if} \quad 0\le r_j\le 1\\ 1 & \text{if} \quad r_j\ge 1\end{cases} \quad . \tag{4.96}$$

The numerical flux function (4.88) with the flux limiter (4.96) is also invariant and TVD.

High resolution invariant numerical flux functions for the inviscid Burgers equation are derived in Section 4.5 by the method of slope limiters.

4.5 INVARIANT SLOPE LIMITERS

An alternative point of view for construction high resolution numerical schemes to that of the flux limiter method is that of the slope limiter method as discussed in LeVeque [6]. In the latter method, data at the nth time level are represented by piecewise linear functions rather than by piecewise constant functions as in the first order Godunov method. Proofs are given below to show that slope limiter algorithms for the advection equation and the inviscid Burgers equation can be constructed in such a way that the numerical flux functions are invariant under four-parameter groups admitted by these two scalar conservation laws.

The basic significance of numerical flux functions can be seen by integrating the conservation law $\partial_t u+\partial_x f(u)=0$ over the nth time interval and the ith spatial cell to obtain

$$\begin{aligned}\frac{1}{h}\int_{x_{j-\frac{1}{2}}}^{x_{j+\frac{1}{2}}} dx\, u(x,t_{n+1})=\frac{1}{h}\int_{x_{j-\frac{1}{2}}}^{x_{j+\frac{1}{2}}} dx\, u(x,t_n)-\frac{\tau}{h}\Bigg\{\frac{1}{\tau}\int_{t_n}^{t_{n+1}} dt\, f\left[u\left(x_{j+\frac{1}{2}},t\right)\right]\\ -\frac{1}{\tau}\int_{t_n}^{t_{n+1}} dt\, f\left[u\left(x_{j-\frac{1}{2}},t\right)\right]\Bigg\} \quad .\end{aligned} \tag{4.97}$$

This shows that

$$\text{numerical flux function} = \frac{1}{\tau}\int_{t_n}^{t_{n+1}} dt\, f\left[u\left(x_{j+\frac{1}{2}},t\right)\right] = F \quad , \tag{4.98}$$

and

$$u_j^{n+1} = \frac{1}{h}\int_{x_{j-\frac{1}{2}}}^{x_{j+\frac{1}{2}}} dx\, u(x,t_{n+1}) \quad . \tag{4.99}$$

To construct slope limited algorithms linear interpolation of the data at the nth time level is used, that is,

$$u^n(x,t_n) = u_j + \sigma_j^n(x - x_j) \quad \text{for} \quad x_{j-\frac{1}{2}} \le x \le x_{j+\frac{1}{2}} \quad , \tag{4.100}$$

and

$$u^n(x,t_n) = u_{j-1}^n + \sigma_{j-1}^n(x - x_{j-1}) \quad \text{for} \quad x_{j-\frac{3}{2}} \le x \le x_{j-\frac{1}{2}} \quad , \tag{4.101}$$

where σ_j^n is the slope in the jth cell.

The exact solution of the advection equation,

$$u_t + cu_x = 0 \tag{4.102}$$

satisfies

$$u(x - c(t + \tau)) = u(x - h - c\,t) \quad , \tag{4.103}$$

so

$$u(x,t_{n+1}) = u(x - c\tau, t_n) \quad . \tag{4.104}$$

Substituting (4.104) into (4.100) and (4.101) and using the results to evaluate (4.99) produces

$$u_j^{n+1} = \frac{1}{h}\int_{x_{j-\frac{1}{2}}}^{x_{j-\frac{1}{2}}+c\tau} dx\left[u_{j-1}^n + \sigma_{j-1}^n(x - c\tau - x_{j-1})\right]$$

$$+\frac{1}{h}\int_{x_{j-\frac{1}{2}}+c\tau}^{x_{j-\frac{1}{2}}} dx\left[u_j^n + \sigma_j^n(x - c\tau - x_j)\right] \quad , \tag{4.105}$$

which simplifies to

$$u_j^{n+1} = u_j^n - \frac{c\tau}{h}(u_j^n - u_{j-1}^n) - \frac{c\tau}{2h}\left(1 - \frac{c\tau}{h}\right)(h\sigma_j^n - h\sigma_{j-1}^n) \quad . \tag{4.106}$$

