LA-12791-T
c.3

LA-12791-T
Thesis

Lie Group Invariant Finite Difference Schemes for the Neutron Diffusion Equation

Los Alamos
NATIONAL LABORATORY

Los Alamos National Laboratory is operated by the University of California for the United States Department of Energy under contract W-7405-ENG-36.

This thesis was accepted by the Department of Nuclear Engineering of the University of Illinois at Urbana-Champaign Graduate College in partial fulfillment of the requirements for the degree of Doctor of Philosophy. The text and illustrations are the independent work of the author and only the front matter has been edited by the CIC-1 staff to conform with Department of Energy and Los Alamos National Laboratory publication policies.

LA-12791-T

UC-705
Issued: June 1994

Lie Group Invariant Finite Difference Schemes for the Neutron Diffusion Equation

*Peter James Jaegers**

**Intern at Los Alamos Group NIS-6.*

Los Alamos
NATIONAL LABORATORY
Los Alamos, New Mexico 87545

ACKNOWLEDGMENTS

I would like to take this opportunity to thank a few people. First, I would like to thank my advisor, Dr. Axford, for his guidance and his helpful suggestions in performing this research. I would also like to thank the folks at LANL, especially Dick Malenfant and Rick Paternoster, who provided me with a desk and the computing time necessary to carry out some of this research. Additionally, I would like to thank the Department of Nuclear Engineering at the University of Illinois, Argonne National Laboratory, and Los Alamos National Laboratory for providing the funding for this endeavor.

TABLE OF CONTENTS

LIST OF TABLES

LIST OF FIGURES

LIE GROUP INVARIANT FINITE DIFFERENCE SCHEMES FOR THE NEUTRON DIFFUSION EQUATION

ABSTRACT

by

Peter James Jaegers

Finite difference techniques are used to solve a variety of differential equations. For the neutron diffusion equation, the typical local truncation error for standard finite difference approximation is on the order of the mesh spacing squared. To improve the accuracy of the finite difference approximation of the diffusion equation, the invariance properties of the original differential equation have been incorporated into the finite difference equations. Using the concept of an invariant difference operator, the invariant difference approximations of the multi-group neutron diffusion equation were determined in one-dimensional slab and two-dimensional Cartesian coordinates, for multiple region problems. These invariant difference equations were defined to lie upon a cell edged mesh as opposed to the standard difference equations, which lie upon a cell centered mesh. Results for a variety of source approximations showed that the invariant difference equations were able to determine the eigenvalue with greater accuracy, for a given mesh spacing, than the standard difference approximation. The local truncation errors for these invariant difference schemes were found to be highly dependent upon the source approximation used, and the type of source distribution played a greater role in determining the accuracy of the invariant difference scheme than the local truncation error.

1 INTRODUCTION

Differential equations play an important role in our understanding of nature. Typically though, the determination of an analytic solution can be extremely difficult. Even if an analytic solution can be found, the numerical evaluation of the solution can be no easy task. It is, therefore, desirable in many situations to use numerical methods to solve differential equations. In the ensuing discussion we will limit ourselves to finite difference techniques for the solution of differential equations.

Numerical methods have the drawback that they usually find an approximate solution to the differential equations being simulated. For typical finite difference simulations the error associated with the simulation is usually a function of the mesh size. This error can be made arbitrarily small by using smaller and smaller mesh spacing. However, with this increase in accuracy comes the requirement of a greater investment in computational resources such as computer memory and time, since more difference equations must be solved. Therefore, it is desirable to determine finite difference formulations that retain accuracy without a prohibitive amount of computational investment.

One would expect that difference schemes that preserve the properties of the solution of an original differential equation would be more accurate. To this end, difference schemes that incorporate the symmetry properties of the original differential equation have been investigated.

In gas dynamics, Shokin [1] has studied difference schemes for which the first differential approximation of the difference equations is invariant under the same group of Lie point transformations as the gas dynamics equations. While Shokin's difference scheme has lead to an improvement in accuracy, the fact that the differential approximation is invariant does not guarantee that higher order approximations are invariant; hence, this method can not produce difference equations whose exact solution coincides with the exact solution to the differential equations being simulated.

Axford has reported in references 2 and 3 that difference schemes which are invariant under the same group of Lie point transformations admitted by the differential equations can lead to difference equations whose exact solution agrees with the exact solution of the simulated differential equations.

The purpose of the author's research has been to investigate invariant finite difference schemes which admit the same group of Lie point transformations that are admitted by the differential equations being simulated. Special emphasis has been placed upon solving the second order ordinary differential equations and second order elliptic partial differential equations that arise in the study of reactor physics, namely, the steady state multi-group diffusion equation given by

$$\nabla\bullet(D_g(\vec{r})\nabla\phi_g(\vec{r})) - \Sigma_{R,g}(\vec{r})\phi_g(\vec{r}) + S_g(\vec{r}) = 0 \qquad (1.1)$$

where $D_g(r)$ is the gth energy group diffusion coefficient, $\Sigma_{r,g}(r)$ is the gth energy group removal cross section, and $\phi_g(r)$ is the gth group neutron flux. $S_g(r)$ is the gth group source, which can include sources from fission, scattering, and external sources as given by

$$S_g(\vec{r}) = \sum_{g'=1}^{G} \Sigma_{g'\rightarrow g}\phi_{g'}(\vec{r}) + \frac{\chi_g}{\lambda}\sum_{g'=1}^{G} \nu\Sigma_{f\,g'}\phi_{g'}(\vec{r}) + S_{g\,ext}(\vec{r}) \qquad (1.2)$$

where $\Sigma_{g'-g}$ is the group g' to g scattering cross section, χ_g is the probability that a fission neutron is born into group g, λ is the eigenvalue, ν is the average number of neutrons per fission, $\Sigma_{f\,g'}$ is the g'th group's fission cross section, and $S_{g\,ext}$ is the external source of neutrons. Equation (1.1) is a particularly useful form, since it easily lends itself to source iteration calculations. Results will be presented that demonstrate that these types of difference schemes offer distinct advantages in that one can achieve greater accuracy with fewer mesh points then is possible with conventional difference schemes. In fact, it will be shown that under certain circumstances, invariant difference schemes will produce the exact solution of the original differential equation.

2 FINITE DIFFERENCE TECHNIQUES

A common method by which differential equations are solved is through the use of finite differences. In the finite difference technique, the differential equation to be solved is simulated by approximating the derivatives with differences over some small interval. This leads to a set of algebraic equations for which the unknowns are to be determined on a set of points defined by some mesh. When formulating finite difference simulations, several things need to be considered: 1) what is the error associated which the simulation; 2) is the finite difference simulation consistent with the original differential equation; 3) does the simulation have the properties of stability and convergence? In this section, we will explore the construction and solution of standard types of difference equations and answer the above questions.

2.1 Construction of a Finite Difference Approximation of the Diffusion Equation

There are several ways to derive finite difference simulations of differential equations. An overview of these methods can be found in references 4 through 10. Typically, derivatives in the differential equation are approximated using some sort of truncated Taylor series.

As an example, we consider the dependent variable U, which depends on the independent variable x. Defining the grid locations $x_{i+1} = x_i + h$ and $x_{i-1} = x_i - h$, where h is the mesh spacing, we can expand $U(x_{i+1})$ and $U(x_{i-1})$ in a Taylor series about x_i to yield

$$U(x_{i+1}) = U(x_i) + h\,U'(x_i) + \frac{h^2}{2}\,U''(x_i) + \cdots \tag{2.1}$$

and

$$U(x_{i-1}) = U(x_i) - h\,U'(x_i) + \frac{h^2}{2}\,U''(x_i) + \cdots \ . \tag{2.2}$$

Subtracting equations (2.1) and (2.2) and truncating the terms of order h^2 and greater yields

$$U(x_{i-1}) - U(x_{i-1}) = 2h\, U'(x_i) \quad . \tag{2.3}$$

Solving for $U'(x_i)$, we obtain the two-point central difference approximation for a first order derivative as

$$U'(x_i) = \frac{U(x_{i+1}) - U(x_{i-1})}{2h} \quad . \tag{2.4}$$

Next adding equations (2.1) and (2.2) and truncating terms of the order h^3 and greater leads to the three point central difference approximation for a second order derivative given by

$$U''(x_i) = \frac{U(x_{i+1}) - U(x_i) + U(x_{i-1})}{h^2} \quad . \tag{2.5}$$

In a similar manner, partial derivatives can also be approximated. Consider the case of a dependent variable U, and the independent variables x and y. We can expand the terms $U(x_{i+1},y_j)$ and $U(x_{i-1},y_j)$, while holding y constant, in a Taylor series as

$$U(x_{i+1},y_j) = U(x_i,y_j) + h\frac{\partial U(x_i,y_j)}{\partial x} + \frac{h^2}{2}\frac{\partial^2 U(x_i,y_j)}{\partial x^2} + \cdots \tag{2.6}$$

and

$$U(x_{i-1},y_j) = U(x_i,y_j) - h\frac{\partial U(x_i,y_j)}{\partial x} + \frac{h^2}{2}\frac{\partial^2 U(x_i,y_j)}{\partial x^2} + \cdots \quad . \tag{2.7}$$

As before, upon adding we arrive at the three-point central difference approximation for the second partial derivative of U with respect to x given by

$$\frac{\partial^2 U(x_i,y_j)}{\partial x^2} = \frac{U(x_{i+1},y_j) - 2U(x_i,y_j) + U(x_{i-1},y_j)}{h^2} \quad . \tag{2.8}$$

Other types of difference approximations can be derived in a similar manner.

We will consider two specific examples of finite difference approximations for the one-energy group neutron diffusion equation with constant material properties. The first case will be one-dimensional in slab geometry, and the second will be two-dimensional in Cartesian coordinates.

The one-group one-dimensional neutron diffusion equation with constant material properties in slab geometry is

$$D\frac{d^2\phi(x)}{dx^2} - \Sigma_R\phi(x) + S(x) = 0 \tag{2.9}$$

where $0 \leq x \leq a$ and the boundary conditions are specified at the right and left hand surfaces as either Neumann or Dirichlet. The finite difference approximation is found by evaluating equation (2.6) at the grid point $x = x_i$ and substituting (2.5) into (2.9) to yield

$$D\frac{\phi(x_{i+1}) - 2\phi(x_i) + \phi(x_{i-1})}{h^2} - \Sigma_R\phi(x_i) + S(x_i) = 0\ . \tag{2.10}$$

Defining $\phi_i = \phi(x_i)$ and $S_i = S(x_i)$, equation (2.10) can be rewritten as

$$D\frac{\phi_{i+1} - 2\phi_i + \phi_{i-1}}{h^2} - \Sigma_R\phi_i + S_i = 0\ . \tag{2.11}$$

Thus we arrive at a set of algebraic equations from which the unknowns ϕ_i can be found.

In two-dimensional Cartesian coordinates, the one-group diffusion equation with constant material properties is

$$D\frac{\partial^2\phi(x,y)}{\partial x^2} + D\frac{\partial^2\phi(x,y)}{\partial y^2} - \Sigma_R\phi(x,y) + S(x,y) = 0\ , \tag{2.12}$$

where $0 \leq x \leq a$ and $0 \leq y \leq b$ and the boundary conditions are either Neumann or Dirichlet at the outer surfaces. As before, the finite difference approximation is found by evaluating this equation at the grid point (x_i,y_j). Difference approximations for the partial derivatives as given by (2.8) and another similar approximation for the partial derivative with respect to y are then substituted into equation (2.12); thus arriving at

$$D\frac{\phi_{i+1,j} - 2\phi_{i,j} + \phi_{i-1,j}}{\Delta x^2} + D\frac{\phi_{i,j+1} - 2\phi_{i,j} + \phi_{i,j-1}}{\Delta y^2} - \Sigma_R\phi_{i,j} + S_{i,j} = 0 \;, \qquad (2.13)$$

where Δx^2 and Δy^2 are the x and y direction mesh spacings respectively.

2.2 Local Truncation Error

Since few finite difference simulations of differential equations produce the exact solution of the differential equation, it is important to know the error associated with the simulation. Considering that most difference schemes are based on a truncated Taylor series, the error associated with the difference scheme at a grid point is called the local truncation error.

The local truncation error, ε_i, can be determined by replacing the unknowns in the difference equation by the exact solution of the differential equation. That is, if the solution, $u = \{u_1, ..., u_N\}$, of the difference equation, $A_i(u) = 0$, is replaced by the solution of the differential equation, U, then the local truncation error is given by $\varepsilon_i = A_i(U)$.

To illustrate this process, we will first consider the one-dimensional diffusion equation as given by (2.9). Let $\Phi(x)$ be the exact solution of this differential equation. A finite difference approximation of (2.9) was found to be (2.11). Substituting the exact solution $\Phi(x)$ into (2.11) yields

$$\varepsilon_i = D\frac{\Phi(x_{i+1}) - 2\Phi(x_i) + \Phi(x_{i-1})}{h^2} - \Sigma_R\Phi(x_i) + S(x_i)\ . \tag{2.14}$$

Next, expanding the exact solution in a Taylor series about the point $x = x_i$ yields

$$\Phi(x_{i+1}) = \Phi(x_i) + h\frac{d\Phi(x_i)}{dx} + \frac{h^2}{2}\frac{d^2\Phi(x_i)}{dx^2} + \cdots \tag{2.15}$$

and

$$\Phi(x_{i-1}) = \Phi(x_i) - h\frac{d\Phi(x_i)}{dx} + \frac{h^2}{2}\frac{d^2\Phi(x_i)}{dx^2} - \cdots\ . \tag{2.16}$$

Substituting (2.15) and (2.16) into (2.14) yields

$$\varepsilon_i = \left[D\Phi''(x_i) - \Sigma_R\Phi(x_i) + S(x_i)\right] + \frac{h^2}{12}\Phi^{(iv)}(x_i) + O(h^4)\ . \tag{2.17}$$

However $\Phi(x_i)$ is the exact solution of equation (2.9) when (2.9) is evaluated at $x = x_i$, so the bracketed term in (2.17) is zero, and the local truncation error is given by

$$\varepsilon_i = \frac{h^2}{12}\Phi^{(iv)}(x_i) + O(h^4) \tag{2.18}$$

where $\Phi^{(iv)}(x_i)$ is the fourth order derivative of $\Phi(x)$ evaluated at grid point x_i.

We will now consider the truncation error for the two-dimensional diffusion equation. As with the one-dimensional case, we let $\Phi(x)$ be the exact solution of (2.12). We then substitute the exact solution into the finite difference approximation (2.13) to give

$$D\frac{\Phi_{i+1,j} - 2\Phi_{i,j} + \Phi_{i-1,j}}{\Delta x^2} + D\frac{\Phi_{i,j+1} - 2\Phi_{i,j} + \Phi_{i,j-1}}{\Delta y^2} - \Sigma_R\Phi_{i,j} + S_{i,j} = 0\ . \tag{2.19}$$

The exact solution is then expanded in a Taylor series to yield

$$\varepsilon_{i,j} = \left[D\frac{\partial^2\Phi_{i,j}}{\partial x^2} + D\frac{\partial^2\Phi_{i,j}}{\partial y^2} - \Sigma_R\Phi_{i,j} + S_{i,j} \right] + \frac{\Delta x^2}{12}\frac{\partial^4\Phi_{i,j}}{\partial x^4} + \frac{\Delta y^2}{12}\frac{\partial^4\Phi_{i,j}}{\partial y^4} + O(\Delta x^4,\Delta y^4) \; . \qquad (2.20)$$

However, since $\Phi(x,y)$ is the exact solution of (2.12) evaluated at the grid point $(x,y) = (x_i,y_j)$, the bracketed term is zero yielding the local truncation error as

$$\varepsilon_{i,j} = \frac{\Delta x^2}{12}\frac{\partial^4\Phi_{i,j}}{\partial x^4} + \frac{\Delta y^2}{12}\frac{\partial^4\Phi_{i,j}}{\partial y^4} + O(\Delta x^4,\Delta y^4) \; . \qquad (2.20)$$

Thus as expected, for both of these finite difference simulations, the local truncation errors depend on the square of the mesh spacing and tend to zero as the mesh spacings become small.

2.3 Consistency of a Finite Difference Scheme

Sometimes it may be possible to derive a difference scheme that produces a solution to a different differential equation than the equation being simulated. Such a difference scheme is said to be inconsistent. A finite difference equation is said to be consistent with a differential equation if the solution of the finite difference equation converges to the solution of the differential equation as the mesh spacing tends to zero. Consistency can be formulated several ways, see reference 5, but the easiest formulation is to say that the local truncation error must go to zero as the mesh spacing goes to zero. In our two example difference schemes, (2.10) and (2.13), it was found that the local truncation errors, as given by (2.18) and (2.20), clearly tended to zero as the mesh spacings tended to zero. Therefore, the difference schemes, (2.10) and (2.13), were consistent with the differential equations being simulated.

2.4 Stability and Convergence

Much has been written in the literature about stability and convergence, see references 10, 14, 16, and 17. In particular it has been shown that the source iteration calculation used to solve the discrete form of the neutron diffusion equation is stable and convergent; references 14, 16, and 17 contain detailed discussions and proofs of the stability and convergence. Since this subject is well known a discussion of this topic will not be presented here.

3 GROUP ANALYSIS OF THE NEUTRON DIFFUSION EQUATION

The determination of a group of point transformations admitted by a differential equation can be found systematically from the transformation theory of differential equations first proposed by Sophus Lie, references 3,11,12, and 13. The group of point transformations admitted by the neutron diffusion equation will be constructed and used later to formulate invariant difference schemes.

3.1 A Brief Introduction to Group Theory

In this section, a brief discussion of the definitions and theory of a group of Lie point transformations is presented.

3.1.1 Continuous Point Transformations

We will consider the case of one dependent variable, y, and one independent variable, x. Let a set of point transformations be given by

$$\bar{x} = f(x,y;a) \tag{3.1a}$$

and

$$\bar{y} = g(x,y;a) \tag{3.1b}$$

where "a" is a parameter. The functions f(x,y;a) and g(x,y;a) are assumed to be continuous and continuously differentiable to all orders in the parameter "a". As the parameter "a" varies, (3.1a) and (3.1b) transform the point P(x,y) into the point P'($\bar{x}$, $\bar{y}$) by

$$\bar{x} = f(x,y;a_0 + \delta a) \tag{3.2a}$$

and

$$\bar{y} = g(x,y;a_0 + \delta a) , \tag{3.2b}$$

where a_0 is an identity element such that

$$x = f(x,y;a_0) \tag{3.3a}$$

and

$$y = g(x,y;a_0). \tag{3.3b}$$

If δa is sufficiently small then the point $P'(\bar{x}, \bar{y})$ can be close to the desired point P(x,y). These transformation are called continuous point transformations.

3.1.2 Definition of a Group of Continuous Point Transformations

For a set of continuous point transformation given by (3.1a) and (3.1b), each value of the parameter "a", called the group parameter, labels a different element of the set. A group is defined as a set of elements together with a binary operation that satisfies the four group axioms namely, closure, existence of an identity element, existence of an inverse element, and associativity of a binary operation. A binary operation is the successive performance of two transformations.

Consider two transformations, the first given by (3.1a) and (3.1b) and the second given by

$$\bar{\bar{x}} = f(\bar{x},\bar{y};b) \tag{3.4a}$$

and

$$\bar{\bar{y}} = g(\bar{x},\bar{y};b). \tag{3.4b}$$

Closure is satisfied if

$$\bar{\bar{x}} = f(f(x,y;a),g(x,y;a);b) = f(x,y;c(a,b)) \tag{3.5a}$$

and

$$\bar{\bar{y}} = g(f(x,y;a),g(x,y;a);b) = g(x,y;c(a,b)) \quad (3.5b)$$

where c(a,b) is called the composition function.

The existence of an identity element axiom is satisfied for some value of the group parameter "a_0" provided that

$$\bar{x} = f(x,y;a_0) = x \quad (3.6a)$$

and

$$\bar{y} = g(x,y;a_0) = y. \quad (3.6b)$$

The existence of an inverse element axiom is satisfied if some value of the group parameter "$\bar{a}$" exists such as

$$x = f(\bar{x},\bar{y};\bar{a}) \quad (3.7a)$$

and

$$y = g(x,y;\bar{a}). \quad (3.7b)$$

Finally, the associativity axiom states given three values of the group parameter a, b, and c and their corresponding transformation denoted by T_a, T_b, and T_c, then

$$(T_a,T_b)T_c = T_a(T_b,T_c). \quad (3.8)$$

If the equations (3.1a) and (3.1b) satisfy the above group axioms, then they are called the finite equations of the group.

3.1.3 Definition of the Coordinate Functions of an Infinitesimal Transformation

Let the group parameter be $a \doteq a_0 + \delta a$, where δa is a small change in the group parameter away from the identity element. Equations (3.1a) and (3.1b) can be written as

$$\bar{x} = f(x,y;a_0 + \delta a) \qquad (3.9a)$$

and

$$\bar{y} = g(x,y;a_0 + \delta a). \qquad (3.9b)$$

Expanding (3.9a) and (3.9b) in a Taylor series about the identity element yields

$$\bar{x} = f(x,y;a_0) + \frac{\partial f(x,y;a_0)}{\partial a}\delta a + \cdots \qquad (3.10a)$$

and

$$\bar{y} = g(x,y;a_0) + \frac{\partial g(x,y;a_0)}{\partial a}\delta a + \cdots. \qquad (3.10b)$$

Since δa is arbitrarily small, the higher order terms in δa can be neglected, and thus with the use of (3.3a) and (3.3b), equations (3.10a) and (3.10b) can be written as

$$\bar{x} = x + \frac{\partial f(x,y;a_0)}{\partial a}\delta a \qquad (3.10a)$$

and

$$\bar{y} = y + \frac{\partial g(x,y;a_0)}{\partial a}\delta a\,. \qquad (3.11b)$$

Defining $\delta x = \bar{x} - x$ and $\delta y = \bar{y} - y$ as the change induced in the variables x and y by a small change in the group parameter away from the identity, we arrive at

$$\delta x = \frac{\partial f(x,y;a_0)}{\partial a}\delta a = \xi(x,y)\delta a \tag{3.12a}$$

and

$$\delta y = \frac{\partial g(x,y;a_0)}{\partial a}\delta a = \eta(x,y)\delta a \ , \tag{3.12b}$$

which are called the infinitesimal transformations of the group. The functions $\xi(x,y)$ and $\eta(x,y)$ are called the coördinate functions of the infinitesimal transformation.

3.1.4 The Definition of the Group Generator of the Infinitesimal Transformation

The change in a function, F(x,y), due to a small change in the group parameter away from the identity can be given by

$$\delta F(x,y) = F(x+\delta x,y+\delta y) - F(x,y) \ . \tag{3.13}$$

Substituting (3.12a) and (3.12b) into (3.3) gives

$$\delta F(x,y) = F(x+\xi\delta a,y+\eta\delta a) - F(x,y) \ . \tag{3.14}$$

Expanding $F(x+\xi\delta a,y+\eta\delta a)$ in a Taylor series and neglecting terms in δa^2 and higher, we obtain

$$\delta F(x,y) = \left[\xi(x,y)\frac{\partial F(x,y)}{\partial x} + \eta(x,y)\frac{\partial F(x,y)}{\partial y}\right]\delta a \ . \tag{3.15}$$

Introducing the notation

$$\hat{U} = \xi(x,y)\frac{\partial}{\partial x} + \eta(x,y)\frac{\partial}{\partial y} \ , \tag{3.16}$$

equation (3.15) can be written as

$$\delta F(x,y) = \hat{U}F(x,y)\delta a \ , \tag{3.17}$$

where $\hat{U}$ is called the group generator or the symbol of the infinitesimal transformation. The group generator can also be defined as

$$\frac{\delta F(x,y)}{\delta a} = \frac{\delta x}{\delta a}\frac{\partial F(x,y)}{\partial x} + \frac{\delta y}{\delta a}\frac{\partial F(x,y)}{\partial y}$$
$$= \xi(x,y)\frac{\partial F(x,y)}{\partial x} + \eta(x,y)\frac{\partial F(x,y)}{\partial y}, \qquad (3.18)$$

where

$$\frac{\delta x}{\delta a} = \xi(x,y) \text{ and } \frac{\delta y}{\delta a} = \eta(x,y). \qquad (3.19)$$

The operator $\delta/\delta a$ is called the group operator or the Lie derivative.

3.1.5 The Invariance Properties of Equations

A function, $F(x,y) = 0$, is said to be invariant under the action of a group of point transformations if

$$\hat{U}F(x,y) = 0. \qquad (3.20)$$

Given a function $F(x,y) = 0$, equation (3.20) can be used to determine the coordinate functions of the infinitesimal transformation.

To examine the invariance of differential equations, it is necessary to know how the derivatives transform; therefore, further coordinate functions are needed. These coordinate functions along with the coordinate functions for the dependent and independent variables comprise the extended infinitesimal transformation. Consider a kth order ordinary differential equation, (ODE), given by $F(x,y,y',\ldots,y^{(k)}) = 0$. Taking the Lie derivative yields

$$\frac{\delta F}{\delta a} = \frac{\delta x}{\delta a}\frac{\partial F}{\partial x} + \frac{\delta y}{\delta a}\frac{\partial F}{\partial y} + \frac{\delta y'}{\delta a}\frac{\partial F}{\partial y'} + \cdots + \frac{\delta y^{(k)}}{\delta a}\frac{\partial F}{\partial y^{(k)}} . \tag{3.21}$$

However, using (3.19) and defining the coordinate function for the jth derivative as

$$\eta^{(j)}(x,y;\cdots y^{(j)}) = \frac{\delta y^{(j)}}{\delta a}$$

equation (3.21) can be rewritten as

$$\frac{\delta F}{\delta a} = \xi(x,y)\frac{\partial F}{\partial x} + \eta(x,y)\frac{\partial F}{\partial y} + \eta^{(1)}(x,y,y')\frac{\partial F}{\partial y'} + \cdots + \eta^{(k)}(x,y,\cdots y^{(k)})\frac{\partial F}{\partial y^{(k)}} . \tag{3.22}$$

Introducing the kth extension of the group generator, equation (3.22) can be written as

$$\frac{\delta F}{\delta a} = \hat{U}^{(k)}F(x,y,y',\cdots y^{(k)}) , \tag{3.23}$$

where

$$\hat{U}^{(k)} = \xi(x,y)\frac{\partial}{\partial x} + \eta(x,y)\frac{\partial}{\partial y} + \eta^{(1)}(x,y,y')\frac{\partial}{\partial y'} + \cdots + \eta^{(k)}(x,y,\cdots y^{(k)})\frac{\partial}{\partial y^{(k)}} . \tag{3.24}$$

The coordinate functions for the derivatives can be written in terms of the derivatives of the coordinate functions of the dependent and independent variables. For one dependent and independent variable, the general formula for the derivative coordinate function is

$$\eta^{(j)}(x,y,\cdots y^{(j)}) = \hat{D}_x\eta^{(j-1)}(x,y,\cdots y^{(j-1)}) - y^{(j)}\hat{D}_x\xi(x,y) , \tag{3.25}$$

where $\hat{D}_x$ is the total derivative operator and for $j = 1$, $\eta^{(0)} = \eta(x,y)$. A kth order ODE is invariant under a group of point transformations if

$$\hat{U}^{(k)}F(x,y,\cdots,y^{(k)}) = 0 , \text{ when } F(x,y,\cdots,y^{(k)}) = 0 . \tag{3.26}$$

Equation (3.26) leads to an over-determined system of partial differential equations, (P.D.E.'s), from which the coordinate functions $\xi(x,y)$ and $\eta(x,y)$ can be found.

3.1.6 More General Lie Algebra

Typically, one encounters a situation in which there are systems of partial differential equations. Consider the case in which there are n independent and m dependent variables; a set of point transformations is given by

$$\bar{x}_i = f_i(x_1,\cdots x_n, y_1,\cdots y_m, a_1,\cdots a_r) \quad 1 \le i \le n \tag{3.27a}$$

and

$$\bar{y}_j = g_j(x_1,\cdots x_n, y_1,\cdots y_m, a_1,\cdots a_r) \quad 1 \le j \le m. \tag{3.27b}$$

Equations (3.27a) and (3.27b) comprise an r-parameter group of point transformation if they satisfy the four group axioms as stated earlier. The corresponding group generator for this case is given by

$$\hat{U}_s = \sum_{i=1}^{n} \xi_{i,s}(\vec{x},\vec{y})\frac{\partial}{\partial x_i} + \sum_{j=1}^{m} \eta_{j,s}(\vec{x},\vec{y})\frac{\partial}{\partial y_j}, \tag{3.28a}$$

where the coordinate functions are given by

$$\xi_{i,s}(\vec{x},\vec{y}) = \frac{\partial f_i}{\partial a_s}\Big|_{\vec{a}=\vec{a}_0}, \tag{3.28b}$$

$$\eta_{j,s}(\vec{x},\vec{y}) = \frac{\partial g_j}{\partial a_s}\Big|_{\vec{a}=\vec{a}_0}, \tag{3.28b}$$

$\vec{x} = \langle x_1,\cdots,x_n\rangle$, $\vec{y} = \langle y_1,\cdots,y_m\rangle$, and $\vec{a} = \langle a_1,\cdots,a_r\rangle$ for s = 1, . . . ,r. As before, in dealing with differential equations the extensions of the group generators are required to determine how the derivatives transform under the action of the group. The formulae for these coordinate functions can become quite complicated.

As a specific example, we will consider the results for one dependent variable, ϕ, and two independent variables, x and y. The second extension of the group generator for this case is

$$\begin{aligned}\hat{U}^{(2)} = \xi_1 \frac{\partial}{\partial x} + \xi_2 \frac{\partial}{\partial y} + \eta \frac{\partial}{\partial \phi} + \eta_x^{(1)} \frac{\partial}{\partial \phi_x} + \eta_y^{(1)} \frac{\partial}{\partial \phi_y} \\ + \eta_{xx}^{(2)} \frac{\partial}{\partial \phi_{xx}} + \eta_{xy}^{(2)} \frac{\partial}{\partial \phi_{xy}} + \eta_{yx}^{(2)} \frac{\partial}{\partial \phi_{yx}} + \eta_{yy}^{(2)} \frac{\partial}{\partial \phi_{yy}} ,\end{aligned} \tag{3.29a}$$

where

$$\eta_x^{(1)} = \frac{\partial \eta}{\partial x} + \left[\frac{\partial \eta}{\partial \phi} - \frac{\partial \xi_1}{\partial x}\right] \phi_x - \frac{\partial \xi_2}{\partial x} \phi_y - \frac{\partial \xi_1}{\partial \phi} (\phi_x)^2 - \frac{\partial \xi_2}{\partial \phi} \phi_x \phi_y , \tag{2.29b}$$

$$\eta_x^{(1)} = \frac{\partial \eta}{\partial x} + \left[\frac{\partial \eta}{\partial \phi} - \frac{\partial \xi_1}{\partial x}\right] \phi_x - \frac{\partial \xi_2}{\partial x} \phi_y - \frac{\partial \xi_1}{\partial \phi} (\phi_x)^2 - \frac{\partial \xi_2}{\partial \phi} \phi_x \phi_y , \tag{2.29c}$$

$$\begin{aligned}\eta_{xx}^{(2)} = \frac{\partial^2 \eta}{\partial x^2} + \left[2 \frac{\partial^2 \eta}{\partial x \partial \phi} - \frac{\partial^2 \xi_1}{\partial x^2}\right] \phi_x - \frac{\partial^2 \xi_2}{\partial x^2} \phi_y + \left[\frac{\partial \eta}{\partial \phi} - 2 \frac{\partial \xi_1}{\partial x}\right] \phi_{xx} - 2 \frac{\partial \xi_2}{\partial x} \phi_{xy} \\ + \left[\frac{\partial^2 \eta}{\partial \phi^2} - 2 \frac{\partial^2 \xi_1}{\partial x \partial \phi}\right] (\phi_x)^2 - 2 \frac{\partial^2 \xi_2}{\partial x \partial \phi} \phi_x \phi_y - \frac{\partial^2 \xi_1}{\partial \phi^2} (\phi_x)^3 - \frac{\partial^2 \xi_2}{\partial \phi^2} (\phi_x)^2 \phi_y \\ - 3 \frac{\partial \xi_1}{\partial \phi} \phi_x \phi_{xx} - \frac{\partial \xi_2}{\partial \phi} \phi_y \phi_{xx} - 2 \frac{\partial \xi_2}{\partial \phi} \phi_x \phi_{xy} ,\end{aligned} \tag{3.29d}$$

$$\begin{aligned}\eta_{xy}^{(2)} = \eta_{yx}^{(2)} = \frac{\partial^2 \eta}{\partial x \partial y} + \left[\frac{\partial^2 \eta}{\partial x \partial \phi} - \frac{\partial^2 \xi_2}{\partial x \partial y}\right] \phi_y + \left[\frac{\partial^2 \eta}{\partial y \partial \phi} - \frac{\partial^2 \xi_1}{\partial x \partial y}\right] \phi_x - \frac{\partial \xi_2}{\partial x} \phi_{yy} \\ + \left[\frac{\partial \eta}{\partial \phi} - \frac{\partial \xi_1}{\partial x} - \frac{\partial \xi_2}{\partial y}\right] \phi_{xy} - \frac{\partial \xi_1}{\partial y} \phi_{xx} - \frac{\partial^2 \xi_2}{\partial x \partial \phi} (\phi_y)^2 + \left[\frac{\partial^2 \eta}{\partial \phi^2} - \frac{\partial^2 \xi_1}{\partial x \partial \phi} - \frac{\partial^2 \xi_2}{\partial y \partial \phi}\right] \phi_x \phi_y \\ - \frac{\partial^2 \xi_1}{\partial y \partial \phi} (\phi_x)^2 - \frac{\partial^2 \xi_2}{\partial \phi^2} \phi_x (\phi_y)^2 - \frac{\partial^2 \xi_1}{\partial \phi^2} (\phi_x)^2 \phi_y - 2 \frac{\partial \xi_2}{\partial \phi} \phi_y \phi_{xy} - 2 \frac{\partial \xi_2}{\partial \phi} \phi_x \phi_{xy} \\ - \frac{\partial \xi_1}{\partial \phi} \phi_y \phi_{xx} - \frac{\partial \xi_2}{\partial \phi} \phi_x \phi_{yy} ,\end{aligned} \tag{3.29e}$$

and

$$\eta_{yy}^{(2)} = \frac{\partial^2\eta}{\partial y^2} + \left[2\frac{\partial^2\eta}{\partial y\partial\phi} - \frac{\partial^2\xi_2}{\partial y^2}\right]\phi_y - \frac{\partial^2\xi_1}{\partial y^2}\phi_x + \left[\frac{\partial\eta}{\partial\phi} - 2\frac{\partial\xi_2}{\partial y}\right]\phi_{yy} - 2\frac{\partial\xi_1}{\partial y}\phi_{xy}$$

$$+ \left[\frac{\partial^2\eta}{\partial\phi^2} - 2\frac{\partial^2\xi_2}{\partial y\partial\phi}\right](\phi_y)^2 - 2\frac{\partial^2\xi_1}{\partial y\partial\phi}\phi_x\phi_y - \frac{\partial^2\xi_2}{\partial\phi^2}(\phi_y)^3 - \frac{\partial^2\xi_1}{\partial\phi^2}(\phi_y)^2\phi_x \qquad (3.29f)$$

$$- 3\frac{\partial\xi_2}{\partial\phi}\phi_y\phi_{yy} - \frac{\partial\xi_1}{\partial\phi}\phi_x\phi_{yy} - 2\frac{\partial\xi_1}{\partial\phi}\phi_y\phi_{xy} .$$

In the next sections, these results will be used to determine the Lie group of point transformations that are admitted by the neutron diffusion equations in one-dimensional slab geometry and two-dimensional Cartesian geometry.

3.2 Determination of the Invariance Condition for the Neutron Diffusion Equation in One-Dimensional Slab Geometry

Here we will consider the case of the multi-group, one-dimensional neutron diffusion equation with constant properties as given by

$$F_g(x,\phi_g(x),\phi_g'(x),\phi_g''(x)) = D_g\phi_g''(x) - \Sigma_{R,g}\phi_g(x) + S_g(x) = 0 , \qquad (3.30)$$

where D_g is the group g diffusion length and $\Sigma_{R,g}$ is the group g removal cross section. We now recognize that equation (3.30) will be of identical form for each energy group; therefore, we can omit the subscript g, and the invariance condition for (3.30) is

$$\hat{U}^{(2)}F(x,\phi(x),\phi'(x),\phi''(x)) = 0 \qquad (3.31)$$

whenever $F(x,\phi(x),\phi'(x),\phi''(x)) = 0$, where $\hat{U}^{(2)}$ is the second extension of the group generator as given by (3.24). Upon performing the differentiations, the expanded invariance condition is

$$\xi S_x(x) - \eta\Sigma_R + D\eta_{xx} + D\phi'(2\eta_{x\phi}-\xi_{xx}) + D\phi'^2(\eta_{\phi\phi}-2\xi_{x\phi})$$
$$- D\phi'^3\xi_{\phi\phi} + D\phi''(\eta_\phi-\xi_x-2\phi'\xi_\phi) = 0 , \qquad (3.32)$$

where the subscripts indicate partial differentiations. Using (3.30), the second derivative of the flux is eliminated from (3.32) with the result that

$$\xi S_x(x) - \eta\Sigma_R + D\eta_{xx} + D\phi'(2\eta_{x\phi}-\xi_{xx}) + D\phi'^2(\eta_{\phi\phi}-2\xi_{x\phi}) - D\phi'^3\xi_{\phi\phi} + (\Sigma_R\phi-S(x))(\eta_\phi-\xi_x-2\phi'\xi_\phi) = 0\ . \tag{3.33}$$

However, since $\xi = \xi(x,\phi)$ and $\eta = \eta(x,\phi)$ the coefficients on the various powers of ϕ' must be equal to zero. This results in a system of P.D.E.'s that are used to solve for the coordinate functions $\xi(x,\phi)$ and $\eta(x,\phi)$; specifically these are

$$\xi_{\phi\phi} = 0\ , \tag{3.34a}$$

$$\eta_{\phi\phi} - 2\xi_{x\phi} = 0\ , \tag{3.34b}$$

$$D(2\eta_{x\phi} - \xi_{xx}) - 2\xi_\phi(\Sigma_R\phi - S(x) = 0\ , \tag{3.34c}$$

and

$$D\eta_{xx} - \Sigma_R\eta + \xi S_x(x) + (\Sigma_R\phi - S(x))(\eta_\phi - \xi_x) = 0\ . \tag{3.34d}$$

If S(x) is assumed to be any general function of x, then it is found that $\xi = 0$ and $\eta = \eta(x)$, where $\eta(x)$ satisfies

$$D\eta_{xx}(x) - \Sigma_R\eta(x) = 0\ , \tag{3.35}$$

or for each energy group

$$D_g\eta_{g,xx}(x) - \Sigma_{R,g}\eta_g(x) = 0\ . \tag{3.36}$$

The group generator for the one dimensional, multi-group diffusion equation is

$$\hat{U}_g = \eta_g(x)\frac{\partial}{\partial\phi_g(x)} \tag{3.37}$$

and is of the special form called an evolutionary vector field.

3.3 Determination of the Invariance Condition for the Neutron Diffusion Equation in Two-Dimensional Cartesian Geometry

The multi-group, two-dimensional neutron diffusion equation is

$$\begin{aligned} &F(x,y,\phi_g(x,y),\phi_{g,x}(x,y),\phi_{g,y}(x,y),\phi_{g,xx}(x,y),\phi_{g,xy}(x,y),\phi_{g,yy}(x,y)) \\ &= D_g\phi_{g,xx}(x,y) + D_g\phi_{g,yy}(x,y) - \Sigma_{R,g}\phi(x,y) + S_g(x,y) = 0 \;. \end{aligned} \tag{3.38}$$

As with the one-dimensional case, we will drop the subscript g since the form of equation (3.38) will be the same for all groups. Using the second extension of the group generator as given by equation (3.29a) with definitions (3.29b) though (3.29f) the invariance condition is

$$\hat{U}^{(2)}\left[F(x,y,\phi(x,y),\phi_x(x,y),\phi_y(x,y),\phi_{xx}(x,y),\phi_{xy}(x,y),\phi_{yy}(x,y))\right] = 0 \;. \tag{3.39}$$

Upon expanding out the terms in equation (3.39) and using equation (3.38) to eliminate ϕ_{xx}, we arrive at a system of P.D.E.'s for which the coordinate functions $\xi_1(x,y,\phi)$, $\xi_2(x,y,\phi)$, and $\eta(x,y,\phi)$ can be solved. Since these expressions are quite complicated they will not be presented here; however, if there are no assumptions about the source S(x,y) then one obtains the evolutionary form of the group generator as

$$\hat{U}_g = \eta_g(x,y)\frac{\partial}{\partial\phi_g(x,y)} \tag{3.40}$$

where the coordinate function $\eta_g(x,y)$ satisfies the homogeneous diffusion equation,

$$D_g\eta_{g,xx}(x,y) + D_g\eta_{g,yy}(x,y) - \Sigma_{R,g}\eta_g(x,y) = 0 \;. \tag{3.41}$$

The results of Sections 3.2 and 3.3 will be used later to obtain an invariant finite difference scheme for the neutron diffusion equation. In particular equations (3.37) and (3.40) will be used in the next section to derive the extension of the group generator to grid points, which will then be used in Chapters 5 and 6 to formulate the invariant finite difference schemes.

4 GROUP INVARIANT DIFFERENCE SCHEMES

As stated earlier, the objective of the author's research is to improve difference schemes by incorporating the invariance properties of the differential equation being simulated into the finite difference simulation to produce invariant difference schemes. There are, however, several definitions of what is meant by an invariant difference scheme.

In reference 1, Shokin defines an invariant difference scheme to be a finite difference scheme whose first differential approximation admits a group of point transformations. Shokin's definition implies that the group acts on a space, whose coordinates include the dependent and independent variables, the grid spacings and derivatives up to one order greater than appears in the original differential equations. Therefore, higher order differential approximations of the difference scheme are not guaranteed to be admitted by the group; thus, Shokin's definition can not lead to difference equations, whose solution agrees with the exact solution of the differential equations being simulated. It is important to note that this type of invariant difference scheme leads to greatly improved difference equations for the solution of the gas dynamics equations.

A second definition is that employed by Axford, references 2 and 3, which states that a difference scheme is invariant under a group of point transformations if it admits the extension of the group to the grid point values of the difference scheme. This definition implies that the extensions of the group generators act upon a space whose coordinates are the dependent and independent variables evaluated at the grid points. Axford has shown in reference 2 that such difference schemes can lead to difference equations whose solution agrees with the exact solution of the differential equation being simulated.

The focus of the author's research is to explore more fully invariant difference schemes of the type based upon Axford's definition of an invariant difference scheme. Considerations such as the consistency of these invariant difference schemes and the truncation error will be addressed.

4.1 Extension of the Group to Grid Point Values for One Dependent and Independent Variable

In this section we will examine the construction of the invariance condition for a finite difference equation. Currently the discussion will be limited to the case of one dependent and independent variable. Consider the finite difference equation as given by

$$H(x_{i-1},x_i,x_{i+1},y_{i-1},y_i,y_{i+1}) = 0\,, \tag{4.1}$$

where the x_i's are the independent variables and the y_i's are the dependent variables evaluated at the grid locations, i.e. $y(x_i) = y_i$. As with a differential equation, the invariance condition can be determined by taking the Lie derivative of (4.1) which is

$$\begin{aligned}\frac{\delta H}{\delta a} = \hat{U}^{(D)}H = \frac{\delta x_{i-1}}{\delta a}\frac{\partial H}{\partial x_{i-1}} + \frac{\delta x_i}{\delta a}\frac{\partial H}{\partial x_i} + \frac{\delta x_{i+1}}{\delta a}\frac{\partial H}{\partial x_i} + \frac{\delta x_i}{\delta a}\frac{\partial H}{\partial x_{i+1}}\\ + \frac{\delta y_{i-1}}{\delta a}\frac{\partial H}{\partial y_{i-1}} + \frac{\delta y_i}{\delta a}\frac{\partial H}{\partial y_i} + \frac{\delta y_{i+1}}{\delta a}\frac{\partial H}{\partial y_{i+1}} = 0\,,\end{aligned} \tag{4.2}$$

where $\hat{U}^{(D)}$ is the symbol or generator of the infinitesimal transformation of the group extended to the grid point values. For a differential equation that admits an evolutionary vector field, the infinitesimal point transformations are given by

$$\overline{x} = x \tag{4.3}$$

and

$$\overline{y} = y + \eta(x,y)\delta a\,. \tag{4.4}$$

Since the independent variable does not transform under the action of the group, the invariance condition (4.2) reduces to

$$\hat{U}^{(D)}H = \frac{\delta y_{i-1}}{\delta a}\frac{\partial H}{\partial y_{i-1}} + \frac{\delta y_i}{\delta a}\frac{\partial H}{\partial y_i} + \frac{\delta y_{i+1}}{\delta a}\frac{\partial H}{\partial y_{i+1}} = 0\,. \tag{4.5}$$

To determine the coordinate functions we need to extend the infinitesimal transformations

$$\overline{x_i} = x_i \tag{4.6}$$

and

$$\overline{y_i} = y(x_i) + \frac{\delta y(x_i)}{\delta a}\delta a = y_i + \eta(x_i,y_i)\delta a \tag{4.7}$$

to

$$\overline{y_{i+1}} = y(x_{i+1}) + \frac{\delta y(x_{i+1})}{\delta a}\delta a \tag{4.8}$$

and

$$\overline{y_{i-1}} = y(x_{i-1}) + \frac{\delta y(x_{i-1})}{\delta a}\delta a \tag{4.9}$$

where $x_{i+1} = x_i + \Delta x^+$ and $x_{i-1} = x_i + \Delta x^-$. We start by expanding $\overline{y}(\overline{x}_{i+1})$ in a Taylor series as

$$\overline{y}(\overline{x}_{i+1}) = \overline{y}(x_{i+1}) = \overline{y}(x_i) + \sum_{k=1}^{\infty}\frac{(\Delta x^+)^k}{k!}\frac{d^k\overline{y}(x_i)}{dx^k}\,. \tag{4.10}$$

However, the kth order derivative transforms as

$$\frac{d^k\overline{y}(\overline{x})}{d\overline{x}^k} = \frac{d^k\overline{y}(x)}{dx^k} = \frac{d^k y(x)}{dx^k} + \eta^{(k)}(x,y)\delta a\,, \tag{4.11}$$

where $\eta^{(k)}(x,y)$ is the coordinate function for the kth derivative given by (3.35). Substituting (4.7) and (4.11) into (4.10) yields

$$\bar{y}(x_{i+1}) = y(x_i) + \sum_{k=1}^{\infty} \frac{(\Delta x^+)^k}{k!} \frac{d^k y(x_i)}{dx^k} + \left[\eta(x_i,y_i) + \sum_{k=1}^{\infty} \frac{(\Delta x^+)^k}{k!} \eta^{(k)}(x_i,y_i) \right] \delta a \quad (4.12)$$

or

$$\bar{y}(x_{i+1}) = y(x_{i+1}) + \left[\eta(x_i,y_i) + \sum_{k=1}^{\infty} \frac{(\Delta x^+)^k}{k!} \eta^{(k)}(x_i,y_i) \right] \delta a \, . \quad (4.13)$$

For an evolutionary vector field ($\xi = 0$) the coordinate functions for the kth order derivatives are simply given by

$$\eta^{(k)}(x,y) = \frac{d^k \eta(x,y)}{dx^k} \, , \quad (4.14)$$

so (4.13) reduces to

$$\bar{y}(x_{i+1}) = y(x_{i+1}) + \left[\eta(x_i,y_i) + \sum_{k=1}^{\infty} \frac{(\Delta x^+)^k}{k!} \frac{d^k \eta(x_i,y_i)}{dx^k} \right] \delta a \, . \quad (4.15)$$

Next comparing (4.8) with (4.15) we see that the coordinate function for the dependent variable at the grid point x_{i+1} is

$$\frac{\delta y(x_{i+1})}{\delta a} = \eta(x_i,y_i) + \sum_{k=1}^{\infty} \frac{(\Delta x^+)^k}{k!} \frac{d^k \eta(x_i,y_i)}{dx^k} \, . \quad (4.16)$$

For the neutron diffusion equation, equation (4.16) can be further simplified by the fact that the dependent variable's coordinate function is only a function of x, $\eta(x,y) = \eta(x)$, thus

$$\frac{\delta y(x_{i+1})}{\delta a} = \eta(x_i) + \sum_{k=1}^{\infty} \frac{(\Delta x^+)^k}{k!} \frac{d^k\eta(x_i)}{dx^k} = \eta(x_{i+1}) \,. \tag{4.17}$$

In a similar manner, we can determine the coordinate function for $y(x_{i-1})$ as

$$\frac{\delta y(x_{i-1})}{\delta a} = \eta(x_i) + \sum_{k=1}^{\infty} \frac{(\Delta x^-)^k}{k!} \frac{d^k\eta(x_i)}{dx^k} = \eta(x_{i-1}) \,. \tag{4.18}$$

Therefore, the group generator extended to neighboring grid points is given by

$$\hat{U}^{(D)} = \eta(x_{i-1}) \frac{\partial}{\partial y_{i-1}} + \eta(x_i) \frac{\partial}{\partial y_i} + \eta(x_{i+1}) \frac{\partial}{\partial y_{i+1}} \,. \tag{4.19}$$

It should be noted that in the derivation of the extension of the group generator to grid points there were no assumptions placed upon the grid spacing; therefore either uniform mesh spacing or variable mesh spacing can be used. This result will be used to determine the invariance condition for the finite difference approximation of the diffusion equation in Chapter 5.