The numerical flux function for this scheme is

$$F\left(u_j^n, \ldots\right) = c u_j^n + \frac{c}{2}\left(1 - \frac{c\tau}{h}\right) h\sigma_j^n \tag{4.107}$$

in terms of the slope limiter. As written, this result is not necessarily invariant; that is, a special case of the invariant numerical flux function obtained in (4.29) for the advection equation. However, examples of choices of the slope limiter in (4.107) that yield invariant numerical flux functions include the following:

(1) If we take

$$\sigma_j^n = 0 \quad , \tag{4.108}$$

then (4.107) reduces to the upwind flux which in invariant.

(2) If we take

$$h\sigma_j^n = u_{j+1}^n - u_j^n \tag{4.109}$$

then (4.107) reduces to the Lax-Wendroff flux,

$$F\left(u_j, u_{j+1}\right) = \frac{c}{2}\left(u_j^n + u_{j+1}^n\right) - \frac{c^2\tau}{2h}\left(u_{j+1}^n - u_j^n\right) \quad , \tag{4.110}$$

which is a special case of the invariant flux (4.29).

(3) If we take

$$h\sigma_j^n = \frac{u_{j+1}^n - u_{j-1}^n}{2} \quad , \tag{4.111}$$

then (4.107) reduces to

$$F\left(u_{j-1}, u_j, u_{j+1}\right) = c\, u_j^n + \frac{c}{4}\left(1 - \frac{\tau c}{h}\right)\left(u_{j+1}^n - u_{j-1}^n\right) \quad . \tag{4.112}$$

This is the numerical flux function for the Fromm algorithm which is the average of those for the Lax-Wendroff and Beam-Warming methods to cancel leading and lagging phase errors. The Fromm numerical flux function is a special case of the general invariant result (4.29), so the slope limiter (4.111) does not break symmetry.

(4) If we take

$$h\sigma_j^n = \min \operatorname{mod}\left(u_{j+1}^n - u_j^n, u_j^n - u_{j-1}^n\right) \quad , \tag{4.113}$$

where the minmod function is defined by

$$\min \bmod = (a, b) = \begin{cases} a, & \text{if} \quad |a| < |b| \quad \text{and} \quad ab > 0, \\ b, & \text{if} \quad |b| < |a| \quad \text{and} \quad ab > 0, \\ 0, & \text{if} \qquad ab < 0, \end{cases} \tag{4.114}$$

then (4.107) becomes

$$F\left(u_{j-1}^n, u_j^n, u_{j+1}^n\right) = c\, u_j^n + \frac{c}{2}\left(1 - \frac{c\tau}{h}\right) \min \bmod \left(u_{j+1}^n - u_j^n, u_j^n - u_{j-1}^n\right) \quad . \tag{4.115}$$

This is seen to be a special case of the general invariant numerical flux function (4.29) for the advection equation. Hence, the use of the minmod function for the slope limiter produces a difference scheme that admits the four-parameter group with the generators (4.13) - (4.16) that is also admitted by the advection equation.

The slope limiter method for the nonlinear scalar conservation law $\partial_t u + \partial_x f(u) = 0$ may be derived as follows. On the interval $u_j^n \leq u \leq u_{j+1}^n$, the flux function is approximated by linear interpolation, that is,

$$f(u) = f\left(u_j^n\right) + \left(u - u_j^n\right) A_j \quad , \tag{4.116}$$

where

$$A_j = \frac{f\left(u_{j+1}^n\right) - f\left(u_j^n\right)}{u_{j+1}^n - u_j^n} \tag{4.117}$$

is interpreted as an approximation of the derivative of the flux function around $x = x_{j+\frac{1}{2}}$. Accordingly, in this neighborhood the conservation law is approximated by