4.2 Extension of the Group to Grid Point Values for One Dependent and Two Independent Variables

Here we will consider the construction of the invariance condition for a finite difference equation which depends on a dependent variable, $\phi_{i,j}$, and the independent variables x_i and y_j. The five point finite difference equation is given by

$$H(x_{i-1},x_i,x_{i+1},y_{j-1},y_j,y_{j+1},\phi_{i-1,j},\phi_{i,j-1},\phi_{i,j},\phi_{i+1,j},\phi_{i,j+1}) = 0 \,. \tag{4.20}$$

As in the previous section, the invariance condition is found by taking the Lie derivative of expression (4.20), thus arriving at

$$\frac{\delta H}{\delta a} = \hat{U}^{(D)}H = \frac{\delta x_{i-1}}{\delta a}\frac{\partial H}{\partial x_{i-1}} + \frac{\delta x_i}{\delta a}\frac{\partial H}{\partial x_i} + \frac{\delta x_{i+1}}{\delta a}\frac{\partial H}{\partial x_{i+1}}$$

$$+ \frac{\delta y_{j-1}}{\delta a}\frac{\partial H}{\partial y_{j-1}} + \frac{\delta y_j}{\delta a}\frac{\partial H}{\partial y_j} + \frac{\delta y_{j+1}}{\delta a}\frac{\partial H}{\partial y_{j+1}} \tag{4.21}$$

$$+ \frac{\delta \phi_{i-1,j}}{\delta a}\frac{\partial H}{\partial \phi_{i-1,j}} + \frac{\delta \phi_{i,j-1}}{\delta a}\frac{\partial H}{\partial \phi_{i,j-1}} + \frac{\delta \phi_{i,j}}{\delta a}\frac{\partial H}{\partial \phi_{i,j}} + \frac{\delta \phi_{i+1,j}}{\delta a}\frac{\partial H}{\partial \phi_{i+1,j}} + \frac{\delta \phi_{i,j+1}}{\delta a}\frac{\partial H}{\partial \phi_{i,j+1}} = 0 .$$

The infinitesimal point transformations of a differential equation that admits an evolutionary vector field are

$$\bar{x} = x , \tag{4.22}$$

$$\bar{y} = y , \tag{4.23}$$

and

$$\bar{\phi}(\bar{x},\bar{y}) = \phi(x,y) + \eta(x,y,\phi)\delta a . \tag{4.24}$$

Equation (4.21) can be simplified to

$$\hat{U}^{(D)}H = \frac{\delta \phi_{i-1,j}}{\delta a}\frac{\partial H}{\partial \phi_{i-1,j}} + \frac{\delta \phi_{i,j-1}}{\delta a}\frac{\partial H}{\partial \phi_{i,j-1}}$$

$$+ \frac{\delta \phi_{i,j}}{\delta a}\frac{\partial H}{\partial \phi_{i,j}} + \frac{\delta \phi_{i+1,j}}{\delta a}\frac{\partial H}{\partial \phi_{i+1,j}} + \frac{\delta \phi_{i,j+1}}{\delta a}\frac{\partial H}{\partial \phi_{i,j+1}} = 0 , \tag{4.25}$$

since the independent variables, x and y, do not transform under the action of the group. As in the previous section, we need to determine the coordinate functions by extending the infinitesimal transformations, as given by equations (4.22) through (4.24) when evaluated at grid point (i,j), to

$$\bar{\phi}_{i-1,j} = \phi_{i-1,j} + \frac{\delta \phi_{i-1,j}}{\delta a}\delta a , \tag{4.26}$$

$$\bar{\phi}_{i,j-1} = \phi_{i,j-1} + \frac{\delta \phi_{i,j-1}}{\delta a}\delta a , \tag{4.27}$$

$$\bar{\phi}_{i+1,j} = \phi_{i+1,j} + \frac{\delta\phi_{i+1,j}}{\delta a}\delta a , \tag{4.28}$$

and

$$\bar{\phi}_{i,j+1} = \phi_{i,j+1} + \frac{\delta\phi_{i,j+1}}{\delta a}\delta a . \tag{4.29}$$

To determine these coordinate functions, we proceed as in the previous section by expanding $\bar{\phi}_{i+1,j}$ in a Taylor series about the point (x_i,y_j) as

$$\bar{\phi}_{i+1,j} = \bar{\phi}_{i,j} + \sum_{k=1}^{\infty} \frac{(\Delta x^+)^k}{k!}\frac{\partial^k\bar{\phi}_{i,j}}{\partial x^k} . \tag{4.30}$$

However, the kth order derivatives of the dependent variable transform as

$$\frac{\partial^k\bar{\phi}(\bar{x},\bar{y})}{\partial\bar{x}^k} = \frac{\partial^k\phi(x,y)}{\partial x^k} + \eta^{(k)}_{i_1\cdots i_k}(x,y,\phi)\delta a , \tag{4.31}$$

where the coordinate function for the kth derivative, $\eta^{(k)}_{i_1\cdots i_k}(x,y,\phi)$ is given by $\eta^{(k)}_{i_1\cdots i_k} = \widehat{D}_{i_k}\eta^{(k-1)}_{i_1\cdots i_{k-1}} - \widehat{D}_{i_k}\xi_j\phi_{i_1\cdots i_{k-1},j}$. Next we substitute (4.24) and (4.31) into (4.30) to yield

$$\begin{aligned}\bar{\phi}_{i+1,j} = \phi_{i,j} + \sum_{k=1}^{\infty} \frac{(\Delta x^+)^k}{k!}\frac{\partial^k\phi_{i,j}}{\partial x^k} \\ + \left[\eta(x_i,y_j,\phi_{i,j}) + \sum_{k=1}^{\infty}\frac{(\Delta x^+)^k}{k!}\eta^{(k)}(x_i,y_j,\phi_{i,j})\right]\delta a\end{aligned} \tag{4.32}$$

or

$$\bar{\phi}_{i+1,j} = \phi_{i+1,j} + \left[\eta(x_i,y_j,\phi_{i,j}) + \sum_{k=1}^{\infty}\frac{(\Delta x^+)^k}{k!}\eta^{(k)}(x_i,y_j,\phi_{i,j})\right]\delta a . \tag{4.33}$$

Upon comparing equations (4.33) and (4.28), we see that the coordinate function of the dependent variable at the grid point (i+1,j) is

$$\frac{\delta\phi_{i+1,j}}{\delta a} = \eta(x_i,y_j,\phi_{i,j}) + \sum_{k=1}^{\infty} \frac{(\Delta x^+)^k}{k!}\,\eta^{(k)}(x_i,y_j,\phi_{i,j}) \;; \tag{4.34}$$

which can be simplified further for the neutron diffusion equation by making use of the fact that the coordinate function, $\eta(x,y,\phi)$, is only a function of x and y to yield

$$\frac{\delta\phi_{i+1,j}}{\delta a} = \eta(x_{i+1},y_j) = \eta_{i+1,j}\,. \tag{4.35}$$

In a similar manner, the coordinate functions for the points (i-1,j), (i,j-1) and (i,j+1) can be found; to yield the extension of the group generator as

$$\hat{U}^{(D)} = \eta_{i-1,j}\frac{\partial}{\partial\phi_{i-1,j}} + \eta_{i,j-1}\frac{\partial}{\partial\phi_{i,j-1}} + \eta_{i,j}\frac{\partial}{\partial\phi_{i,j}} + \eta_{i+1,j}\frac{\partial}{\partial\phi_{i+1,j}} + \eta_{i,j+1}\frac{\partial}{\partial\phi_{i,j+1}}\,. \tag{4.36}$$

This result will be used in Chapter 6 to determine the invariance condition for the two-dimensional neutron diffusion equation.

4.3 More General Extensions of the Group to Grid Points

In the previous two sections, we explored the invariance conditions for finite difference equations which depended only on the independent variables and the dependent variable evaluated at the grid points. In many situations, it is desirable to have difference formulations which also depend upon derivatives of the dependent variable evaluated at the grid points. In a manner similar to the two previous sections we can extend the extensions of the group generator to grid point values. As an example, we consider the first extension of the evolutionary vector field, as given by

$$\hat{U}^{(1)} = \eta(x)\frac{\partial}{\partial\phi(x)} + \eta_x(x)\frac{\partial}{\partial\phi_x(x)} \ . \tag{4.37}$$

We wish to extend this vector field to grid point values as

$$\hat{U}^{(1D)} = \hat{U}^{(D)} + \frac{\delta\phi_{x,i-1}}{\delta a}\frac{\partial}{\partial\phi_{x,i-1}} + \frac{\delta\phi_{x,i}}{\delta a}\frac{\partial}{\partial\phi_{x,i}} + \frac{\delta\phi_{x,i+1}}{\delta a}\frac{\partial}{\partial\phi_{x,i+1}} \ , \tag{4.38}$$

where the extension of the group to grid point values, $\hat{U}^{(D)}$, was determined in Section 4.1. For the first extension of the evolutionary vector field that is admitted by the neutron diffusion equation, the infinitesimal point transformations are

$$\bar{x} = x \ , \tag{4.39}$$

$$\bar{\phi}(\bar{x}) = \phi(x) + \eta(x)\delta a \ , \tag{4.40}$$

and

$$\bar{\phi}_x(\bar{x}) = \phi_x(x) + \eta_x(x)\delta a \ , \tag{4.41}$$

where $\eta(x)$ is the solution of the homogeneous diffusion equation. In order to determine the coordinate functions, we need to extend the infinitesimal transformations as given by equations (4.39) through (4.41), when evaluated at the grid point $x = x_i$, to

$$\bar{\phi}_x(\overline{x_{i+1}}) = \bar{\phi}_x(x_{i+1}) = \phi_x(x_{i+1}) + \frac{\delta\phi_x(x_{i+1})}{\delta a}\delta a \tag{4.42}$$

and

$$\bar{\phi}_x(\overline{x_{i-1}}) = \bar{\phi}_x(x_{i-1}) = \phi_x(x_{i-1}) + \frac{\delta\phi_x(x_{i-1})}{\delta a}\delta a \ . \tag{4.43}$$

As in Section 4.1, we begin by expanding $\bar{\phi}_x(x_{i+1})$ in a Taylor series as

$$\bar{\phi}_x(x_{i+1}) = \bar{\phi}_x(x_i) + \sum_{k=1}^{\infty} \frac{(\Delta x^+)^k}{k!} \frac{d^k \bar{\phi}_x(x_i)}{dx^k} . \tag{4.44}$$

However, the kth plus one derivative transforms as

$$\frac{d^{k+1}\bar{\phi}(\bar{x})}{d\bar{x}^{k+1}} = \frac{d^{k+1}\bar{\phi}(x)}{dx^{k+1}} = \frac{d^{k+1}\phi(x)}{dx^{k+1}} + \eta_{x_1,\ldots x_{k+1}}(x)\delta a , \tag{4.45}$$

where $\eta_{x_1,\ldots x_{k+1}}(x)$ is the kth plus one derivative of $\eta(x)$ with respect to x. We now substitute equations (4.45) and (4.41) into (4.44) to yield

$$\bar{\phi}_x(x_{i+1}) = \phi_x(x_i) + \sum_{k=1}^{\infty} \frac{(\Delta x^+)^k}{k!} \frac{d^{k+1}\phi(x)}{dx^{k+1}} + \left[\eta_x(x_i) + \sum_{k=1}^{\infty} \frac{(\Delta x^+)^k}{k!} \eta_{x_1,\ldots x_{k+1}}(x_i) \right] \delta a \tag{4.44}$$

or

$$\bar{\phi}_x(x_{i+1}) = \phi_x(x_{i+1}) + \eta_x(x_{i+1})\delta a \ . \tag{4.45}$$

Comparing equations (4.45) and (4.42) we see that the coordinate function for $\phi_x(x_{i+1})$ is

$$\frac{\delta\phi_x(x_{i+1})}{\delta a} = \eta_x(x_{i+1}) \ . \tag{4.46}$$

The coordinate functions for other derivatives can be found in a similar manner. Results such as these will be used in subsequent chapters to derive the group invariant difference equations for the neutron diffusion equation. It should be noted that extending a group of point transformations to grid points is relatively easy for the case at hand, i.e. for the evolutionary vector field whose coordinate function depends only on the independent variable; it is not particularly clear how to handle more general types of point transformations.

5 LIE GROUP INVARIANT FINITE DIFFERENCE SCHEMES FOR THE NEUTRON DIFFUSION EQUATION IN ONE-DIMENSIONAL SLAB GEOMETRY

We begin this chapter by deriving the Lie group invariant finite difference approximation for the neutron diffusion equation in slab geometry. Additionally the necessary interface equations for multiple region problems will be derived. Specific numerical results will be provided to show the utility of such difference schemes. Along the way, the issues of local truncation error, consistency, and stability of the difference approximation will be addressed.

5.1 The Grid Space upon which the Solution is Determined

Before we begin the actual derivation of the invariant finite difference equations it is useful to discuss the issue of upon which type of grid space the difference equations are to be based. There are two types of grid spaces; the first is the cell centered mesh, and the second is the cell edged mesh. Cell centered meshes get their name from the fact that the mesh points lie at the center of the cell interval and do not fall on a interface, where as for the cell edged mesh, some mesh points fall on an interface. Figures 5.1 and 5.2 show the differences between the cell centered and cell edged mesh.

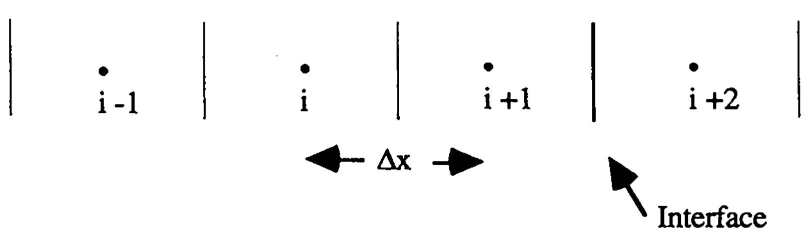

Figure 5.1 Cell Centered Mesh

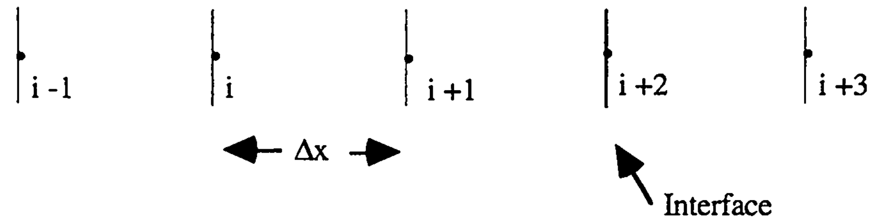

Figure 5.2 Cell Edged Mesh

In most reactor calculations, the cell centered mesh is used [9, 16,17]. Experience has shown that standard finite difference schemes perform better when calculated on the cell centered mesh as opposed to the cell edged mesh. This fact will be demonstrated later in Section 5.5.3. However, for the invariant difference schemes yet to be derived, we will use the cell edged. The reason for choosing the cell edged mesh stems from the manner by which the invariant difference equations at the interface are derived. We will later demonstrate that this choice of mesh is acceptable.

5.2 Derivation of the Group Invariant Finite Difference Equations for the One-Dimensional Region with Constant Material Properties

We begin our derivation of the group invariant difference equations be considering the multi-group diffusion equation in one-dimensional slab geometry as given by

$$\frac{d}{dx}\left(D_g(x)\frac{d\phi_g(x)}{dx}\right) - \Sigma_{R,g}\phi_g(x) + S_g(x) = 0\ , \tag{5.1}$$

where $S_g(x)$ contains both the sources due to fission and scattering. Since equation (5.2a) has the same form for all energy groups, we will omit the subscript g in the ensuing discussion. Additionally, we will assume that the material properties are piecewise constant; we will use the diffusion equation in the form

$$D\frac{d^2\phi(x)}{dx^2} - \Sigma_R\phi(x) + S(x) = 0\,. \tag{5.2a}$$

For multiple material region problems the necessary interface conditions are continuity of current and flux as given by

$$D^-\frac{d\phi^-(x_a)}{dx} = D^+\frac{d\phi^+(x_a)}{dx} \tag{5.2b}$$

and

$$\phi^-(x_a) = \phi^+(x_a)\,, \tag{5.2c}$$

where the superscripts + and - refer to the right and left hand sides of the interface and x_a is the interface location.

In Section 3.2, we found that equation (5.2a) admitted a group of point transformations whose evolutionary vector field was given by

$$\hat{U} = \eta(x)\frac{\partial}{\partial\phi(x)}\,, \tag{5.3}$$

where the coordinate function, $\eta(x)$, satisfied the homogenous diffusion equation

$$D\frac{d^2\eta(x)}{dx^2} - \Sigma_R\eta(x) = 0\,. \tag{5.4}$$

The general solution of the homogeneous diffusion equation, (5.4), is readily found to be

$$\eta(x) = A\cosh(\alpha x) + B\sinh(\alpha x)\,, \tag{5.5}$$

where $\alpha^2 = \Sigma_R / D$, and A and B are coefficients which will shown later to cancel out. It is of interest to note that this particular group of point transformations is not admitted by the boundary conditions, since both A and B are not zero; therefore, we only have partial invariance. As will be shown, partial invariance will pose no difficulty in constructing the invariant difference equations.

We now introduce the concept of an invariant difference operator [19]. This concept is similar to the differential operator in the study of differential equations. As an example of a differential operator, we can rewrite equation (5.2a) as

$$\hat{L}\phi(x) + S(x) = 0 , \tag{5.6a}$$

where the differential operator is

$$\hat{L} = D\frac{d^2}{dx^2} - \Sigma_R . \tag{5.6b}$$

The solution of equation (5.2a) can be written in terms of the homogeneous solution and the particular solution as

$$\phi(x) = \phi_H(x) + \phi_P(x) , \tag{5.7}$$

where $\phi_H(x)$ is the homogeneous solution and $\phi_P(x)$ is the particular solution, which, respectively, satisfy

$$\hat{L}\phi_H(x) = 0 \tag{5.8}$$

and

$$\hat{L}\phi_P(x) + S(x) = 0 . \tag{5.9}$$

We now define the invariant difference equation as

$$\hat{\Omega}\phi_i + Q_i = 0 , \tag{5.10}$$

where $\hat{\Omega}$ is the invariant difference operator and Q_i is the inhomogeneous source. The solution of equation (5.2a) can be written as

$$\phi_i = \phi_{H,i} + \phi_{P,i} , \qquad (5.11)$$

where $\phi_{H,i}$ is the homogeneous solution which satisfies

$$\hat{\Omega}\phi_{H,i} = 0 , \qquad (5.12)$$

and $\phi_{P,i}$ is the particular solution that satisfies

$$\hat{\Omega}\phi_{P,i} + Q_i = 0 . \qquad (5.13)$$

Now the invariant difference operator, $\hat{\Omega}$, is determined such that equation (5.2a) is invariant under the action of the group extended to grid points. The inhomogeneous source, Q_i, is then determined from equation (5.13) using the particular solution of equation (5.2a) as

$$Q_i = - \hat{\Omega}\phi_{P,i} . \qquad (5.14)$$

5.2.1 Construction of the Invariant Difference Operator

There are several methods by which the invariant difference operator, $\hat{\Omega}$, may be constructed. We will consider the three point central difference form of the invariant difference operator as

$$\hat{\Omega} = P_i\left[\hat{E}^{-1} - 2\hat{E}^{0} + \hat{E}^{+1}\right] - \Sigma_R\hat{E}^{0} , \qquad (5.15)$$

where $\hat{E}^n$ is the shift operator such that n = -1 is the backward shift, n = 0 is the null shift, and n = +1 is the forward shift. The explicit form of equation (5.12) for the difference operator, (5.15), is

$$\hat{\Omega}\phi_{H,i} = P_i\left[\phi_{H,i-1} - 2\phi_{H,i} + \phi_{H,i+1}\right] - \Sigma_R\phi_{H,i} = 0 . \qquad (5.16)$$

We now determine P_i, such that equation (5.16) is invariant with respect to the group generator, (5.3), when extended to grid points. In Section 4.1, we found that the extension of the group generator to grid points was

$$\hat{U}^{(D)} = \eta_{i-1}\frac{\partial}{\partial\phi_{i-1}} + \eta_i\frac{\partial}{\partial\phi_i} + \eta_{i+1}\frac{\partial}{\partial\phi_{i+1}} . \tag{5.17}$$

Operating on equation (5.16) with the group generator (5.17) yields

$$P_i\left[\eta_{i-1} - 2\eta_i + \eta_{i+1}\right] - \Sigma_R\eta_i = 0 , \tag{5.18}$$

where the η_i are given by equation (5.5) when evaluated at the grid points. Solving for P_i yields

$$P_i = \frac{\Sigma_R\eta_i}{\eta_{i-1} - 2\eta_i + \eta_{i+1}} . \tag{5.19}$$

If uniform mesh spacing is assumed for a given region, equation (5.29) can be simplified to

$$P_i = \frac{\Sigma_R}{4\,\mathrm{Sinh}^2\left[\alpha\,\frac{\Delta x}{2}\right]} , \tag{5.20}$$

where the coefficients A and B have canceled, and the invariant difference operator is

$$\hat{\Omega} = \frac{\Sigma_R\left(\hat{E}^{-1} - 2\hat{E}^0 + \hat{E}^{+1}\right)}{4\,\mathrm{Sinh}^2\left[\alpha\,\frac{\Delta x}{2}\right]} - \Sigma_R\hat{E}^0 . \tag{5.21}$$

An alternative method by which the invariant difference operator may be derived consists of using the second extension of the group generator extended to grid points. This method essentially consists of determining the invariant difference approximation of the derivatives and substituting these approximations into the differential operator. Using the arguments put forth in Section 4.3, we find that the second extension of the group generator, (5.3), extended to grid points is

$$
\begin{aligned}
\hat{U}^{(2D)} &= \eta_{i-1}\frac{\partial}{\partial\phi_{i-1}} + \eta_i\frac{\partial}{\partial\phi_i} + \eta_{i+1}\frac{\partial}{\partial\phi_{i+1}} \\
&+ \eta_{x,i-1}\frac{\partial}{\partial\phi_{x,i-1}} + \eta_{x,i}\frac{\partial}{\partial\phi_{x,i}} + \eta_{x,i+1}\frac{\partial}{\partial\phi_{x,i+1}} \\
&+ \eta_{xx,i-1}\frac{\partial}{\partial\phi_{xx,i-1}} + \eta_{xx,i}\frac{\partial}{\partial\phi_{xx,i}} + \eta_{xx,i+1}\frac{\partial}{\partial\phi_{xx,i+1}} .
\end{aligned}
\tag{5.22}
$$

We begin by operating on the flux, $\phi_H(x)$ with the differential operator (5.7) and evaluate this expression at the grid point $x = x_i$ as

$$\hat{L}\phi_H(x)\big|_{x=x_i} = D\frac{d^2\phi_{H,i}}{dx^2} + \Sigma_R\phi_{H,i} . \tag{5.23}$$

We next operate on the flux, $\phi_{H,i}$, with the candidate difference operator, (5.25), to obtain

$$\hat{\Omega}\phi_{H,i} = P_i\left[\phi_{H,i-1} - 2\phi_{Hi} + \phi_{H,i+1}\right] + \Sigma_R\phi_{H,i} . \tag{5.24}$$

Equating equations (5.23) and (5.24) yields

$$D\frac{d^2\phi_{H,i}}{dx^2} - \Sigma_R\phi_{H,i} = P_i\left[\phi_{H,i-1} - 2\phi_{H,i} + \phi_{H,i+1}\right] - \Sigma_R\phi_{H,i} \tag{5.25}$$

or

$$D\frac{d^2\phi_{H,i}}{dx^2} = P_i\left[\phi_{H,i-1} - 2\phi_{H,i} + \phi_{H,i+1}\right] . \tag{5.26}$$

We now operate on equation (5.26) with the second extension of the group generator extended to grid points as given by (5.22), which yields

$$D\frac{d^2\eta_i}{dx^2} = P_i\left[\eta_{i-1} - 2\eta_i + \eta_{i+1}\right] , \tag{5.27}$$

and solving for P_i we obtain

$$P_i = \frac{D \frac{d^2\eta_i}{dx^2}}{[\eta_{i-1} - 2\eta_i + \eta_{i+1}]} . \quad (5.28)$$

Again if uniform mesh spacing is assumed, equation (5.28) reduces to

$$P_i = \frac{D\,\alpha^2}{4\,\mathrm{Sinh}^2(\alpha\Delta x/2)} = \frac{\Sigma_R}{4\,\mathrm{Sinh}^2(\alpha\Delta x/2)} . \quad (5.29)$$

Equation (5.29) is identical to equation (5.20); and the invariant difference operator is again given by

$$\hat{\Omega} = \frac{\Sigma_R\left[\hat{E}^{-1} - 2\hat{E}^0 + \hat{E}^{+1}\right]}{4\,\mathrm{Sinh}^2(\alpha\Delta x/2)} - \Sigma_R\hat{E}^0 . \quad (5.30)$$

Since equations (5.30) and (5.21) are identical, these two methods are consistent with each other. The later method of deriving the invariant difference operator will prove to be of particular use when deriving the interface equations for multiple region problems.