$$u_t + A_j u_x = 0 \quad . \tag{4.118}$$

For the time interval $t_n \leq t \leq t_{n+1}$ the exact solution of (4.118) is

$$u(x,t) = g\left[x - A_j\left(t - t_n\right)\right] \tag{4.119}$$

in which g is a function of the indicated argument. By using linear interpolation of the data at the nth time level, namely,

$$u(x,t) = u_j^n + \sigma_j^n\left(x - x_j\right) \tag{4.120}$$

together with (4.119), we construct the approximation

$$u(x,t) = u_j^n + \sigma_j^n\left[x - x_j - \left(t - t_n\right)A_j\right] \quad . \tag{4.121}$$

From (4.116) we have

$$f\left[u\left(x_{j+\frac{1}{2}},t\right)\right]=f(u_j^n)+\left[u\left(x_{j+\frac{1}{2}},t\right)-u_j^n\right]A_j \quad , \tag{4.122}$$

which with (4.121) becomes

$$f\left[u\left(x_{j+\frac{1}{2}},t\right)\right]=f(u_j^n)+A_j\left[\frac{h}{2}-(t-t_n)A_j\right]\sigma_j^n \quad . \tag{4.123}$$

By substituting (4.123) into the integral for the numerical flux function given in (4.98) it is found that

$$F(u_j^n,\ldots)=f(u_j^n)+\frac{A_j}{2}\left(1-\frac{\tau}{h}A_j\right)h\sigma_j^n \quad . \tag{4.124}$$

The corresponding difference scheme in conservation form is

$$u_j^{n+1}=u_j^n-\frac{\tau}{h}\left[f(u_j^n)-f(u_{j-1}^n)+\frac{A_j}{2}\left(1-\frac{\tau}{h}A_j\right)h\sigma_j^n-\frac{A_{j-1}}{2}\left(1-\frac{\tau}{h}A_{j-1}\right)h\sigma_{j-1}^n\right] \tag{4.125}$$

in terms of the slope limiter. For a given flux function $f(u)$ in the conservation law, $\partial_t u+\partial_x f(u)=0$, the choice of the slope limiter may or may not yield an invariant difference scheme (4.125).

For the inviscid Burgers equation the flux function is $u^2/2$, and the numerical flux function (4.124) becomes

$$F=\frac{(u_j^n)^2}{2}+\left(\frac{u_{j+1}^n+u_j^n}{4}\right)\left[1-\frac{\tau}{2h}(u_{j+1}^n+u_j^n)\right]h\sigma_j^n \quad . \tag{4.126}$$

If the slope limiter in this equation is selected so that it becomes a special case of the general invariant numerical flux function obtained in (4.69) for the inviscid Burgers equation, then the conservative difference scheme (4.125) will also be invariant. With the slope limiter (4.109) the numerical flux function (4.126) reduces to that of the Lax-Wendroff method given in (4.72) for the inviscid Burgers equation. By writing (4.126) in the form,

$$\frac{F}{h^2}=\frac{1}{2}\left(\frac{u_j^n}{h}\right)^2+\frac{1}{4}\left(\frac{u_{j+1}^n}{h}+\frac{u_j^n}{h}\right)\left[1-\frac{\tau}{2}\left(\frac{u_{j+1}^n}{h}+\frac{u_j^n}{h}\right)\right]\sigma_j^n \quad , \tag{4.127}$$

and the minmod function (4.113) as

$$\sigma_j^n=\min\bmod\left(\frac{u_{j+1}^n}{h}-\frac{u_j^n}{h},\ \frac{u_j^n}{h}-\frac{u_{j-1}^n}{h}\right) \quad , \tag{4.128}$$

we see that the numerical flux function (4.126) with the minmod function for a slope limiter becomes a special case of the general invariant flux function in (4.69). Accordingly, when the minmod function is used as a slope limiter in numerical flux functions in conservative difference schemes for both in inviscid Burgers equation and the advection equation, these schemes are invariant under the four-parameter groups admitted by these equations.

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