5.2.2 Determination of the Inhomogeneous Source Term

Now that the invariant difference operator, $\hat{\Omega}$, has been determined, we need to determine the inhomogeneous source term Q_i. As stated earlier, the inhomogeneous source term is determined by operating on the particular solution of equation (5.2a), when evaluated at the grid points, with the invariant difference operator, (5.21) as

$$Q_i = -\,\hat{\Omega}\,\phi_{P,i} . \quad (5.31)$$

Therefore, we need to determine the particular solution of (5.2a). However, since the source distribution, S(x), is based upon the unknown flux, the source distribution can not be determined beforehand, and, therefore, the particular solution can not be determined. To get around this problem, we will use an approximation for the source distribution.

There are several ways to approximate the source distribution; the simplest is to use a curve fit. If we have some estimate of the flux at several points in the neighborhood of $x = x_i$, then we can estimate the source distribution due to fission and scattering in this neighborhood. As an example, we can use a quadratic curve fit as given by

$$S(x) = \frac{S_{i-1} - 2S_i + S_{i+1}}{2\Delta x^2} (x - x_i)^2 + \frac{S_{i+1} - S_{i-1}}{2\Delta x} (x-x_i) + S_i \, , \tag{5.32}$$

where the S_i's are the sources evaluated at the grid points. Using equation (5.2a) and the source distribution as given by (5.28), we find that the particular solution is

$$\begin{aligned} \phi_P(x) = \frac{1}{\Sigma_R}\left[\frac{S_{i-1} - 2S_i + S_{i+1}}{2\Delta x^2} (x - x_i)^2 + \frac{S_{i+1} - S_{i-1}}{2\Delta x} (x-x_i) + S_i\right] \\ + \frac{S_{i-1} - 2S_i + S_{i+1}}{\alpha^2 \Sigma_R \Delta x^2} \, . \end{aligned} \tag{5.33}$$

Now operating on this particular solution with the invariant difference operator, we find that

$$Q_i = S_i + (S_{i-1} - 2S_i + S_{i+1})\left[\frac{1}{(\alpha\Delta x)^2} - \frac{1}{4 \, \mathrm{Sinh}^2[\alpha\Delta x/2]}\right] . \tag{5.34}$$

Thus, the invariant finite difference equation of the neutron diffusion equation for this particular example is

$$\begin{aligned} \frac{\Sigma_R\left(\phi_{i-1} - 2\phi_i + \phi_{i+1}\right)}{4 \, \mathrm{Sinh}^2\left[\alpha \frac{\Delta x}{2}\right]} - \Sigma_R\phi_i + S_i \\ + (S_{i-1} - 2S_i + S_{i+1})\left[\frac{1}{(\alpha\Delta x)^2} - \frac{1}{4 \, \mathrm{Sinh}^2[\alpha\Delta x/2]}\right] = 0 \, . \end{aligned} \tag{5.35}$$

For the multiple energy group problem, equation (5.31) becomes for energy group g, $1 \le g \le G$,

$$\frac{\Sigma_{R,g}\left(\phi_{g,i-1} - 2\phi_{g,i} + \phi_{g,i+1}\right)}{4\,\mathrm{Sinh}^2\left[\alpha_g \frac{\Delta x}{2}\right]} - \Sigma_{R,g}\phi_{g,i} + S_{g,i}$$
$$+ \left(S_{g,i-1} - 2S_{g,i} + S_{g,i+1}\right)\left[\frac{1}{(\alpha_g \Delta x)^2} - \frac{1}{4\,\mathrm{Sinh}^2\left[\alpha_g \Delta x/2\right]}\right] = 0\,. \tag{5.36}$$

This is by no means the only possible form of a curve fit possible; one could assume that the source distribution is simply equal to S_i in the immediate neighborhood of $x = x_i$, or one might try higher order curve fits. Table 5.1 lists some sample source distributions and their corresponding invariant source terms, Q_i. The results presented thus far are only valid for a single region that has uniform mesh spacing or constant material properties. In the next section, we will present results that will allow for changes in the mesh spacing or material properties, both of which will be dealt with using an invariant finite difference scheme at an interface.

5.3 Determination of the Group Invariant Difference Equations for an Interface between Two Regions

In Section 5.2 we determined the multi-group invariant difference equations for the diffusion equation at points that were interior to a given region in which the material properties and the mesh spacing were uniform. We now need to determine the invariant difference equations for an interface in order to link together the various regions.

We begin by deriving the Lie group invariant difference form of the net current interface *condition*. The net current condition states that the neutron current exiting from one side of the interface must equal the current entering the other side of the interface; mathematically this is given by

Table 5.1 Sample Source Distributions and the Corresponding Invariant Finite Difference Source Terms

Sample Curve Fits of the Source Distribution	Inhomogeneous Source Terms for the Invariant Finite Difference Equation
$S(x) = S_i$	$Q_i = S_i$
$S(x) = \frac{S_{i-1} - 2S_i + S_{i+1}}{2\Delta x^2}(x-x_i)^2 + \frac{S_{i+1} - S_{i-1}}{2\Delta x}(x-x_i) + S_i$	$Q_i = S_i + (S_{i-1} - 2S_i + S_{i+1})\left[\frac{1}{(\alpha\Delta x)^2} - \frac{1}{4\ \mathrm{Sinh}^2(\alpha\Delta x)}\right]$
$S(x) = \frac{S_i - 2S_{i-1} + S_{i-2}}{2\Delta x^2}(x-x_i)^2 + \frac{3S_i - 4S_{i-1} + S_{i-2}}{2\Delta x}(x-x_i) + S_i$	$Q_i = S_i + (S_i - 2S_{i-1} + S_{i-2})\left[\frac{1}{(\alpha\Delta x)^2} - \frac{1}{4\ \mathrm{Sinh}^2(\alpha\Delta x)}\right]$
$S(x) = \frac{S_i - 2S_{i+1} + S_{i+2}}{2\Delta x^2}(x-x_i)^2 - \frac{3S_i - 4S_{i+1} + S_{i+2}}{2\Delta x}(x-x_i) + S_i$	$Q_i = S_i + (S_i - 2S_{i+1} + S_{i+2})\left[\frac{1}{(\alpha\Delta x)^2} - \frac{1}{4\ \mathrm{Sinh}^2(\alpha\Delta x)}\right]$
$S(x) = \frac{S_{i+1} - 3S_i + 3S_{i-1} - S_{i-2}}{6\Delta x^3}(x-x_i)^3 + \frac{S_{i+1} - 2S_i + S_{i-1}}{2\Delta x^2}(x-x_i)^2 + \frac{2S_{i+1} + 3S_i - 6S_{i-1} + S_{i-2}}{6\Delta x}(x-x_i) + S_i$	$Q_i = S_i + (S_{i-1} - 2S_i + S_{i+1})\left[\frac{1}{(\alpha\Delta x)^2} - \frac{1}{4\ \mathrm{Sinh}^2(\alpha\Delta x)}\right]$
$S(x) = \frac{S_{i-2} - 4S_{i-1} + 6S_i - 4S_{i+1} + S_{i+2}}{24\Delta x^4}(x-x_i)^4 + \frac{-S_{i-2} + 2S_{i-1} - 2S_{i+1} + S_{i+2}}{12\Delta x^3}(x-x_i)^3 + \frac{-S_{i-2} + 16S_{i-1} - 30S_i + 16S_{i+1} - S_{i+2}}{24\Delta x^2}(x-x_i)^2 + \frac{S_{i-2} - 8S_{i-1} + 8S_{i+1} - S_{i+2}}{12\Delta x}(x-x_i) + S_i$	$Q_i = \left[\frac{S_{i-2} - 4S_{i-1} + 6S_i - 4S_{i+1} + S_{i+2}}{\alpha^2\Delta x^2} + \frac{-S_{i-2} + 16S_{i-1} - 30S_i + 16S_{i+1} - S_{i+2}}{12}\right] \mathrm{x} \left[\frac{1}{(\alpha\Delta x)^2} - \frac{1}{4\ \mathrm{Sinh}^2(\alpha\Delta x/2)}\right] - \frac{S_{i-2} - 4S_{i-1} + 6S_i - 4S_{i+1} + S_{i+2}}{48\ \mathrm{Sinh}^2(\alpha\Delta x/2)} + S_i$

$$D^{-}\frac{d\phi(x)}{dx}\Big|_{x=x_s^-} = D^{+}\frac{d\phi(x)}{dx}\Big|_{x=x_s^+} . \tag{5.37}$$

As before, the solution, $\phi(x)$, can be written in terms of the homogeneous and particular portions as

$$\phi(x) = \phi_H(x) + \phi_P(x) , \tag{5.38}$$

and the neutron current can be written as

$$D\frac{d\phi(x)}{dx} = D\frac{d\phi_H(x)}{dx} + D\frac{d\phi_P(x)}{dx} . \tag{5.39}$$

We now seek an invariant difference approximation of the neutron current as

$$D\frac{d\phi(x)}{dx}\Big|_{x=x_i} \approx T_i\,(\phi_{i+1} - \phi_{i-1}) + QX , \tag{5.40}$$

where T_i is determined from

$$D\frac{d\phi_H(x)}{dx}\Big|_{x=x_i} = T_i\,(\phi_{H,i+1} - \phi_{H,i-1}) \tag{5.41}$$

such that equation (4.41) is invariant under the action of the group, and QX is determined using the particular solution as

$$QX = D\frac{d\phi_P(x)}{dx}\Big|_{x=x_i} - T_i\,(\phi_{P,i+1} - \phi_{P,i-1}) . \tag{5.42}$$

Using the first extension of the group generator extended to grid points as

$$\begin{aligned}\hat{U}^{(1D)} &= \eta_{i-1}\frac{\partial}{\partial\phi_{i-1}} + \eta_i\frac{\partial}{\partial\phi_i} + \eta_{i+1}\frac{\partial}{\partial\phi_{i+1}} \\ &+ \eta_{x,i-1}\frac{\partial}{\partial\phi_{x,i-1}} + \eta_{x,i}\frac{\partial}{\partial\phi_{x,i}} + \eta_{x,i+1}\frac{\partial}{\partial\phi_{x,i+1}} ,\end{aligned} \tag{5.43}$$

we operate on equation (5.41) to obtain

$$D\frac{d\eta_i}{dx} = T_i\,(\eta_{i+1} - \eta_{i-1}) \tag{5.44}$$

or

$$T_i = \frac{D\frac{d\eta_i}{dx}}{(\eta_{i+1} - \eta_{i-1})}\,, \tag{5.45}$$

and if uniform mesh spacing is assumed equation (5.45) can be reduced to

$$T_i = \frac{D\,\alpha}{2\,\mathrm{Sinh}(\alpha\Delta x)}\,. \tag{5.46}$$

Thus the invariant difference approximation to the neutron current is

$$D\frac{d\phi(x)}{dx}\Big|_{x=x_i} \approx \frac{D\alpha(\phi_{i+1} - \phi_{i-1})}{2\,\mathrm{Sinh}(\alpha\Delta x)} + QX\,, \tag{5.47}$$

where QX is determined from equation (5.42) for some given form of the particular solution; and the invariant difference approximation of the net neutron current interface condition is

$$\frac{D^-\alpha^-(\phi^-_{i+1} - \phi^-_{i-1})}{2\,\mathrm{Sinh}(\alpha^-\Delta x^-)} + QX^- = \frac{D^+\alpha^+(\phi^+_{i+1} - \phi^+_{i-1})}{2\,\mathrm{Sinh}(\alpha^+\Delta x^+)} + QX^+\,. \tag{5.48}$$

We will now consider a specific example of the invariant difference equations at an interface. Since the sources due to material properties on the left-hand side of the interface are not known on the right-hand side of the interface and vise versa, we can use a backward and forward curve fit of the source distributions, as given by the third and fourth entries in Table 5.1. This leads to explicit expressions for QX^- and QX^+ as

$$QX^- = \frac{3S_i^- - 4S_{i-1}^- + S_{i-2}^-}{2\alpha^-}\left[\frac{1}{\alpha^-\Delta x^-} - \frac{1}{\mathrm{Sinh}(\alpha^-\Delta x^-)}\right] \tag{5.49}$$

and

$$QX^+ = \frac{-3S_i^+ + 4S_{i+1}^+ - S_{i+2}^+}{2\alpha^+}\left[\frac{1}{\alpha^+\Delta x^+} - \frac{1}{\mathrm{Sinh}(\alpha^+\Delta x^+)}\right], \tag{5.50}$$

where the superscripts - and + indicate whether material properties on the left-hand side and the right-hand side of the interface are respectively used.

We are now ready to formulate the invariant difference equation at the interface for a general one-dimensional problem. We start by writing the invariant three point central difference equations for the left and right-hand sides of the interface as

$$\frac{\Sigma_R^-\left(\phi_{i-1}^- - 2\phi_i^- + \phi_{i+1}^-\right)}{4\,\mathrm{Sinh}^2\left[\alpha^-\frac{\Delta x^-}{2}\right]} - \Sigma_R^-\phi_i^- + Q_i^- = 0 \tag{5.51}$$

and

$$\frac{\Sigma_R^+\left(\phi_{i-1}^+ - 2\phi_i^+ + \phi_{i+1}^+\right)}{4\,\mathrm{Sinh}^2\left[\alpha^+\frac{\Delta x^+}{2}\right]} - \Sigma_R^+\phi_i^+ + Q_i^+ = 0\,, \tag{5.52}$$

where the Q_i's are determined from equation (5.31) using the appropriate particular solutions. Now the unknowns ϕ_{i+1}^- and ϕ_{i-1}^+ can not be determined since these points do not really exist. Therefore, using equations (5.51), (5.52) and the current interface equation (5.48), we eliminate the terms, ϕ_{i+1}^- and ϕ_{i-1}^+, to arrive at

$$\frac{D^-\alpha^-}{\mathrm{Sinh}(\alpha^-\Delta x^-)}\phi_{i-1}^- - \frac{D^-\alpha^-}{\mathrm{Sinh}(\alpha^-\Delta x^-)}\left[1 + 2\mathrm{Sinh}^2(\alpha^-\frac{\Delta x^-}{2})\right]\phi_i^-$$
$$- \frac{D^+\alpha^+}{\mathrm{Sinh}(\alpha^+\Delta x^+)}\left[1 + 2\mathrm{Sinh}^2(\alpha^+\frac{\Delta x^+}{2})\right]\phi_i^+ + \frac{D^+\alpha^+}{\mathrm{Sinh}(\alpha^+\Delta x^+)}\phi_{i+1}^+ \tag{5.53}$$
$$+ 2\frac{\mathrm{Sinh}^2(\alpha^-\frac{\Delta x^-}{2})}{\alpha^-\mathrm{Sinh}(\alpha^-\Delta x^-)}Q_i^- + 2\frac{\mathrm{Sinh}^2(\alpha^+\frac{\Delta x^+}{2})}{\alpha^+\mathrm{Sinh}(\alpha^+\Delta x^+)}Q_i^+ - QX^- + QX^+ = 0\,.$$

We now apply the interface condition of continuity of the flux as $\phi_i^- = \phi_i^+$, and upon dropping the superscripts on the flux, we arrive at the invariant three point central difference equation for an interface as given by

$$\frac{D^-\alpha^-}{\mathrm{Sinh}(\alpha^-\Delta x^-)}\phi_{i-1}$$
$$-\left[\frac{D^-\alpha^-}{\mathrm{Sinh}(\alpha^-\Delta x^-)}\left(1+ 2\mathrm{Sinh}^2(\alpha^-\frac{\Delta x^-}{2})\right) + \frac{D^+\alpha^+}{\mathrm{Sinh}(\alpha^+\Delta x^+)}\left(1+ 2\mathrm{Sinh}^2(\alpha^+\frac{\Delta x^+}{2})\right)\right]\phi_i$$
$$+ \frac{D^+\alpha^+}{\mathrm{Sinh}(\alpha^+\Delta x^+)}\phi_{i+1} \tag{5.54}$$
$$+ 2\frac{\mathrm{Sinh}^2(\alpha^-\frac{\Delta x^-}{2})}{\alpha^-\mathrm{Sinh}(\alpha^-\Delta x^-)}Q_i^- + 2\frac{\mathrm{Sinh}^2(\alpha^+\frac{\Delta x^+}{2})}{\alpha^+\mathrm{Sinh}(\alpha^+\Delta x^+)}Q_i^+ - QX^- + QX^+ = 0\,.$$

For the multi-group case, equation (5.54) can be written as

$$\frac{D_g^-\alpha_g^-}{\mathrm{Sinh}(\alpha_g^-\Delta x^-)}\phi_{g,i-1}$$
$$-\left[\frac{D_g^-\alpha_g^-}{\mathrm{Sinh}(\alpha_g^-\Delta x^-)}\left(1+ 2\mathrm{Sinh}^2(\alpha_g^-\frac{\Delta x^-}{2})\right) + \frac{D_g^+\alpha_g^+}{\mathrm{Sinh}(\alpha_g^+\Delta x^+)}\left(1+ 2\mathrm{Sinh}^2(\alpha_g^+\frac{\Delta x^+}{2})\right)\right]\phi_{g,i}$$
$$+ \frac{D_g^+\alpha_g^+}{\mathrm{Sinh}(\alpha_g^+\Delta x^+)}\phi_{g,i+1} \tag{5.55}$$
$$+ 2\frac{\mathrm{Sinh}^2(\alpha_g^-\frac{\Delta x^-}{2})}{\alpha_g^-\mathrm{Sinh}(\alpha_g^-\Delta x^-)}Q_{g,i}^- + 2\frac{\mathrm{Sinh}^2(\alpha_g^+\frac{\Delta x^+}{2})}{\alpha_g^+\mathrm{Sinh}(\alpha_g^+\Delta x^+)}Q_{g,i}^+ - QX_g^- + QX_g^+ = 0\,.$$

It should be pointed out that equation (5.55) is the generic form of the invariant difference equation at an interface, and that the source terms $Q^-_{g,i}$, $Q^+_{g,i}$, QX^-_g, and QX^+_g depend only on the particular solution chosen and, hence, on the form of the source curve fit used. To fill out the set of example source distributions at an interface, we will list some other types of curve fits that are possible.

If the source is varying slowly, one can assume that the source distribution is constant in the neighborhood of $x = x_i$, therefore $S(x) = S_i$. We find that

$$Q^-_i = S^-_i \text{ and } Q^+_i = S^+_i \,, \tag{5.56a}$$

and that

$$QX^-_i = 0 \text{ and } QX^+_i = 0 \,. \tag{5.56b}$$

The invariant interface difference equation is then

$$\begin{aligned}
&\frac{D^-\alpha^-}{\mathrm{Sinh}(\alpha^-\Delta x^-)}\phi_{i-1} \\
&-\left[\frac{D^-\alpha^-}{\mathrm{Sinh}(\alpha^-\Delta x^-)}\left(1+2\mathrm{Sinh}^2(\alpha^-\frac{\Delta x^-}{2})\right)+\frac{D^+\alpha^+}{\mathrm{Sinh}(\alpha^+\Delta x^+)}\left(1+2\mathrm{Sinh}^2(\alpha^+\frac{\Delta x^+}{2})\right)\right]\phi_i \\
&+\frac{D^+\alpha^+}{\mathrm{Sinh}(\alpha^+\Delta x^+)}\phi_{i+1} \\
&+2\frac{\mathrm{Sinh}^2(\alpha^-\frac{\Delta x^-}{2})}{\alpha^-\mathrm{Sinh}(\alpha^-\Delta x^-)}S^-_i+2\frac{\mathrm{Sinh}^2(\alpha^+\frac{\Delta x^+}{2})}{\alpha^+\mathrm{Sinh}(\alpha^+\Delta x^+)}S^+_i = 0\,.
\end{aligned} \tag{5.57}$$

It is interesting to note that equation (5.57) is identical to equation 6 in reference 15, as derived by Wachpress. Later, we will show that this equation is exact under certain situations.

Another example of a curve fit consists of fitting the source with a fourth order polynomial across the interface as given by

$$S(x) = a(x-x_i)^4 + b(x-x_i)^3 + c(x-x_i)^2 + d(x-x_i) + S_i^- \,, \tag{5.58a}$$

where

$$a = \frac{\left[\begin{array}{c} (\Delta x^+)^2(2\Delta x^+ + \Delta x^-)S_{i-2} - 4(\Delta x^+)^2(\Delta x^+ + 2\Delta x^-)S_{i-1} \\ + (2(\Delta x^+)^3 + 7(\Delta x^+)^2\Delta x^- + 7\Delta x^+(\Delta x^-)^2 + (\Delta x^-)^3)S_i \\ - 4(\Delta x^-)^2(2\Delta x^+ + \Delta x^-)S_{i+1} + (\Delta x^-)^2(\Delta x^+ + 2\Delta x^-)S_{i+2} \end{array}\right]}{4(\Delta x^+\Delta x^-)^2(\Delta x^+ + \Delta x^-)(2\Delta x^+ + 5\Delta x^+\Delta x^- + 2\Delta x^-)} \,, \tag{5.58b}$$

$$b = \frac{\left[\begin{array}{c} (\Delta x^+)^2((\Delta x^-)^2 - \Delta x^+\Delta x^- - 6(\Delta x^+)^2)S_{i-2} \\ + 4(\Delta x^+)^2(3(\Delta x^+)^2 + 4\Delta x^+\Delta x^- - 4(\Delta x^-)^2)S_{i-1} \\ + 3(2(\Delta x^-)^4 + 5\Delta x^+(\Delta x^-)^3 - 5\Delta x^-(\Delta x^+)^3 - 2(\Delta x^+)^4)S_i \\ + 4(\Delta x^-)^2(4(\Delta x^-)^2 + 4\Delta x^+\Delta x^- - 3(\Delta x^+)^2)S_{i+1} \\ + (\Delta x^-)^2(6(\Delta x^-)^2 + \Delta x^+\Delta x^- - (\Delta x^+)^2)S_{i+2} \end{array}\right]}{4(\Delta x^+\Delta x^-)^2(\Delta x^+ + \Delta x^-)(2\Delta x^+ + 5\Delta x^+\Delta x^- + 2\Delta x^-)} \,, \tag{5.58c}$$

$$c = \frac{\left[\begin{array}{c} (\Delta x^+)^3(4(\Delta x^-)^3 - 4\Delta x^+\Delta x^- - 3(\Delta x^+)^2)S_{i-2} \\ + 8(\Delta x^+)^3(-(\Delta x^+)^2 + \Delta x^+\Delta x^- + 6(\Delta x^-)^2)S_{i-1} \\ +(4(\Delta x^-)^4(\Delta x^- - \Delta x^+) - 45(\Delta x^-)^2(\Delta x^+)^2(\Delta x^+ + \Delta x^-) + 4(\Delta x^+)^4(\Delta x^+ - \Delta x^-)S_i \\ + 8(\Delta x^-)^3(6(\Delta x^+)^2 + \Delta x^+\Delta x^- - (\Delta x^-)^2)S_{i+1} \\ + (\Delta x^-)^3(4(\Delta x^-)^2 - 4\Delta x^+\Delta x^- - 3(\Delta x^+)^2)S_{i+2} \end{array}\right]}{4(\Delta x^+\Delta x^-)^2(\Delta x^+ + \Delta x^-)(2\Delta x^+ + 5\Delta x^+\Delta x^- + 2\Delta x^-)} \,, \tag{5.58d}$$

and

$$d = \frac{\left[\begin{array}{c} (\Delta x^+)^3(\Delta x^- + 2\Delta x^+)S_{i-2} - 8(\Delta x^+)^3(\Delta x^+ + 2\Delta x^-)S_{i-1} \\ + 3(2(\Delta x^-)^4 + 5\Delta x^+(\Delta x^-)^3 + 5\Delta x^-(\Delta x^+)^3 + 2(\Delta x^+)^4)S_i \\ + 8(\Delta x^-)^3(2\Delta x^+ + \Delta x^-)S_{i+1} - (\Delta x^-)^3(\Delta x^+ + 2\Delta x^-)S_{i+2} \end{array}\right]}{2\Delta x^+\Delta x^-(\Delta x^+ + \Delta x^-)(2\Delta x^+ + 5\Delta x^+\Delta x^- + 2\Delta x^-)} \,. \tag{5.58e}$$

Performing a calculation similar to that already performed for the quadratic curve fit, we find that

$$Q_i^s = S_i + 2\left(c + \frac{12a}{(\alpha^s)^2}\right)\left(\frac{1}{(\alpha^s)^2} - \frac{(\Delta x^s)^2}{4\mathrm{Sinh}^2(\alpha^s\Delta x^s/2)}\right) - \frac{2a(\Delta x^s)^4}{4\mathrm{Sinh}^2(\alpha^s\Delta x^s/2)} \qquad (5.59)$$

and

$$QX_i^s = \left(e + \frac{6b}{(\alpha^s)^2}\right)\left(\frac{1}{(\alpha^s)^2} - \frac{\Delta x^s}{\alpha^s\mathrm{Sinh}(\alpha^s\Delta x^s)}\right) - \frac{b(\Delta x^s)^3}{\alpha^s\mathrm{Sinh}(\alpha^s\Delta x^s)}, \qquad (5.60)$$

where the superscript s is respectively either - or + for the left or right-hand sides. There are several options as to what to use for the sources in equations (5.58a) through (5.58e). The most obvious is to use the sources as calculated on the left and right-hand sides of the interface and assign the appropriate source at the interface as in the earlier examples. The second option is to extend the material properties of one region into the other region for the sole purpose of calculating the source distribution. In Section 5.5.3, results will be presented for both these options.

5.4 Local Truncation Error, Consistency, and the Relationship between the Lie Group Invariant Finite Difference Equations and Standard Difference Equations

Before we present specific numerical results, it is useful to discuss the local truncation error of the invariant finite difference equations. Additionally, we will demonstrate that the invariant difference equations are consistent with the original differential equations and that it is possible to recover standard difference equations from the invariant difference equations.

We begin by discussing the invariant finite difference equations in which the source distribution was simply approximated by a constant, $S(x) = S_i$, in the neighborhood of $x = x_i$. The equation for points interior a to given region was determined in Section 5.2 as

$$\frac{\Sigma_R\left(\phi_{i-1} - 2\phi_i + \phi_{i+1}\right)}{4\text{Sinh}^2(\alpha\Delta x/2)} - \Sigma_R\phi_i + S_i = 0 \,. \qquad (5.61)$$

We can recover the standard three-point difference approximation of equation (5.2a) by expanding the hyperbolic-sine in a series expansion as

$$4\text{Sinh}^2(\alpha\frac{\Delta x}{2}) = (\alpha\Delta x)^2 + \frac{(\alpha\Delta x)^4}{12} + \frac{(\alpha\Delta x)^6}{360} + \cdots \,. \qquad (5.62)$$

Upon truncating the series in terms Δx^4 and greater yields

$$\frac{\Sigma_R\left(\phi_{i-1} - 2\phi_i + \phi_{i+1}\right)}{(\alpha\Delta x)^2} - \Sigma_R\phi_i + S_i = 0 \,, \qquad (5.63)$$

or using $\alpha^2 = \Sigma_R/D$ we arrive at the standard three-point central difference equation,

$$\frac{D\left(\phi_{i-1} - 2\phi_i + \phi_{i+1}\right)}{\Delta x^2} - \Sigma_R\phi_i + S_i = 0 \,. \qquad (5.64)$$

The local truncation error for equation (5.61) may be determined by expanding the equation in a series about the point $x = x_i$, as Δx becomes small, to obtain

$$\begin{aligned}\tau_\varepsilon &= D\,\phi_i'' - \Sigma_R\phi_i + S_i + \frac{\Delta x^2}{12}\left[D\,\phi_i^{(iv)} - \Sigma_R\phi_i''\right] \\ &+ \Delta x^4\left[\frac{1}{360}\left(D\,\phi_i^{(vi)} - \Sigma_R\phi_i^{(iv)}\right) + \frac{\Sigma_R}{240\,D}\left(\Sigma_R\phi_i'' - D\,\phi_i^{(iv)}\right)\right] + \cdots \,.\end{aligned} \qquad (5.65)$$

Next, we eliminate the original differential equation and its higher order differentials to yield

$$\tau_\varepsilon = \frac{\Delta x^2}{12}\left[\,-S_i''\,\right] + \Delta x^4\left[\frac{1}{360}\left(\,-S_i^{(iv)}\right) + \frac{\Sigma_R}{240\,D}\left(\,S_i''\,\right)\right] + O(\Delta x^6) \qquad (5.66)$$

or

$$\tau_\varepsilon = \frac{\Delta x^2}{12}\left[\,-S_i''\,\right] + O(\Delta x^4) \,. \qquad (5.67)$$

It is readily seen that the local truncation error vanishes as Δx goes to zero; thus the invariant finite difference equation, (5.61) is consistent with the original differential equation, (5.2a).

It is interesting to note that in formulating the invariant difference equation, we assumed that the source distribution was constant in the neighborhood of $x = x_i$, and if indeed the source is a constant across all mesh in this region, the local truncation error is zero. It will be shown in Section 5.5 that the invariant finite difference equation, (5.61), is exact for problems in which the source distribution is constant. Consider a diffusing media, in which there are no sources present, i.e., $S(x) = 0$, an interesting consequence of the fact that the local truncation error vanishes for a constant source is that the invariant finite difference equation

$$\frac{\Sigma_R\left(\phi_{i-1} - 2\phi_i + \phi_{i+1}\right)}{4\mathrm{Sinh}^2(\alpha\Delta x/2)} - \Sigma_R\phi_i = 0 \tag{5.68}$$

is an exact discrete representation of the differential equation

$$D\frac{d^2\phi(x)}{dx^2} - \Sigma_R\phi(x) = 0\ . \tag{5.69}$$

This implies that the more information Q_i contains about the source distribution at $x = x_i$, the better the invariant difference equation will simulate the original differential equation. This also suggests that the quality of the information represented in Q_i, i.e., the type of curve fit used to model the source distribution, will play a larger role in determining the accuracy of the invariant difference equation than the local truncation error will play. This final conclusion will be demonstrated in Section 5.5.

We now consider the invariant finite difference approximation at an interface in which the constant source approximation was used as given by

$$\frac{D^-\alpha^-}{\mathrm{Sinh}(\alpha^-\Delta x^-)}\phi_{i-1}$$
$$-\left[\frac{D^-\alpha^-}{\mathrm{Sinh}(\alpha^-\Delta x^-)}\left(1+2\mathrm{Sinh}^2(\alpha^-\frac{\Delta x^-}{2})\right)+\frac{D^+\alpha^+}{\mathrm{Sinh}(\alpha^+\Delta x^+)}\left(1+2\mathrm{Sinh}^2(\alpha^+\frac{\Delta x^+}{2})\right)\right]\phi_i$$
$$+\frac{D^+\alpha^+}{\mathrm{Sinh}(\alpha^+\Delta x^+)}\phi_{i+1} \tag{5.70}$$
$$+2\frac{\mathrm{Sinh}^2(\alpha^-\frac{\Delta x^-}{2})}{\alpha^-\mathrm{Sinh}(\alpha^-\Delta x^-)}S_i^-+2\frac{\mathrm{Sinh}^2(\alpha^+\frac{\Delta x^+}{2})}{\alpha^+\mathrm{Sinh}(\alpha^+\Delta x^+)}S_i^+=0\,.$$

As with the previous equation, (5.61), we can recover the standard finite difference formulation by expanding the hyperbolic-sines in series; truncating the series to the first term yields

$$\frac{D^-}{\Delta x^-}\phi_{i-1}-\left[\frac{D^-}{\Delta x^-}+\frac{\Sigma_R^-\Delta x^-}{2}+\frac{D^+}{\Delta x^+}+\frac{\Sigma_R^+\Delta x^+}{2}\right]\phi_i+\frac{D^+}{\Delta x^+}\phi_{i+1}$$
$$+\frac{\Delta x^-}{2}S_i^-+\frac{\Delta x^+}{2}S_i^+=0\,, \tag{5.71}$$

which is the cell edged standard finite difference approximation of the diffusion equation.

The local truncation error for equation (5.70) is determined in a similar process to that of equation (5.61); expanding the terms in (5.70) in a series about the point $x = x_i$ and eliminating all differential forms of the diffusion equation, we obtain

$$\tau_\varepsilon=\frac{1}{6}\left[(\Delta x^-)^2\,(S_i^-)'-(\Delta x^+)^2\,(S_i^+)'\right]+O\left[(\Delta x^-)^3,(\Delta x^+)^3\right]. \tag{5.72}$$

It is readily seen that as the mesh spacing tends to zero the local truncation error goes to zero; therefore, the invariant finite difference equation is consistent with the original differential equation. We again note that if the source distribution is a constant, the local truncation error vanishes, and the invariant difference equation is exact. This claim of exactness will be supported with a numerical calculation in the next section.

Since there are a large number of curve fits that can be used to model the source distribution, we will not present the details for determining the local truncation error, but, instead, we will present the local truncation error for some sample curve fits. The following cases will be the basis for the numerical calculations to be presented in Section 5.5.

Case 1, Second Order Invariant Finite Difference Scheme

The in-region source curve fit is

$$S(x) = S_i \; . \tag{5.73a}$$

The corresponding inhomogeneous source term for the invariant difference equation is

$$Q_i = S_i \; , \tag{5.73b}$$

and the local truncation error for the in-region invariant finite difference equation is given by

$$\tau_\varepsilon = -\frac{\Delta x^2}{12} S_i'' + O(\Delta x^4) \; . \tag{5.73c}$$

At the interface, the source curve fits is taken as

$$S(x_a^-) = S_i^- \text{ and } S(x_a^+) = S_i^+ \; . \tag{5.73d}$$

The inhomogeneous source terms for the invariant finite difference equation are

$$Q_i^- = S_i^- \, , \;\; Q_i^+ = S_i^+ \, , \;\; QX^- = 0 \, , \text{ and } \;\; QX^+ = 0 \; . \tag{5.73e}$$

The local truncation error for the interface equation was determined to be

$$\tau_\varepsilon = \frac{1}{6}\left[(\Delta x^-)^2 (S_i^-)' - (\Delta x^+)^2 (S_i^+)'\right] + O\left[(\Delta x^-)^3,(\Delta x^+)^3\right] . \qquad (5.73f)$$

Case 2, Forth Order Invariant Finite Difference Scheme

The in-region source curve fit is taken as

$$S(x) = \frac{S_{i-1} - 2S_i + S_{i+1}}{2\Delta x^2} (x-x_i)^2 + \frac{S_{i+1} - S_{i-1}}{2\Delta x} (x-x_i) + S_i . \qquad (5.74a)$$

The invariant inhomogeneous source is

$$Q_i = S_i +(S_{i-1} - 2S_i + S_{i+1})\left[\frac{1}{(\alpha\Delta x)^2} - \frac{1}{4\mathrm{Sinh}^2(\alpha\Delta x/2)}\right] , \qquad (5.74b)$$

and the local truncation error for this in-region invariant difference equation is

$$\tau_\varepsilon = \frac{\Delta x^4}{240} S_i^{(iv)} + O(\Delta x^6) . \qquad (5.74c)$$

At the interface two quadratic curve fits are used as

$$S(x_a^-) = \frac{S_i^- - 2S_{i-1}^- + S_{i-2}^-}{2(\Delta x^-)^2} (x-x_i)^2 + \frac{3S_i^- - 4S_{i-1}^- + S_{i-2}^-}{2\Delta x^-} (x-x_i) + S_i^- \qquad (5.74d)$$

and

$$S(x_a^+) = \frac{S_i^+ - 2S_{i+1}^+ + S_{i+2}^+}{2(\Delta x^+)^2} (x-x_i)^2 + \frac{3S_i^+ - 4S_{i+1}^+ + S_{i+2}^+}{2\Delta x^+} (x-x_i) + S_i^+ . \qquad (5.74e)$$

The corresponding inhomogeneous source terms are

$$Q_i^- = S_i^- + (S_i^- - 2S_{i-1}^- + S_{i-2}^-)\left[\frac{1}{(\alpha^-\Delta x^-)^2} - \frac{1}{4\mathrm{Sinh}^2(\alpha^-\Delta x^-/2)}\right] , \qquad (5.74f)$$

$$Q_i^+ = S_i^+ + (S_i^+ - 2S_{i+1}^+ + S_{i+2}^+)\left[\frac{1}{(\alpha^+\Delta x^+)^2} - \frac{1}{4\mathrm{Sinh}^2(\alpha^+\Delta x^+/2)}\right] , \qquad (5.74g)$$

$$QX^- = \frac{3S_i^- - 4S_{i-1}^- + S_{i-2}^-}{2\alpha^-}\left[\frac{1}{\alpha^-\Delta x^-} - \frac{1}{\text{Sinh}(\alpha^-\Delta x^-)}\right], \tag{5.74h}$$

and

$$QX^+ = \frac{3S_i^+ - 4S_{i+1}^+ + S_{i+2}^+}{2\alpha^+}\left[\frac{1}{\alpha^+\Delta x^+} - \frac{1}{\text{Sinh}(\alpha^+\Delta x^+)}\right]. \tag{5.74i}$$

The local truncation error for this particular set of curve fits at the interface was determined to be

$$\tau_\varepsilon = \frac{1}{45}\left[\,(\Delta x^-)^4(\,S_i^-\,)''' - (\Delta x^+)^4(\,S_i^+\,)'''\,\right] + O(\Delta x^6)\,. \tag{5.74j}$$

Case 3, Sixth Order Invariant Finite Difference Scheme

In determining this sixth order difference scheme, we will use two in-region curve fits. The first is used as one moves away from the interface and consists of a fourth order polynomial. The second is a fifth order polynomial curve fit of the source distribution that is used as one approaches the interface. At interior points away from the interface the polynomial fit of the source distribution is

$$S(x) = a(x-x_i)^4 + b(x-x_i)^3 + c(x-x_i)^2 + d(x-x_i) + S_i\,, \tag{5.75a}$$

where

$$a = \frac{S_{i-2} - 4S_{i-1} + 6S_i - 4S_{i+1} + S_{i+2}}{24\Delta x^4},$$

$$b = \frac{-S_{i-2} + 2S_{i-1} - 2S_{i+1} + S_{i+2}}{12\Delta x^3},$$

$$c = \frac{-S_{i-2} + 16S_{i-1} - 30S_i + 16S_{i+1} - S_{i+2}}{24\Delta x^2},$$

and

$$d = \frac{S_{i-2} - 8S_{i-1} + 8S_{i+1} - S_{i+2}}{12\Delta x} .$$

The invariant inhomogeneous source term is

$$Q_i = S_i + 2\left(\frac{12a}{\alpha^2} + c\right)\left[\frac{1}{\alpha^2} - \frac{\Delta x^2}{4\mathrm{Sinh}^2(\alpha\Delta x/2)}\right] - \frac{2a\Delta x^4}{4\mathrm{Sinh}^2(\alpha\Delta x/2)} , \qquad (5.75b)$$

and the local truncation error is

$$\tau_\varepsilon = -\frac{31\ \Delta x^6}{60480} S_i^{(vi)} + O(\Delta x^8) . \qquad (5.75c)$$

The in-region curve fit of the source distribution to the left of the interface is

$$S(x) = a(x\text{-}x_i)^5 + b(x\text{-}x_i)^4 + c(x\text{-}x_i)^3 + d(x\text{-}x_i)^2 + e(x\text{-}x_i) + S_i , \qquad (5.75d)$$

where

$$a = \frac{- S_{i-4} + 5S_{i-3} - 10S_{i-2} + 10S_{i-1} - 5S_i + S_{i+1}}{120\ \Delta x^5} ,$$

$$b = \frac{- S_{i-4} + 6S_{i-3} - 14S_{i-2} + 16S_{i-1} - 9S_i + 2S_{i+1}}{24\Delta x^4} ,$$

$$c = \frac{- S_{i-4} + 7S_{i-3} - 22S_{i-2} + 34S_{i-1} - 25S_i + 7S_{i+1}}{24\Delta x^3} ,$$

$$d = \frac{S_{i-4} - 6S_{i-3} + 14S_{i-2} - 4S_{i-1} - 15S_i + 10S_{i+1}}{24\Delta x^2} ,$$

and

$$e = \frac{3S_{i-4} - 20S_{i-3} + 60S_{i-2} - 120S_{i-1} + 65S_i + 12S_{i+1}}{60\Delta x} .$$

The invariant source term was determined to be

$$Q_i = S_i + 2\left(\frac{12b}{\alpha^2} + d\right)\left[\frac{1}{\alpha^2} - \frac{1}{4\mathrm{Sinh}^2(\alpha\Delta x/2)}\right] - \frac{2b\Delta x^4}{4\mathrm{Sinh}^2(\alpha\Delta x/2)}\,, \qquad (5.75e)$$

and the local truncation error for this invariant finite difference equation is

$$\tau_\varepsilon = \frac{221\ \Delta x^6}{60480}\, S_i^{(vi)} + O(\Delta x^8)\,. \qquad (5.75f)$$

We can arrive at a similar set of equations for the in-region difference equation that is to the right of the interface, where the source distribution is given by equation (5.75d) but the coefficients are

$$a = \frac{-S_{i-1} + 5S_i - 10S_{i+1} + 10S_{i+2} - 5S_{i+3} + S_{i+4}}{120\ \Delta x^5}\,,$$

$$b = \frac{2S_{i-1} - 9S_i + 16S_{i+1} - 14S_{i+2} + 6S_{i+3} - 2S_{i+4}}{24\Delta x^4}\,,$$

$$c = \frac{-7S_{i-1} + 25S_i - 34S_{i+1} + 22S_{i+2} - 7S_{i+3} + S_{i+4}}{24\Delta x^3}\,,$$

$$d = \frac{10S_{i-1} - 15S_i - 4S_{i+1} + 14S_{i+2} - 6S_{i+3} + S_{i+4}}{24\Delta x^2}\,,$$

and

$$e = \frac{-12S_{i-1} - 65S_i + 120S_{i+1} - 60S_{i+2} + 20S_{i+3} - 3S_{i+4}}{60\Delta x}\,.$$

The inhomogeneous source term for the invariant difference equation is given by (5.75e), and the local truncation error for this scheme is given by (5.75f).

At the interface, there are several possibilities as far as curve fits for the source distribution are concerned. For this particular case will use a fifth order backward and forward polynomial as given by

$$S(x) = a(x-x_i)^5 + b(x-x_i)^4 + c(x-x_i)^3 + d(x-x_i)^2 + e(x-x_i) + S_i\,. \qquad (5.75g)$$

To the left of the interface, the coefficients are

$$a^- = \frac{S_i^- - 5S_{i-1}^- + 10S_{i-2}^- - 10S_{i-3}^- + 5S_{i-4}^- - S_{i-5}^-}{120(\Delta x^-)^5},$$

$$b^- = \frac{3S_i^- - 14S_{i-1}^- + 26S_{i-2}^- - 24S_{i-3}^- + 11S_{i-4}^- - 2S_{i-5}^-}{24(\Delta x^-)^4},$$

$$c^- = \frac{17S_i^- - 71S_{i-1}^- + 118S_{i-2}^- - 98S_{i-3}^- + 41S_{i-4}^- - 7S_{i-5}^-}{24(\Delta x^-)^3},$$

$$d^- = \frac{45S_i^- - 154S_{i-1}^- + 241S_{i-2}^- - 156S_{i-3}^- + 61S_{i-4}^- - 10S_{i-5}^-}{24(\Delta x^-)^2},$$

and

$$e^- = \frac{137S_i^- - 300S_{i-1}^- + 300S_{i-2}^- - 200S_{i-3}^- + 75S_{i-4}^- - 12S_{i-5}^-}{60\Delta x^-}.$$

To the right of the interface, the coefficient are

$$a^+ = \frac{- S_i^+ + 5S_{i+1}^+ - 10S_{i+2}^+ + 10S_{i+3}^+ - 5S_{i+4}^+ + S_{i+5}^+}{120(\Delta x^+)^5},$$

$$b^+ = \frac{3S_i^+ - 14S_{i+1}^+ + 26S_{i+2}^+ - 24S_{i+3}^+ + 11S_{i+4}^+ - 2S_{i+5}^+}{24(\Delta x^+)^4},$$

$$c^+ = \frac{- 17S_i^+ + 71S_{i+1}^+ - 118S_{i+2}^+ + 98S_{i+3}^+ - 41S_{i+4}^+ + 7S_{i+5}^+}{24(\Delta x^+)^3},$$

$$d^+ = \frac{45S_i^+ - 154S_{i+1}^+ + 241S_{i+2}^+ - 156S_{i+3}^+ + 61S_{i+4}^+ - 10S_{i+5}^+}{24(\Delta x^+)^2},$$

and

$$e^+ = \frac{- 137S_i^+ + 300S_{i+1}^+ - 300S_{i+2}^+ + 200S_{i+3}^+ - 75S_{i+4}^+ + 12S_{i+5}^+}{60\Delta x^+}.$$

The inhomogeneous source terms Q^+, Q^-, QX^+, and QX^- are

$$Q^+ = S_i^+ + 2\left(\frac{12b^+}{(\alpha^+)^2} + e^+\right)\left[\frac{1}{(\alpha^+)^2} - \frac{(\Delta x^+)^2}{4\mathrm{Sinh}^2(\alpha^+\Delta x^+/2)}\right] - \frac{2b^+(\Delta x^+)^4}{4\mathrm{Sinh}^2(\alpha^+\Delta x^+/2)}, \quad (5.75h)$$

$$Q^- = S_i^- + 2\left(\frac{12b^-}{(\alpha^+)^2} + e^-\right)\left[\frac{1}{(\alpha^-)^2} - \frac{(\Delta x^-)^2}{4\mathrm{Sinh}^2(\alpha^-\Delta x^-/2)}\right] - \frac{2b^-(\Delta x^-)^4}{4\mathrm{Sinh}^2(\alpha^-\Delta x^-/2)}, \quad (5.75i)$$

$$QX^+ = \left[e^+ + \frac{6}{(\alpha^+)^2}\left(\frac{2a^+}{(\alpha^+)^2} + c^+\right)\right]\left[\frac{1}{(\alpha^+)^2} - \frac{\Delta x^+}{\alpha^+\mathrm{Sinh}(\alpha^+\Delta x^+)}\right] - \frac{a^+(\Delta x^+)^5 + \left(\frac{20a^+}{(\alpha^+)^2} + c^+\right)(\Delta x^+)^3}{\alpha^+\,\mathrm{Sinh}(\alpha^+\Delta x^+)}, \quad (5.75j)$$

and

$$QX^- = \left[e^- + \frac{6}{(\alpha^-)^2}\left(\frac{2a^-}{(\alpha^-)^2} + c^-\right)\right]\left[\frac{1}{(\alpha^-)^2} - \frac{\Delta x^-}{\alpha^-\mathrm{Sinh}(\alpha^-\Delta x^-)}\right] - \frac{a^-(\Delta x^-)^5 + \left(\frac{20a^-}{(\alpha^-)^2} + c^-\right)(\Delta x^-)^3}{\alpha^-\,\mathrm{Sinh}(\alpha^-\Delta x^-)}. \quad (5.75k)$$

Now, the local truncation error for this particular case is

$$\tau_\varepsilon = \frac{199\,(\Delta x^-)^7}{24192}\,(S_i^-)^{(vi)} + \frac{199\,(\Delta x^+)^7}{24192}\,(S_i^+)^{(vi)} + O(\Delta x^8). \quad (5.75l)$$

Though the local truncation error for the interface is Δx^7, the overall truncation error is Δx^6.

Case 4 A Second Sixth Order Invariant Finite Difference Scheme

This case is essentially the same as Case 3, but the curve fit at the interface is different. At points interior to a region, we will use the invariant difference equations as given by equations (5.75a) through (5.75f). However, at the interface we will use a fourth order polynomial fit across the interface as given by equations (5.58a) through (5.58e). The invariant inhomogeneous source terms are given by equations (5.59) and (5.60). As stated earlier, there are two options as to what to use for the sources in the curve fit of the source distribution. In this case, we will use the actual material properties at the grid locations to determine the sources. We therefore use the following source definitions:

$$S_{i-2} = S^-_{i-2},\ S_{i-1} = S^-_{i-1},\ S_{i+1} = S^+_{i+1},\ \text{and}\ S_{i+2} = S^+_{i+2}\ .$$

For the S_i terms we will use the corresponding sources, i.e. for Q^+ and QX^+ we will use $S_i = S^+_i$, and for Q^- and QX^- we will use $S_i = S^-_i$.

The local truncation error for this type of interface equation is

$$\begin{aligned}\tau_\varepsilon &= \left[\frac{(\Delta x^-)^6}{5040} + \frac{(\Delta x^-)^5\Delta x^+}{800} + \frac{(\Delta x^-)^4(\Delta x^+)^2}{450}\right](S^-_i)^{(v)} \\ &- \left[\frac{(\Delta x^+)^6}{5040} + \frac{(\Delta x^+)^5\Delta x^-}{800} + \frac{(\Delta x^+)^4(\Delta x^-)^2}{450}\right](S^+_i)^{(v)} + O(\Delta x^7)\ .\end{aligned} \quad (5.76)$$

Case 5 The Final Sixth Order Invariant Finite Difference Scheme

This case is identical to Case 4a, with the exception that the material properties used to determine the sources at the grid points are different. In this case, we will extend the material properties from one region, across the interface, and into the other region. This results in the following source definitions:

For Q^- and QX^- we will use

$$S_{i-2} = S^-_{i-2},\ S_{i-1} = S^-_{i-1},\ S_i = S^-_i,\ S_{i+1} = S^-_{i+1},\ \text{and}\ S_{i+2} = S^-_{i+2},$$

where at the points x_{i+1} and x_{i+2}, the material properties from the left side of the interface are used with the fluxes on the right side of the interface to determine the sources. Similarly, for Q^+ and QX^+ we will use

$$S_{i-2} = S^+_{i-2},\ S_{i-1} = S^+_{i-1},\ S_i = S^+_i,\ S_{i+1} = S^+_{i+1},\ \text{and}\ S_{i+2} = S^+_{i+2},$$

where at the points x_{i-1} and x_{i-2}, the material properties from the right-hand side of the interface are used with the fluxes on the left side of the interface to determine the sources. As with Case 4a, the local truncation error for the interface equation is given by expression (5.76).

5.5 Numerical Results for Specific Examples of the Group Invariant Finite Difference Equations

In this section, we will provide numerical results for the Lie group invariant difference equations as derived thus far. We will begin by discussing the special case of a multiple material region, one-energy group problem with a constant source. We will then discuss the source iteration technique for the solution of multiple region, multi-group eigenvalue problems. Numerical results for the different approximations of the source distributions as presented in Section 5.4 will be given.

5.5.1 Solutions of the Multiple Material Region, One Energy Group Diffusion Problem with a Constant Source

In this section, we will consider a diffusion problem in which only one energy group is used, and the multiple material regions have piecewise constant material properties. Consider a two-region problem, as shown in Figure 5.3, where region I is a core type region and region II is a reflector type region.

The diffusion equations for this problem are

$$D_I \frac{d^2\phi_I(x)}{dx^2} - \Sigma_{R,I}\, \phi_I(x) + S = 0 \qquad (5.77a)$$

and

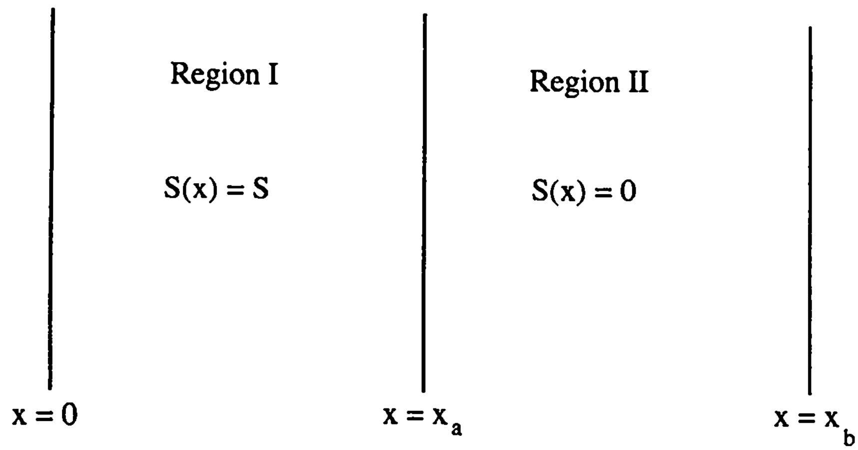

Figure 5.3 Schematic of the Two Region Problem

$$D_{II} \frac{d^2\phi_{II}(x)}{dx^2} - \Sigma_{R,II}\, \phi_{II}(x) = 0 \,, \qquad (5.77b)$$

where the subscripts I and II refer to regions I and II, respectively, and the boundary conditions are

$$D_I \frac{d\phi_I(0)}{dx} = 0 \,, \qquad (5.77c)$$

$$- D_I \frac{d\phi_I(x_a)}{dx} = - D_{II} \frac{d\phi_{II}(x_a)}{dx} \,, \qquad (5.77d)$$

$$\phi_I(x_a) = \phi_{II}(x_a) \,, \qquad (5.77e)$$

and

$$\phi_{II}(x_b) = 0 \,. \qquad (5.77f)$$

The analytic solutions of equations (5.77) are

$$\phi_I(x) = \frac{S}{D_I}\left[1 - \frac{\mathrm{Cosh}[\alpha_{II}(x_b - x_a)]\ \mathrm{Cosh}[\alpha_I x]}{\mathrm{Cosh}[\alpha_I x_a]\mathrm{Cosh}[\alpha_{II}(x_b - x_a)] + \frac{\alpha_I D_I}{\alpha_{II} D_{II}}\mathrm{Sinh}[\alpha_I x_a]\mathrm{Sinh}[\alpha_{II}(x_b - x_a)]}\right] \tag{5.78a}$$

$$0 \le x \le x_a$$

and

$$\phi_{II}(x) = \frac{\frac{S}{D_I}\mathrm{Sinh}[\alpha_I x_a]\ \mathrm{Sinh}[\alpha_{II}(x_b - x)]}{\frac{\alpha_I D_I}{\alpha_{II} D_{II}}\mathrm{Cosh}[\alpha_I x_a]\mathrm{Cosh}[\alpha_{II}(x_b - x_a)] + \mathrm{Sinh}[\alpha_I x_a]\mathrm{Sinh}[\alpha_{II}(x_b - x_a)]} \tag{5.78b}$$

$$x_a \le x \le x_b\ .$$

The invariant difference equations for this case are: in region I

$$\frac{\Sigma_{R,I}\left[\phi_{i-1} - 2\phi_i + \phi_{i+1}\right]}{4\mathrm{Sinh}^2(\alpha_I \Delta x_I/2)} - \Sigma_{R,I}\,\phi_i + S = 0 \quad \text{for } 0 \le x_i < x_a\ , \tag{5.79a}$$

at the interface

$$\begin{aligned} &\frac{D_I\,\alpha_I}{\mathrm{Sinh}(\alpha_I \Delta x_I)}\phi_{i-1} \\ &- \left[\frac{D_I\,\alpha_I}{\mathrm{Sinh}(\alpha_I \Delta x_I)}\left(1 + 2\mathrm{Sinh}^2(\alpha_I \frac{\Delta x_I}{2})\right) + \frac{D_{II}\,\alpha_{II}}{\mathrm{Sinh}(\alpha_{II} \Delta x_{II})}\left(1 + 2\mathrm{Sinh}^2(\alpha_{II} \frac{\Delta x_{II}}{2})\right)\right]\phi_i \\ &+ \frac{D_{II}\,\alpha_{II}}{\mathrm{Sinh}(\alpha_{II} \Delta x_{II})}\phi_{i+1} \\ &+ 2\,\frac{\mathrm{Sinh}^2(\alpha_I \frac{\Delta x_I}{2})}{\alpha_I \mathrm{Sinh}(\alpha_I \Delta x_I)} S = 0 \text{ at } x_i = x_a\ , \end{aligned} \tag{5.79b}$$

and in region II

$$\frac{\Sigma_{R,II}\left[\phi_{i-1} - 2\phi_i + \phi_{i+1}\right]}{4\mathrm{Sinh}^2(\alpha_{II} \Delta x_{II}/2)} - \Sigma_{R,II}\,\phi_i = 0 \quad \text{for } x_a < x_i \le x_b\ . \tag{5.79c}$$

Since this is a relatively simple example, it is fairly easy to show that the invariant difference equations, (5.79a) through (5.79c), are exact for this problem. Substituting the analytic solutions of the diffusion equation, expressions (5.78a) and (5.78b), into the difference equations, we find that all terms cancel; and therefore the difference equations are exact. Alternatively, one can solve the difference equations with a computer and compare this solution with the analytic solution evaluated at the grid points to reach the same conclusion.

5.5.2 The Source Iteration Solution Algorithm

We now begin to consider the more general case in which the sources are dependent upon the neutron flux. This type of problem arises in the determination of the dominant eigenvalue, or the multiplication, of a reactor system. In the ensuing discussion we will assume that there is no self-scattering. We can rewrite the invariant finite difference equations as

$$\frac{\Sigma_{R,g}(\phi_{g,i-1} - 2\phi_{g,i} + \phi_{g,i+1})}{4\text{Sinh}^2(\alpha_g \Delta x/2)} - \Sigma_{R,g}\phi_{g,i} + \sum_{\substack{g'=1 \\ g'\neq g}}^{G} Q_{sc,g'\to g,i} + \frac{\chi_g}{\lambda}\sum_{g'=1}^{G} Q_{f,g',i} = 0 \, , \quad (5.80)$$

where $Q_{sc,g',i}$ and $Q_{f,g',i}$ are the invariant source terms due to scattering and fission respectively, and are determined using the expression for Q_i. As a specific example, we can consider the constant source approximation, $Q_i = S_i$, to yield

$$\frac{\Sigma_{R,g}(\phi_{g,i-1} - 2\phi_{g,i} + \phi_{g,i+1})}{4\text{Sinh}^2(\alpha_g \Delta x/2)} - \Sigma_{R,g}\phi_{g,i} + \sum_{\substack{g'=1 \\ g'\neq g}}^{G} \Sigma_{s,g'\to g}\phi_{g',i} + \frac{\chi_g}{\lambda}\sum_{g'=1}^{G} \Sigma_f\phi_{g',i} = 0 \, . \quad (5.81)$$

Equation (5.80) can be rewritten in matrix form as

$$A_g\vec{\phi}_g - \sum_{\substack{g'=1 \\ g'\neq g}}^{G} Q_{s,g'\to g}\vec{\phi}_{g'} = \frac{\chi_g}{\lambda}\sum_{g'=1}^{G} Q_{F,g'}\vec{\phi}_{g'} \, , \; 1 \le g \le G \, . \quad (5.82)$$

The matrices $\mathbf{A}_g$ are diagonally dominant tridiagional, and the diagonal elements are

$$a_{g,i,i} = \Sigma_{R,g}\left(1 + \frac{1}{2\mathrm{Sinh}^2(\alpha_g \Delta x/2)}\right) \tag{5.83}$$

while the lower and upper diagonal elements are

$$a_{g,i,i-1} = a_{g,i,i+1} = \frac{-\Sigma_{R,g}}{4\mathrm{Sinh}^2(\alpha_g \Delta x/2)} . \tag{5.84}$$

The matrices $\mathbf{Q}_{s,g'\rightarrow g}$ and $\mathbf{Q}_{F,g'}$ are banded, non-negative matrices, whose number of bands depends upon the order of the curve fit used to approximate the source distribution.

As the matrices $\mathbf{A}_g$, $\mathbf{Q}_{s,g'\rightarrow g}$, and $\mathbf{Q}_{F,g'}$ have the same properties as their corresponding counterparts in references 7, 16, and 17, namely, that the matrices $\mathbf{A}_g$ are irreducible Stieltjes matrices, and that the matrices $\mathbf{Q}_{s,g'\rightarrow g}$ and $\mathbf{Q}_{F,g'}$ are non-negative matrices, the same arguments that apply to the stability and convergence of the solution process for the standard difference equations also apply to the solution process for the invariant finite difference equations. The fact that the matrix properties of the invariant finite difference equations are the same as those of the standard difference equations is not surprising, since the standard difference equations can be recovered from the invariant difference equations.

The method chosen for the solution of the neutron flux and the eigenvalue was the power method, see reference 7. The power method was chosen for its simplicity and the fact that it provides the basis for other solution methods. The power method does have the drawback that it is not as efficient as other methods; however, since our primary concern is demonstrating that the invariant finite difference equations are more accurate for a given mesh spacing than the standard difference equations, the choice of solution method is irrelevant.

The power method can be broken down into two portions; the first is the outer iteration in which the fission source and the eigenvalue are determined, and the second is the inner iteration in which the neutron flux is determined from the source. The inner iterations get their name from the fact that for problems in which there is up scattering, iterations must be carried out over the groups in order to determine accurately the scattering sources. The solution process begins by making an estimate of the neutron flux, $\phi_{g,i}^{(0)}$, and the eigenvalue, $\lambda^{(0)}$, where the superscripts indicate the iteration number. The fission source is then determined from the estimate of the flux by

$$\vec{y}_g^{(0)} = \mathbf{Q}_{F,g} \vec{\phi}_g^{(0)} , \; 1 \leq g \leq G. \tag{5.85}$$

Now that the fission source and the eigenvalue have been estimated, we determine the neutron flux via the inner iterations. The inner iterations begin with the determination of the flux in energy group one; we then work through the energy groups to group G, updating the scattering source along the way. The new neutron flux is determined from

$$\vec{\phi}_g^{(k)} = \mathbf{A}_g^{-1} \vec{S}_g^{(k)} , \tag{5.86}$$

where

$$\vec{S}_g^{(k)} = \sum_{g'=1}^{g-1} \mathbf{Q}_{s,g' \to g} \vec{\phi}_g^{(k)} + \vec{y}_g^{(k-1)} . \tag{5.87}$$

This process is carried out for groups $1 \leq g \leq G$. Using these new group fluxes, a new fission source is determined as

$$\vec{y}_g^{(k)} = Q_{F,g}\,\vec{\phi}_g^{(k)}, \ 1 \le g \le G \tag{5.88}$$

and the new eigenvalue is determined from

$$\lambda^{(k)} = \lambda^{(k-1)} \frac{\sum_{g=1}^{G} \left\langle \vec{w}_g, \vec{y}_g^{(k-1)} \right\rangle}{\sum_{g=1}^{G} \left\langle \vec{w}_g, \vec{y}_g^{(k)} \right\rangle}, \tag{5.89}$$

where $\vec{w}_g$ is a weighting factor, and $\left\langle \vec{w}_g, \vec{y}_g^{(k-1)} \right\rangle$ is the scalar produce of the two vectors. Lastly, we test for the convergence of the eigenvalue and the neutron flux. This is by no means the only convergence test possible; one could equally test the convergence of the eigenvalue and the fission source. This process is repeated until convergence is achieved. Figure 5.4 shows a schematic of this solution process. This solution algorithm was used in several computer codes that were written to solve the invariant finite difference equations, results of which will be presented in the next section.

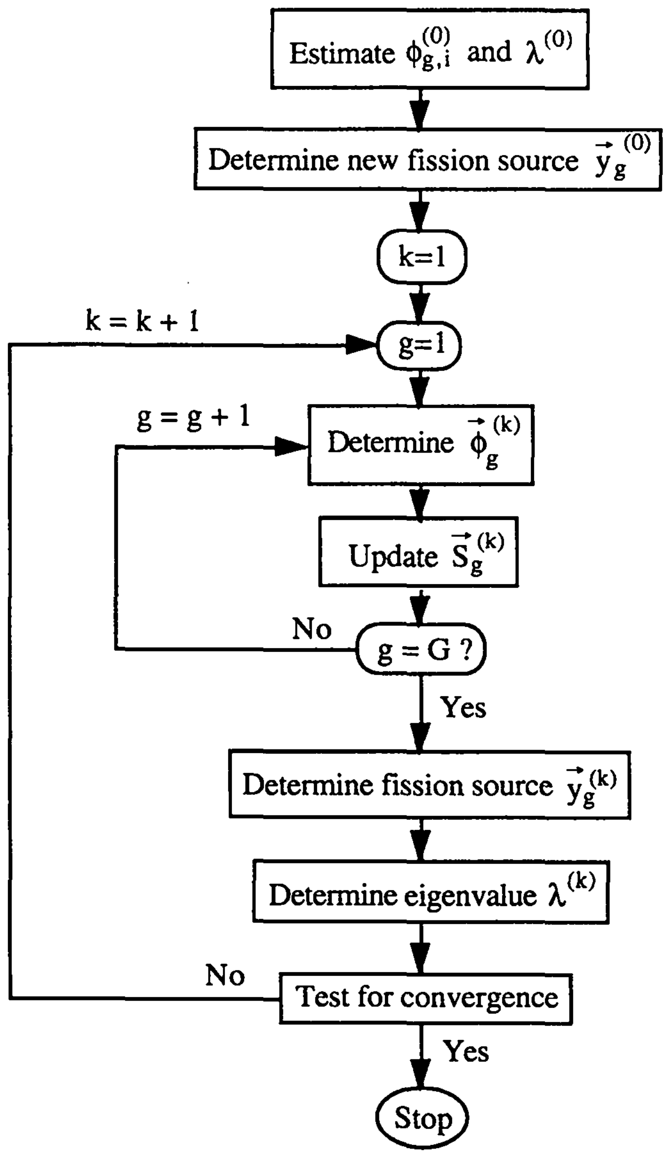

Figure 5.4 Schematic of the Solution Process of the Invariant Finite Difference Equations

5.5.3 Numerical Results for a Sample Problem

In this section, we will present numerical results for a sample problem consisting of a two-region slab reactor model using two energy groups. Figure 5.4 shows a schematic of the sample problem.

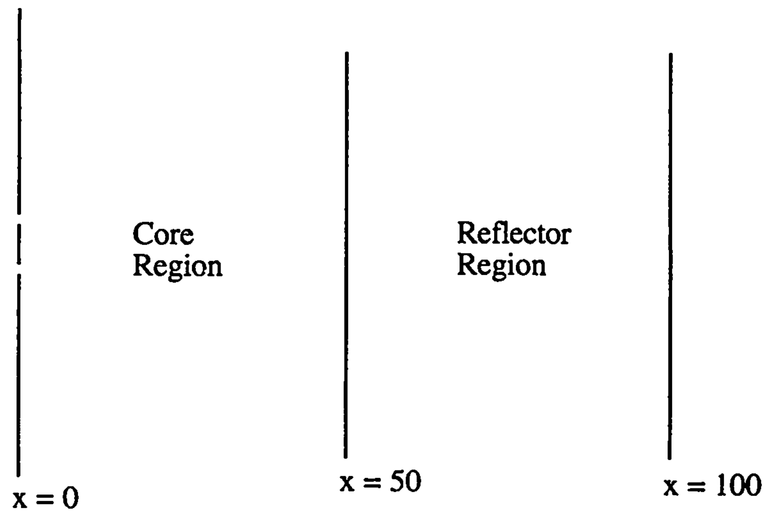

Figure 5.5 Schematic of the Slab Reactor Sample Problem

The cross sections used in these calculations where taken from the IAEA thermal reactor benchmark problem, reference 16, and are listed in Table 5.2.

Several calculations were performed on this sample problem using the invariant difference equations as given by the five cases in Section 5.4. Two additional calculations were performed on this sample case The first calculation used the cell edged standard difference equations as given by equations 5.64 and 5.71 in Section 5.4. The second calculation was performed using the computer code DIF3D, reference 16, which employs cell centered standard difference equations.

The various methods used to calculate the solution of this sample problem produced very similar flux profiles for a given mesh spacing. The group one and group two flux profiles, as shown in Figures 5.6 and 5.7, respectively, were determined using a mesh spacing of 1.0 cm. For all the computational methods used, the flux profiles for this mesh spacing were indistinguishable.

Table 5.2 Two Energy Group Cross Sections

	Core Region Group 1	Core Region Group 2	Reflector Region Group 1	Reflector Region Group 2
Diffusion Coefficient, D_g (cm)	1.5	0.4	1.999996	0.3
Removal Cross Section, $\Sigma_{R,g}$ (cm^{-1})	0.03	0.08	0.04	0.01
Fission Cross Section, $\nu\Sigma_{f,g}$ (cm^{-1})	0.0	0.135	0.0	0.0
Probability of a Fission Neutron Born into Group g, χ_g	1.0	0.0	1.0	0.0
Scattering Cross Section, $\Sigma_{s,g'g}$ (cm^{-1})	$1\rightarrow1$ 0.0 $2\rightarrow1$ 0.0	$1\rightarrow2$ 0.02 $2\rightarrow2$ 0.0	$1\rightarrow1$ 0.0 $2\rightarrow1$ 0.0	$1\rightarrow2$ 0.04 $2\rightarrow2$ 0.0

Since the local truncation error is a function of the mesh spacing, one expects that as the mesh spacing goes to zero, the accuracy of the of the numerical solution should increase. It is therefore useful to examine the accuracy of the eigenvalue as a function of the mesh spacing. Also of interest is the absolute value of the relative error in the eigenvalue as a function the mesh spacing as calculated by

$$e = \left| \frac{\lambda - \lambda_{converged}}{\lambda_{converged}} \right| . \qquad (5.90)$$

The converged eigenvalue is defined to be the eigenvalue to which all the computational methods converged as the mesh spacing went to zero.

We will begin comparing the various computational methods by examining the eigenvalues as a function of the mesh spacing for the five example Cases of the invariant difference schemes outlined in Section 5.4. Figure 5.8 shows the eigenvalue, as calculated by the five invariant difference schemes, as a function of the mesh spacing. The local truncation errors for the five Cases are: second order for Case 1, fourth order for Case 2, and sixth order for Cases 3, 4, and 5. Since the invariant Case 3 approaches the converged eigenvalue from below, it is easier to compare the five methods by examining the absolute value of the error, as shown in Figure 5.9. There are several interesting things to note about how the eigenvalues behave as a function of the mesh spacing. If we compare the sixth order difference schemes, as given by Cases 3 and 4, to say the fourth order scheme, Case 2, we find that they are not as accurate as the fourth order scheme. On the other hand though, we find that the sixth order scheme used in Case 5 is more accurate than the fourth order scheme. Since the only differences between the sixth order schemes is in the source approximations at the interface, we conclude that the type of curve fit approximation used is more important than the local truncation error in determining the accuracy of the invariant difference scheme. Secondly we can also conclude that as the order of the curve fit of the source distribution increases, the accuracy of the difference scheme increases, provided that the curve fit is a good representation of the source distribution.

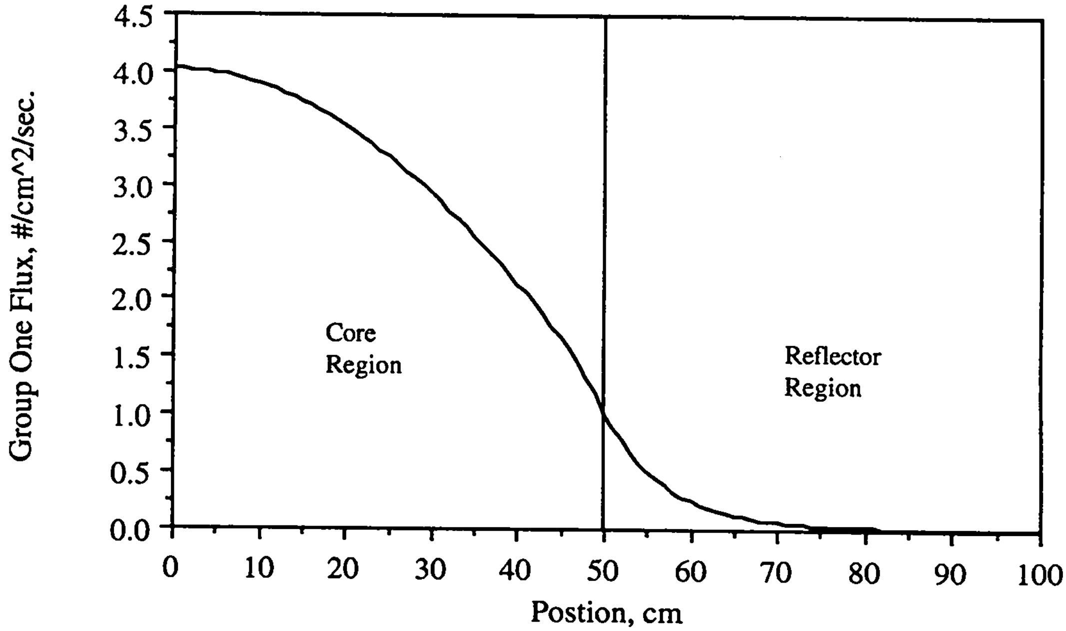

Figure 5.6 Group One Flux Profile for the Sample Problem

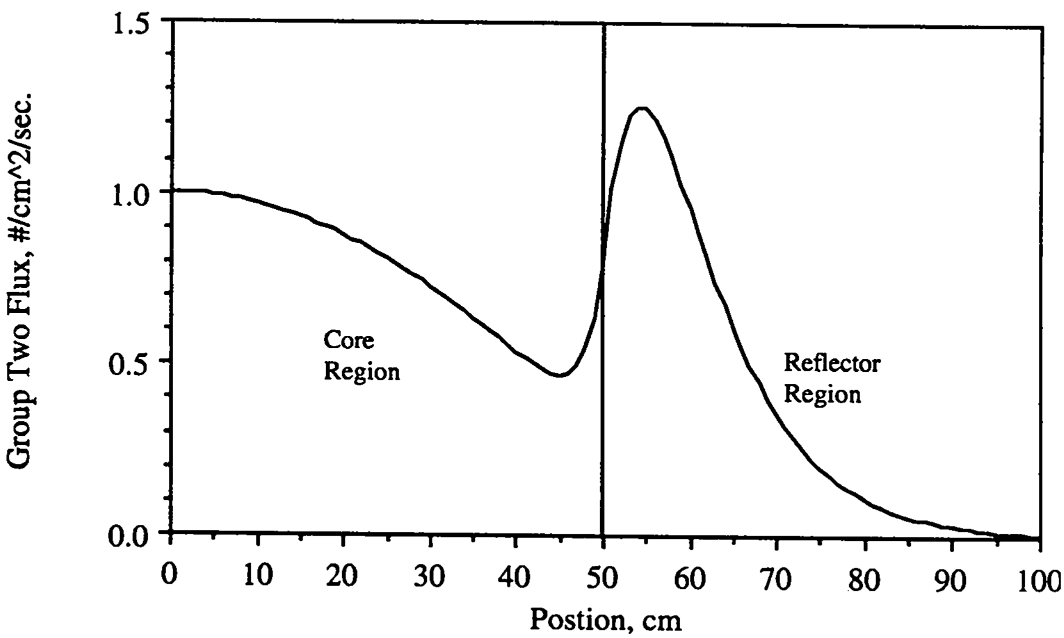

Figure 5.7 Group Two Flux Profile for the Sample Problem

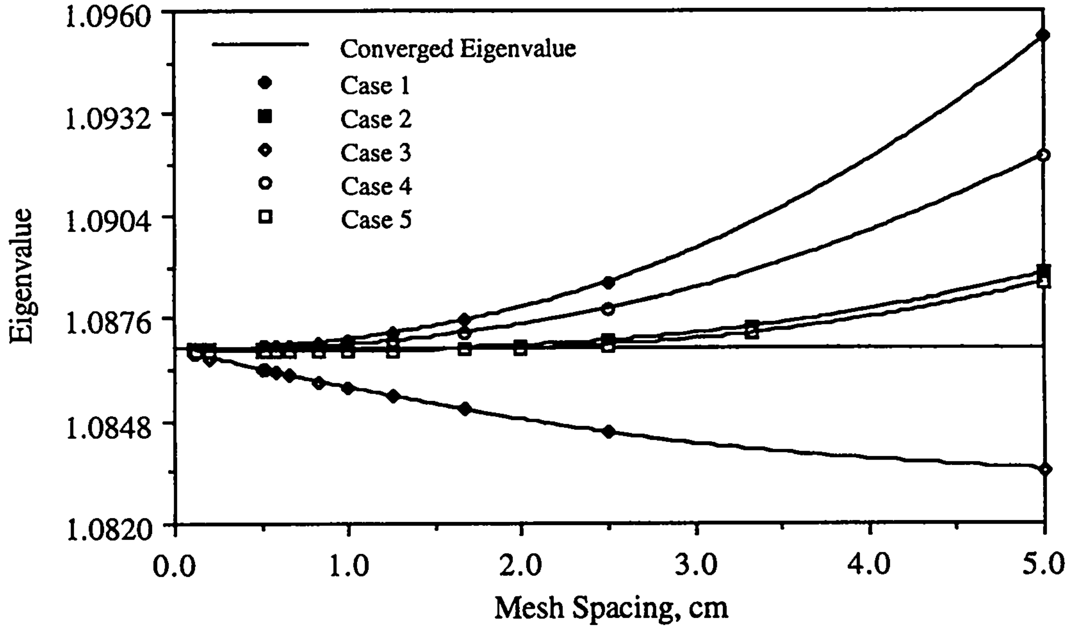

Figure 5.8 Eigenvalue as a Function of the Mesh Spacing for the Five Invariant Difference Schemes

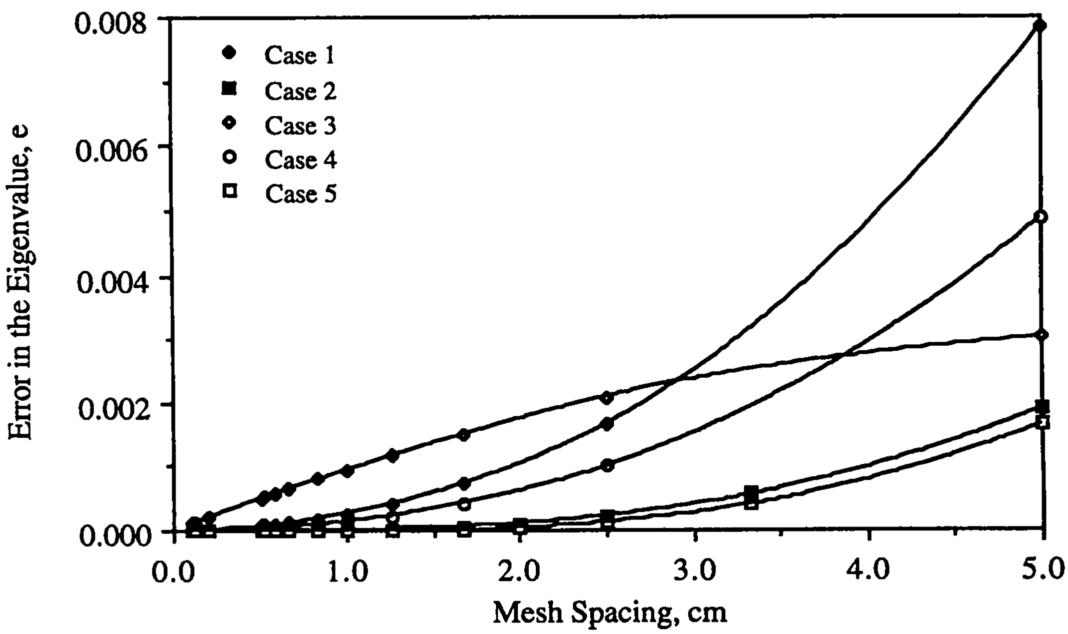

Figure 5.9 Absolute Value of the Relative Error in the Eigenvalue as a Function of the Mesh Spacing for the Five Invariant Difference Schemes

We now compare the eigenvalues as computed by the invariant difference schemes as given by Cases 1, 2, and 5, to the eigenvalue as computed by the two standard difference schemes, the cell centered and cell edged difference equations; the cell centered difference scheme being calculated by the computer code DIF3D. Figure 5.10 shows the eigenvalues as a function mesh spacing for these cases. Since the eigenvalues as calculated by DIF3D approaches the converged eigenvalue from below, it is again useful to compare the methods by examining the absolute value of the error, as shown in Figure 5.11. Examining Figure 5.11, we find, as expected, that the cell edged difference scheme is not as accurate as the cell centered difference scheme employed in DIF3D. Secondly if we compare the difference schemes with a second order local truncation error, i.e., the cell edged scheme, DIF3D, and the invariant Case 1, we find that the performance of the invariant difference scheme leaves something to be desired. However, one must consider that the curve fit used in formulating the difference scheme of Case 1 consisted of setting the sources adjacent to $x=x_i$ equal to the source at $x=x_i$, which in reality is not the case, since the source has some spatial dependence. In particular, this assumption breaks down at an interface since there can be a radical chance in the material properties, and hence the source, as one crosses the interface. The fact that this assumption breaks down particularly at interfaces can be demonstrate by replacing the interface equations in Case 1 with the quadratic curve fit interface equations of Case 2. This yields an invariant difference scheme, labeled Case 1-a, whose overall local truncation error is second order. Figure 5.12 is a plot of the error in the eigenvalue for Cases 1 and 1-a. As one can see, by simply changing the difference equations at the interface, the accuracy increases significantly. This shows that the assumptions made about the source distribution for Case 1 did indeed break down at the interface.

Lastly, we compare the results of the invariant difference schemes Cases 2, and 5 to the results obtained from the computer code DIF3D, as shown in Figure 5.13. As one can see, DIF3D produces a more accurate values of the eigenvalue for the large mesh spacing of between four and five cm. However, as the mesh spacing is reduced to less than four cm, the invariant difference schemes produced more accurate values of the eigenvalue. The results for the mesh spacings greater than four cm are somewhat suspect, since these mesh spacings are approximately twice the diffusion length, 2.236 cm; and secondly none of the computer codes could resolve the neutron fluxes with any reasonable degree of accuracy. Ignoring the eigenvalue data for which the neutron flux could not be determined accurately, we find that the invariant difference schemes could determine the eigenvalue more accurately for a given mesh spacing than the standard finite difference formulations as employed by DIF3D. This result can be restated; for a desired level of accuracy in the eigenvalue one can use fewer mesh points with the invariant difference schemes than are required with the standard difference approximations.

In the next chapter, we will explore the construction of invariant difference schemes for two-dimensional diffusion theory in Cartesian coordinates. Many of the results presented in this chapter will be found to have a similar counterpart for the two-dimensional case.

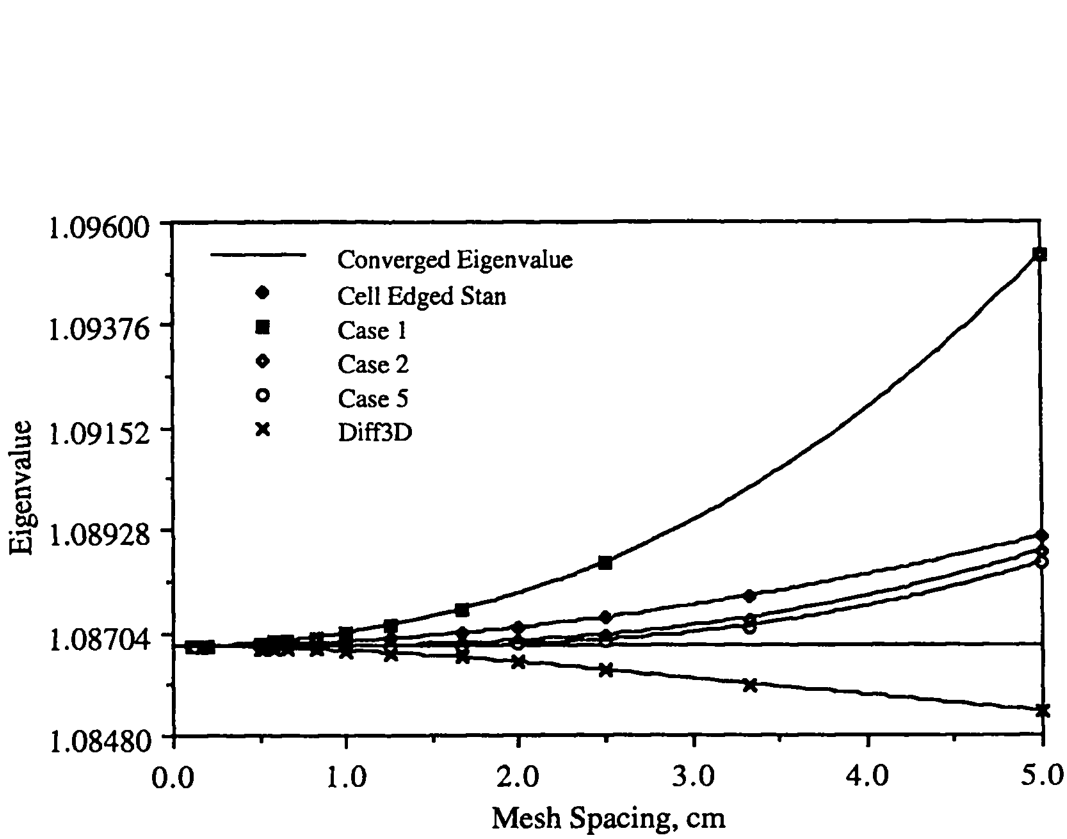

Figure 5.10 Eigenvalue as a Function of the Mesh Spacing as Calculated by the Computer Code DIF3D, the Standard Cell Edged Scheme, and the Invariant Finite Difference cases 1, 2, and 5

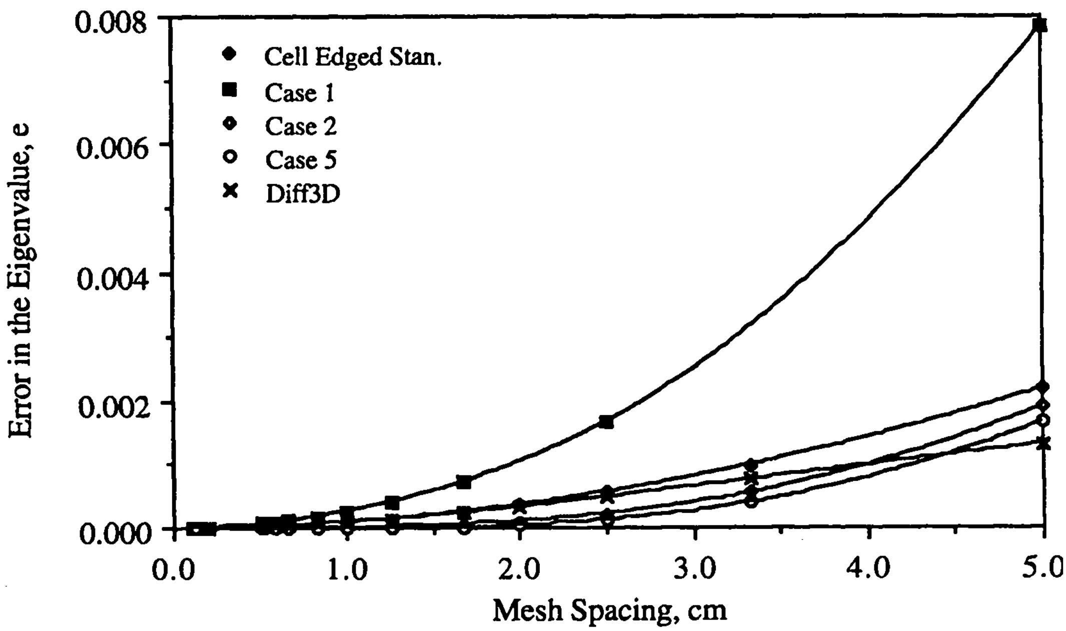

Figure 5.11 Absolute Value of the Relative Error in the Eigenvalue as a Function of the Mesh Spacing for the Computer Code DIF3D, the Standard Cell Edged Scheme, and the Invariant Finite Difference cases 1, 2, and 5

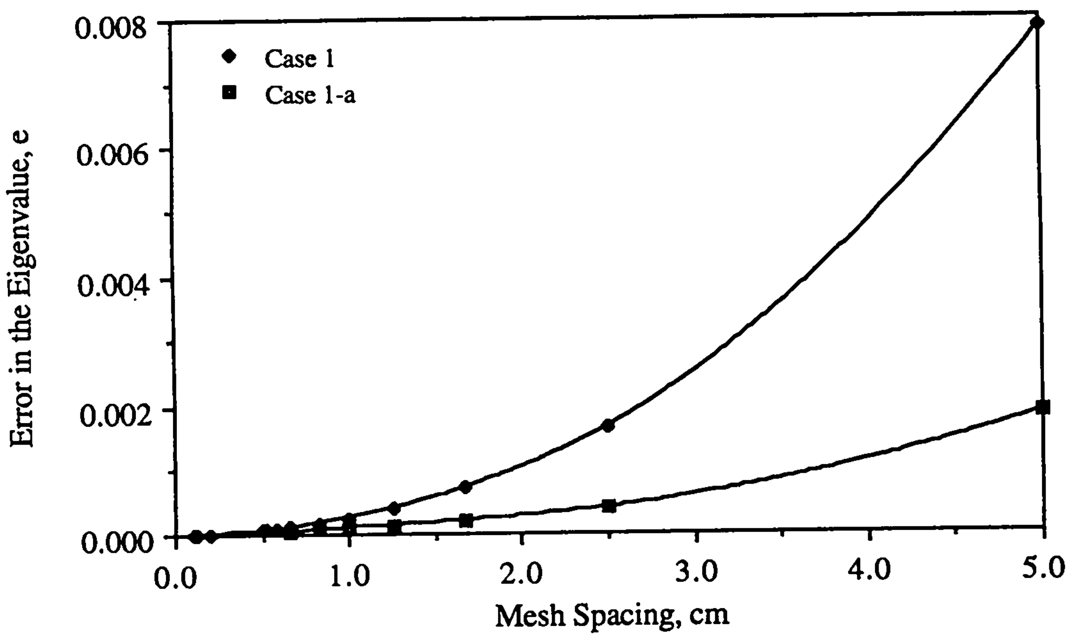

Figure 5.12 Absolute Value of the Relative Error in the Eigenvalue as a Function of the Mesh Spacing for the Invariant Difference Cases 1 and 1-a

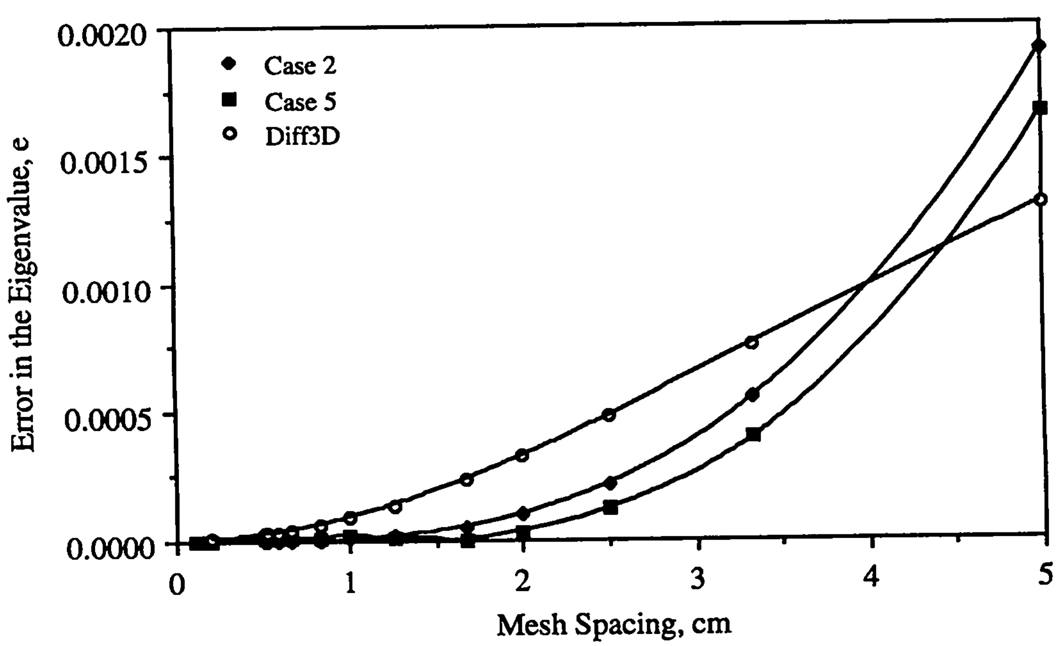

Figure 5.13 Absolute Value of the Relative Error in the Eigenvalue as a Function of the Mesh Spacing for the Invariant Difference 2, and 5 and for the Computer Code DIF3D

6 GROUP INVARIANT FINITE DIFFERENCE EQUATIONS FOR THE TWO-DIMENSIONAL DIFFUSION EQUATION IN CARTESIAN COORDINATES

In this chapter, we will discuss the construction of the group invariant finite difference equations for the neutron diffusion equation with material properties assumed to be piecewise constant as given by

$$D_g\phi_{g,xx}(x,y) + D_g\phi_{g,yy}(x,y) - \Sigma_{R,g}\phi_g(x,y) + S_g(x,y) = 0 , \tag{6.1}$$

where the source is

$$S_g(x,y) = \sum_{\substack{g'=1 \\ g'\neq g}}^{G} \Sigma_{s\, g'\to g}\phi_{g'}(x,y) + \frac{\chi_g}{\lambda}\sum_{g'=1}^{G} \nu\Sigma_{f,g'}\phi_{g'}(x,y) \tag{6.2}$$

for $1 \le g \le G$. Equation (6.1) can be written in operator form as

$$\hat{L}_g\phi_g(x,y) = S_g(x,y) , \tag{6.3}$$

where the differential operator, $\hat{L}_g$, is given by

$$\hat{L}_g = D_g\frac{\partial^2}{\partial x^2} + D_g\frac{\partial^2}{\partial y^2} - \Sigma_{R,g} . \tag{6.4}$$

The boundary and interface conditions are similar to those used in the one-dimensional case: the neutron flux is zero at all outside surfaces, or if symmetry permits, the net neutron current along a line of symmetry is zero. The interface conditions are again that the net neutron current and the neutron flux are equal at the interface as given by

$$\begin{aligned} -D_g^-\phi_{g,x}^-(x_b^-,y) &= -D_g^+\phi_{g,x}^+(x_b^+,y) \\ \phi_g^-(x_b^-,y) &= \phi_g^+(x_b^+,y) \end{aligned} \tag{6.5}$$

and

$$-D_g^-\phi_{g,y}^-(x,y_b^-) = -D_g^+\phi_{g,y}^+(x,y_b^+)$$
$$\phi_g^-(x,y_b^-) = \phi_g^+(x,y_b^+)\ . \qquad (6.6)$$

We will begin by constructing the invariant finite difference equation interior to a given region. We will then go on to construct the difference equations for the three types of interfaces to link together multiple regions. Modifications to the solution algorithm presented in Section 5.5.2 for the solution of the two-dimensional problem will then be discussed. Finally, results will be presented for the two-dimensional equivalent of the sample problem presented in Chapter 5.

6.1 The Two-Dimensional Grid upon which the Solution is Determined

The grid space upon which the solution of the invariant difference equations are to be solved is an orthogonal cell edged mesh. Figure 6.1 shows a schematic representation of the cell edged grid.

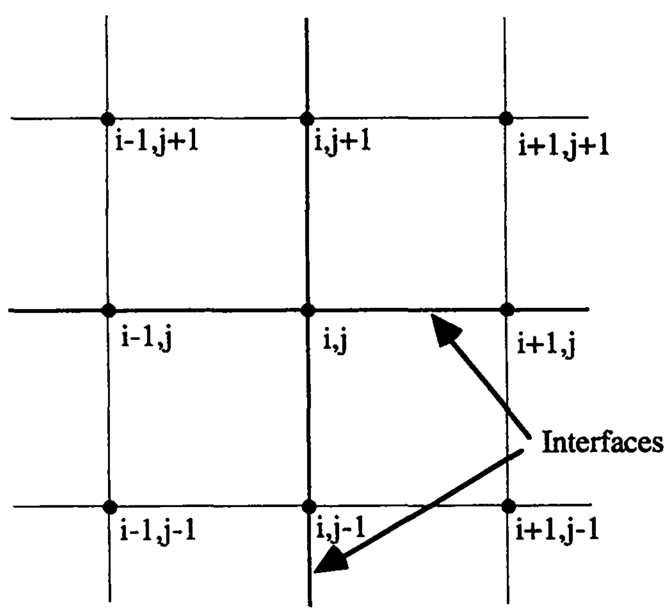

Figure 6.1 The Cell Edged Mesh

This contrasts to the cell centered mesh shown in Figure 6.2, that is employed in the conventional finite difference approximations of the diffusion equation. As with the one-dimensional case, the reasons for choosing the cell edged mesh stems from the method by which the interface equations are formulated.

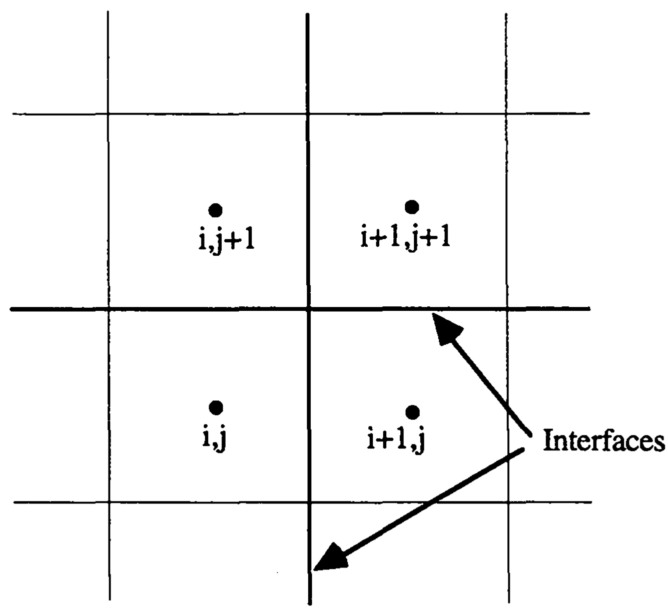

Figure 6.2 The Cell Centered Mesh

6.2 Derivation of the Two-Dimensional Group Invariant Finite Difference Equations for the Multigroup Neutron Diffusion Equation

We will begin this section by deriving the invariant finite difference equations for the two-dimensional diffusion equation for a given region away from the interfaces. This result will then be used with a discrete form of the interface conditions, much like in the one-dimensional case, to determine the invariant finite difference equations for three different type of interfaces.

6.2.1 The In-Region Invariant Finite Difference Equations in Two-Dimensions

In Section 3.3, we found that the diffusion equation, as given by equation (6.1), admitted a group of point transformations whose group generator was

$$\hat{U}_g = \eta_g(x,y) \frac{\partial}{\partial \phi_g(x,y)} , \qquad (6.7)$$

where the coordinate functions, $\eta_g(x,y)$, satisfied

$$D_g \eta_{g,xx}(x,y) + D_g \eta_{g,yy}(x,y) - \Sigma_{R,g} \eta_g(x,y) = 0 . \qquad (6.8)$$

Setting $\alpha_g^2 = \Sigma_{R,g}/D_g$, the solution of equation (6.8) can be determined using separation of variables as

$$\eta_g(x,y) = X_g(x) Y_g(y) , \qquad (6.9)$$

where the equations for $X_g(x)$ and $Y_g(y)$ are respectively

$$X_{g,xx}(x) - \beta_g^2 X_g(x) = 0 \qquad (6.10)$$

and

$$Y_{g,yy}(y) - (\alpha_g^2 - \beta_g^2) Y_g(y) = 0 . \qquad (6.11)$$

Since there is no group of point transformations that preserve both the invariance of the diffusion equation and its boundary conditions, we have only partial invariance; therefore, there is not a complete set of boundary conditions that can be used to determine the coordinate function. Thus, the eigenvalues, β_g, of the coordinate function are continuous and have the range of $-\infty \le \beta_g^2 \le +\infty$. This range of eigenvalues can be broken up into three classes: class 1, $-\infty \le \beta_g^2 \le 0$, class 2, $0 < \beta_g^2 < \alpha_g^2$, and class 3, $\alpha_g^2 \le \beta_g^2 \le +\infty$. The general solutions of equations (6.10) and (6.11) for these three classes are:

class 1

$$X_g(x) = A_{1,g}\,\mathrm{Cos}(\beta_g x) + B_{1,g}\,\mathrm{Sin}(\beta_g x)$$
$$Y_g(y) = A_{2,g}\,\mathrm{Cosh}\left(\sqrt{\alpha_g^2 + |\beta_g^2|}\,y\right) + B_{2,g}\,\mathrm{Sinh}\left(\sqrt{\alpha_g^2 + |\beta_g^2|}\,y\right), \tag{6.12}$$

class 2

$$X_g(x) = A_{1,g}\,\mathrm{Cosh}(\beta_g x) + B_{1,g}\,\mathrm{Sinh}(\beta_g x)$$
$$Y_g(y) = A_{2,g}\,\mathrm{Cosh}\left(\sqrt{\alpha_g^2 - \beta_g^2}\,y\right) + B_{2,g}\,\mathrm{Sinh}\left(\sqrt{\alpha_g^2 - \beta_g^2}\,y\right), \tag{6.13}$$

and class 3

$$X_g(x) = A_{1,g}\,\mathrm{Cosh}(\beta_g x) + B_{1,g}\,\mathrm{Sinh}(\beta_g x)$$
$$Y_g(y) = A_{2,g}\,\mathrm{Cos}\left(\sqrt{|\alpha_g^2 - \beta_g^2|}\,y\right) + B_{2,g}\,\mathrm{Sin}\left(\sqrt{|\alpha_g^2 - \beta_g^2|}\,y\right). \tag{6.14}$$

Now the question arises as to which of the solutions, equations (6.12), (6.13) or (6.14), is the best solution for our particular problem. To answer this question, we consider a one-region symmetric reactor as shown in Figure 6.3.

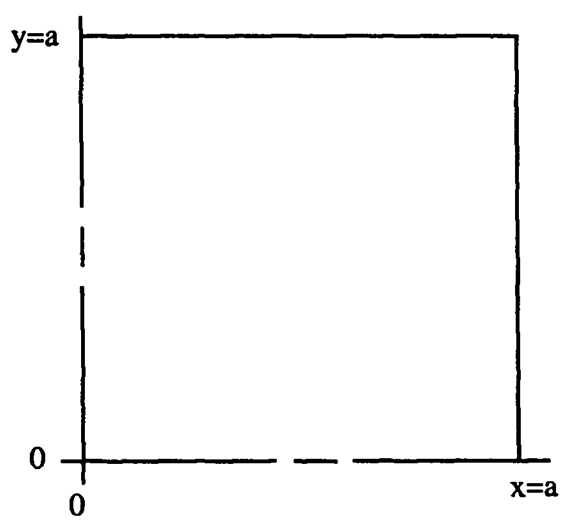

Figure 6.3 Schematic Representation of a One-Region Symmetric Reactor System

One would expect that for such a reactor system that the coordinate function, $\eta_g(x,y)$, would be symmetric, since the neutron flux is symmetric. Therefore, classes 1 and 3 can be eliminated since these solutions are not symmetric. The expression for the coordinate function that will be used is

$$\eta_g(x,y) = \left[A_{1,g}\,\mathrm{Cosh}(\beta_g x) + B_{1,g}\,\mathrm{Sinh}(\beta_g x)\right] \left[A_{2,g}\,\mathrm{Cosh}(\sqrt{\alpha_g^2 - \beta_g^2}\; y) + B_{2,g}\,\mathrm{Sinh}(\sqrt{\alpha_g^2 - \beta_g^2}\; y)\right]. \tag{6.15}$$

Now that we have an expression for the coordinate function, we are ready to determine the invariant difference equation, in a manner similar to that used in Chapter 5. The invariant difference equation is

$$\hat{\Omega}_g\, \phi_{g,i,j} + Q_{g,i,j} = 0\,, \tag{6.16}$$

where $\hat{\Omega}_g$ is the invariant difference operator. A candidate invariant difference operator is

$$\hat{\Omega}_g = A_g\left[\hat{E}^{\,i-1,0} - 2\hat{E}^{\,0,0} + \hat{E}^{\,i+1,0}\right] + \left[\hat{E}^{\,0,j-1} - 2\hat{E}^{\,0,0} + \hat{E}^{\,0,j+1}\right] - \Sigma_{R,g}\hat{E}^{\,0,0}, \tag{6.17}$$

where the $\hat{E}$ are the shift operators.

Equation 6.3 can be rewritten in terms of the homogeneous solution, $\phi_{H,g}(x,y)$, and the particular solution, $\phi_{P,g}(x,y)$, as

$$\hat{L}_g \phi_{H,g}(x,y) = 0 \tag{6.18}$$

and

$$\hat{L}_g \phi_{P,g}(x,y) + S_g(x,y) = 0\,. \tag{6.19}$$

In a manner similar to that employed in Chapter 5, the invariant difference operator, $\hat{\Omega}_g$, is determined such that

$$\hat{\Omega}_g \, \phi_{H,g}(x_i,y_j) = 0 \tag{6.20}$$

is invariant under the action of the group generator extended to grid points. The invariant source term, $Q_{g,i,j}$, is then determined using a particular solution of equation 6.3 as

$$Q_{g,i,j} = - \hat{\Omega}_g \, \phi_{P,g}(x_i,y_j) \, . \tag{6.21}$$

Using the arguments put forth in Section 4.3, the second extension of the group generator extended to grid points was determined to be

$$\begin{aligned}
\hat{U}_g^{(2D)} = {} & \eta_{g,i-1,j} \frac{\partial}{\partial \phi_{g,i-1,j}} + \eta_{g,i,j-1} \frac{\partial}{\partial \phi_{g,i,j-1}} + \eta_{g,i,j} \frac{\partial}{\partial \phi_{g,i,j}} \\
& + \eta_{g,i+1,j} \frac{\partial}{\partial \phi_{g,i+1,j}} + \eta_{g,i,j+1} \frac{\partial}{\partial \phi_{g,i,j+1}} + \cdots \\
& + \eta_{g,xx,i-1,j} \frac{\partial}{\partial \phi_{g,xx,i-1,j}} + \eta_{g,xx,i,j} \frac{\partial}{\partial \phi_{g,xx,i,j}} + \eta_{g,xx,i+1,j} \frac{\partial}{\partial \phi_{g,xx,i+1,j}} + \cdots \\
& + \eta_{g,yy,i,j-1} \frac{\partial}{\partial \phi_{g,yy,i,j-1}} + \eta_{g,yy,i,j} \frac{\partial}{\partial \phi_{g,yy,i,j}} + \eta_{g,yy,i,j+1} \frac{\partial}{\partial \phi_{g,yy,i,j+1}} + \cdots \, .
\end{aligned} \tag{6.22}$$

The coefficients, A_g and B_g, of the invariant difference operator are determined by equating equations (6.18) and (6.20), and then operating upon the result with the second extension of the group generator extended to grid points to yield

$$\begin{aligned}
D_g\eta_{g,xx,i,j} + D_g\eta_{g,yy,i,j} = {} & A_g[\eta_{g,i-1,j} - 2\eta_{g,i,j} + \eta_{g,i+1,j}] \\
& + B_g[\eta_{g,i,j-1} - 2\eta_{g,i,j} + \eta_{g,i,j+1}] \, .
\end{aligned} \tag{6.23}$$

Splitting equation (6.23) into its x and y components, we can solve for the coefficients as

$$A_g = \frac{D_g\eta_{g,xx,i,j}}{\eta_{g,i-1,j} - 2\eta_{g,i,j} + \eta_{g,i+1,j}} \tag{6.24}$$

and

$$B_g = \frac{D_g \eta_{g,yy,i,j}}{\eta_{g,i,j-1} - 2\eta_{g,i,j} + \eta_{g,i,j+1}} . \tag{6.25}$$

If uniform mesh spacing is assumed in both the x and y directions, then equations (6.24) and (6.25) can be simplified with the use of some hyperbolic-trigonometric identities to yield

$$A_g = \frac{D_g \beta_g^2}{4\mathrm{Sinh}^2(\beta_g \Delta x/2)} \tag{6.26}$$

and

$$B_g = \frac{D_g(\alpha_g^2 - \beta_g^2)}{4\mathrm{Sinh}^2(\sqrt{\alpha_g^2 - \beta_g^2}\,\Delta y/2)} , \tag{6.27}$$

where $0 < \beta_g^2 < \alpha_g^2$. The coefficients A_g and B_g have a striking resemblance to the coefficient of the derivative in the one-dimension case, a result which is not surprising, since second order derivatives are being approximated. If we make the substitution $\beta_g^2 = \alpha_g^2 p^2$ and make use of $\alpha_g^2 = \Sigma_{R,g}/D_g$, the invariant difference operator becomes

$$\hat{\Omega}_g = \frac{\Sigma_{R,g} p_g^2 \left[\hat{E}^{\,i+1,0} - 2\hat{E}^{\,0,0} + \hat{E}^{\,i+1,0}\right]}{4\mathrm{Sinh}^2(\alpha_g p_g \Delta x/2)} + \frac{\Sigma_{R,g}(1-p_g^2)\left[\hat{E}^{\,0,j-1} - 2\hat{E}^{\,0,0} + \hat{E}^{\,0,j+1}\right]}{4\mathrm{Sinh}^2(\alpha_g\sqrt{1 - p_g^2}\,\Delta y/2)} - \Sigma_{R,g}\hat{E}^{\,0,0} , \tag{6.28}$$

where $0 < p_g < 1$. The invariant difference equation is therefore,

$$\frac{\Sigma_{R,g} p_g^2 \left[\phi_{g,i-1,j} - 2\phi_{g,i,j} + \phi_{g,i+1,j}\right]}{4\mathrm{Sinh}^2(\alpha_g p_g \Delta x/2)} + \frac{\Sigma_{R,g}(1-p_g^2)\left[\phi_{g,i,j-1} - 2\phi_{g,i,j} + \phi_{g,i,j+1}\right]}{4\mathrm{Sinh}^2(\alpha_g\sqrt{1 - p_g^2}\,\Delta y/2)} - \Sigma_{R,g}\phi_{g,i,j} + Q_{g,i,j} = 0 \quad \text{for } 1 \le g \le G, \tag{6.29}$$

where $0 < p_g < 1$ and $Q_{g,i,j}$ is the invariant source term, that has yet to be determined. As we shall see later, there are only certain acceptable values of p_g that will be allowed.

To determine the invariant source term, we will need a particular solution of equation (6.1). As with the one-dimensional problem, we will have to make some approximation of the source distribution in order to determine a particular solution. In deriving expressions for the invariant source terms, we will examine only two forms of source distributions: the first case will consist of assuming a constant source distribution, and the second will consist of using a two-dimensional quadratic curve fit.

For the first source distribution, we will assume that the source is a constant in the neighborhood of the point x_i,y_j, i.e., the source as all points adjacent to the point x_i,y_j are equal to the source at the point x_i,y_j; therefore, the source distribution is

$$S_g(x,y) = S_{g,i,j} \, . \tag{6.30}$$

Using this source distribution, we find that the particular solution of equation (6.1) is

$$\phi_{P,g}(x,y) = \frac{1}{\Sigma_{R,g}} S_{g,i,j} \, . \tag{6.31}$$

Operating upon this particular solution with the invariant difference operator, (6.28), the invariant source term was determined to be

$$Q_{g,i,j} = S_{g,i,j} \, ; \tag{6.32}$$

therefore, the in-region invariant finite difference approximation of the two-dimensional neutron diffusion equation for the first case is

$$\frac{\Sigma_{R,g}p_g^2\left[\phi_{g,i-1,j} - 2\phi_{g,i,j} + \phi_{g,i+1,j}\right]}{4\mathrm{Sinh}^2(\alpha_g p_g \Delta x/2)} + \frac{\Sigma_{R,g}(1-p_g^2)\left[\phi_{g,i,j-1} - 2\phi_{g,i,j} + \phi_{g,i,j+1}\right]}{4\mathrm{Sinh}^2(\alpha_g\sqrt{1-p_g^2}\Delta y/2)}$$
$$- \Sigma_{R,g}\phi_{g,i,j} + S_{g,i,j} = 0 \quad \text{for } 1 \le g \le G. \tag{6.33}$$

We now consider the second case, in which a two-dimensional quadratic fit is used as an approximation of the source distribution as given by

$$S_g(x,y) = \frac{S_{g,i-1,j} - 2S_{g,i,j} + S_{g,i+1,j}}{2\Delta x^2}(x - x_i)^2 + \frac{S_{g,i+1,j} - S_{g,i-1,j}}{2\Delta x}(x - x_i)$$
$$+ \frac{S_{g,i,j-1} - 2S_{g,i,j} + S_{g,i,j+1}}{2\Delta y^2}(y - y_j)^2 + \frac{S_{g,i,j+1} - S_{g,i,j-1}}{2\Delta y}(y - y_j) + S_{g,i,j}\,. \tag{6.34}$$

Using the source distribution (6.34) and the differential equation (6.1), the particular solution was found to be

$$\phi_{P,g}(x,y) = \frac{1}{\Sigma_{R,g}}\left[\frac{S_{g,i-1,j} - 2S_{g,i,j} + S_{g,i+1,j}}{2\Delta x^2}(x - x_i)^2 + \frac{S_{g,i+1,j} - S_{g,i-1,j}}{2\Delta x}(x - x_i)\right]$$
$$+ \frac{1}{\Sigma_{R,g}}\left[\frac{S_{g,i,j-1} - 2S_{g,i,j} + S_{g,i,j+1}}{2\Delta y^2}(y - y_j)^2 + \frac{S_{g,i,j+1} - S_{g,i,j-1}}{2\Delta y}(y - y_j)\right] \tag{6.35}$$
$$+ \frac{1}{\Sigma_{R,g}}\left[\frac{S_{g,i-1,j} - 2S_{g,i,j} + S_{g,i+1,j}}{2\alpha_g^2\Delta x^2} + \frac{S_{g,i,j-1} - 2S_{g,i,j} + S_{g,i,j+1}}{2\alpha_g^2\Delta y^2} + S_{g,i,j}\right].$$

Operating upon this particular solution with the invariant difference operator (6.28), we find that the invariant source term, $Q_{g,i,j}$, is

$$Q_{g,i,j} = (S_{g,i-1,j} - 2S_{g,i,j} + S_{g,i+1,j})\left[\frac{1}{(\alpha_g\Delta x)^2} - \frac{p_g^2}{4\mathrm{Sinh}^2(\alpha_g p_g\Delta x/2)}\right]$$
$$+ (S_{g,i,j-1} - 2S_{g,i,j} + S_{g,i,j+1})\left[\frac{1}{(\alpha_g\Delta y)^2} - \frac{1 - p_g^2}{4\mathrm{Sinh}^2(\alpha_g\sqrt{1-p_g^2}\Delta y/2)}\right] + S_{g,i,j}\,. \tag{6.36}$$

The invariant finite difference approximation of the diffusion equation, for the two-dimensional quadratic curve fit of the source, is

$$
\begin{aligned}
&\frac{\Sigma_{R,g}p_g^2\left[\phi_{g,i-1,j} - 2\phi_{g,i,j} + \phi_{g,i+1,j}\right]}{4\mathrm{Sinh}^2(\alpha_g p_g \Delta x/2)} + \frac{\Sigma_{R,g}(1-p_g^2)\left[\phi_{g,i,j-1} - 2\phi_{g,i,j} + \phi_{g,i,j+1}\right]}{4\mathrm{Sinh}^2(\alpha_g\sqrt{1-p_g^2}\Delta y/2)} \\
&- \Sigma_{R,g}\phi_{g,i,j} + (S_{g,i-1,j} - 2S_{g,i,j} + S_{g,i+1,j})\left[\frac{1}{(\alpha_g\Delta x)^2} - \frac{p_g^2}{4\mathrm{Sinh}^2(\alpha_g p_g\Delta x/2)}\right] \\
&+ (S_{g,i,j-1} - 2S_{g,i,j} + S_{g,i,j+1})\left[\frac{1}{(\alpha_g\Delta y)^2} - \frac{1-p_g^2}{4\mathrm{Sinh}^2(\alpha_g\sqrt{1-p_g^2}\Delta y/2)}\right] \\
&+ S_{g,i,j} = 0 \quad \text{for } 1 \le g \le G.
\end{aligned} \tag{6.37}
$$

Now that we have the in-region finite difference equations for the two cases, we will go on to derive the interface equations required to link together several regions.

6.2.2 The Invariant Finite Difference Equations for Interfaces

Interface equations are required in order to handle problems in which there are changes in the material properties or changes in the mesh spacing, both of which will be dealt with in the same manner. There are essentially three types of interfaces for which we need to derive the invariant finite difference equations. The three types of interfaces are: 1) a cross type, which consists of the intersection of four material regions, 2) a vertical type in which two material regions meet such that the interface is parallel to the y-axis, and 3) the horizontal interface, that consists of two material regions which meet such that the interface is parallel to the x-axis. All other types of interfaces can be modeled with some variation of these three types.

We begin the derivation of the interface conditions with the cross type, since the other two types of interfaces are simply special cases of this interface. Since the invariant difference equations have the same form for all energy groups, we will omit the energy group subscript, g, in the ensuing discussion. Figure 6.4 shows a schematic representation of the cross type interface. The derivation of the interface equations will follow in a manner similar to that employed in

Chapter 5. We now need to determine the discrete form of the interface conditions, (6.5) and (6,6). The discrete forms of the interface conditions will then be used to couple together the four invariant difference equations, which have the form of equation (6.29).

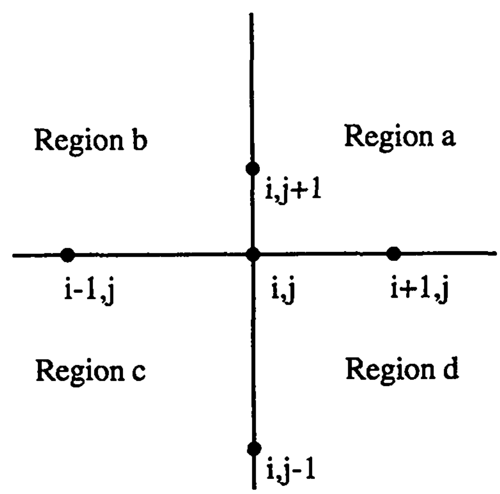

Figure 6.4 A Schematic of the Cross Type of Interface

The invariant discrete forms of the interface conditions are determined using the same procedure as used in Section 5.3. As a specific example, we will examine the construction of the discrete form of the net current across a vertical interface as given by

$$-D_g^-\phi_{g,x}^-(x_b^-,y) = -D_g^+\phi_{g,x}^+(x_b^+,y)\ . \tag{6.38}$$

The solution, $\phi(x,y)$, can be written in terms of the homogeneous and particular solutions as

$$\phi(x,y) = \phi_H(x,y) + \phi_P(x,y)\ , \tag{6.39}$$

and the neutron current, $-D\phi(x,y)$, can be rewritten as

$$\frac{\partial\phi(x,y)}{\partial x} = \frac{\partial\phi_H(x,y)}{\partial x} + \frac{\partial\phi_P(x,y)}{\partial x}\ . \tag{6.40}$$

We now approximate the neutron current as

$$D\frac{\partial\phi(x,y)}{\partial x}\Big|_{x=x_i}^{y=y_j} \approx T_i(\phi_{i+1,j} - \phi_{i-1,j}) + QX, \tag{6.41}$$

where T_i is determined, such that

$$D\frac{\partial\phi_H(x,y)}{\partial x}\Big|_{x=x_i}^{y=y_j} = T_i(\phi_{H,i+1,j} - \phi_{H,i-1,j}) \tag{6.42}$$

is invariant under the action of the group extended to grid points, and QX is determined using

$$QX = D\frac{\partial\phi_P(x,y)}{\partial x}\Big|_{x=x_i}^{y=y_j} - T_i(\phi_{p,i+1,j} - \phi_{p,i-1,j}) \,. \tag{6.43}$$

Operating on equation (6.42) with the second extension of the group generator extended to grid points, as given by (6.22), and determining T_i, assuming uniform mesh spacing, we find that the invariant difference approximation of the neutron current is

$$D\frac{\partial\phi(x,y)}{\partial x}\Big|_{x=x_i}^{y=y_j} \approx \frac{Dp\alpha(\phi_{i+1,j} - \phi_{i-1,j})}{2\text{Sinh}(p\alpha\Delta x)} + QX \,, \tag{6.44}$$

where QX will be determined later. In a manner identical to that outlined above, we find that the neutron current in the y-direction is

$$D\frac{\partial\phi(x,y)}{\partial y}\Big|_{x=x_i}^{y=y_j} \approx \frac{D\alpha\sqrt{1 - p^2}(\phi_{i,j+1} - \phi_{i,j-1})}{2\text{Sinh}(\alpha\Delta y\sqrt{1-p^2})} + QY \,, \tag{6.45}$$

where QY will again be determined later.

Now that we have the discrete form of the neutron current, we can write the current boundary conditions. The net current boundary conditions are: from region b to region a

$$\frac{D_a p_a \alpha_a(\phi_{a,i+1,j} - \phi_{a,i-1,j})}{2\mathrm{Sinh}(p_a\alpha_a\Delta x_a)} + QX_a = \frac{D_b p_b \alpha_b(\phi_{b,i+1,j} - \phi_{b,i-1,j})}{2\mathrm{Sinh}(p_b\alpha_b\Delta x_b)} + QX_b\,, \qquad (6.46)$$

from region c to region d

$$\frac{D_c p_c \alpha_c(\phi_{c,i+1,j} - \phi_{c,i-1,j})}{2\mathrm{Sinh}(p_c\alpha_c\Delta x_c)} + QX_c = \frac{D_d p_d \alpha_d(\phi_{d,i+1,j} - \phi_{d,i-1,j})}{2\mathrm{Sinh}(p_d\alpha_d\Delta x_d)} + QX_d\,, \qquad (6.47)$$

from region c to region b

$$\frac{D_c\sqrt{1-p_c^2}\,\alpha_c(\phi_{c,i,j+1} - \phi_{c,i,j-1})}{2\mathrm{Sinh}(\sqrt{1-p_c^2}\,\alpha_c\Delta x_c)} + QY_c = \frac{D_b\sqrt{1-p_b^2}\,\alpha_b(\phi_{b,i,j+1} - \phi_{b,i,j-1})}{2\mathrm{Sinh}(\sqrt{1-p_b^2}\,\alpha_b\Delta x_b)} + QY_b\,, \quad (6.48)$$

and from region d to region a

$$\frac{D_a\sqrt{1-p_a^2}\,\alpha_c(\phi_{a,i,j+1} - \phi_{a,i,j-1})}{2\mathrm{Sinh}(\sqrt{1-p_a^2}\,\alpha_a\Delta x_a)} + QY_a = \frac{D_d\sqrt{1-p_d^2}\,\alpha_d(\phi_{d,i,j+1} - \phi_{d,i,j-1})}{2\mathrm{Sinh}(\sqrt{1-p_d^2}\,\alpha_d\Delta x_d)} + QY_d\,, \quad (6.49)$$

where the subscripts a, b, c, and d refer to the four regions respectively. We also have four invariant finite difference equations for the four regions as given by

$$\frac{\Sigma_{R,r}p_r^2\left[\phi_{r,i-1,j} - 2\phi_{r,i,j} + \phi_{r,i+1,j}\right]}{4\mathrm{Sinh}^2(\alpha_r p_r \Delta x_r/2)} + \frac{\Sigma_{R,r}(1-p_r^2)\left[\phi_{r,i,j-1} - 2\phi_{r,i,j} + \phi_{r,i,j+1}\right]}{4\mathrm{Sinh}^2(\alpha_r\sqrt{1-p_r^2}\,\Delta y_r/2)}$$
$$- \Sigma_{R,r}\phi_{r,i,j} + Q_{r,i,j} = 0\;, \qquad (6.50)$$

where the subscripts r indicate which region, either a, b, c, or d. Additionally, we have the flux interface condition

$$\phi_{a,i,j} = \phi_{b,i,j} = \phi_{c,i,j} = \phi_{d,i,j}\,. \qquad (6.51)$$

The object now is to eliminate the eight fluxes, $\phi_{a,i-1,j}$, $\phi_{a,i,j-1}$, $\phi_{b,i+1,j}$, $\phi_{b,i,j-1}$, $\phi_{c,i+1,j}$, $\phi_{c,i,j+1}$, $\phi_{d,i-1,j}$, and $\phi_{d,i,j+1}$, using the four invariant difference equations, (6.50), and the four invariant net current interface equations; then apply the flux interface conditions (6.51). The algebra involved in this process is very involved, and, therefore, will not be presented. Knowing that we have an orthogonal grid, we can make use of the fact that $\Delta x_c = \Delta x_b$, $\Delta x_a = \Delta x_d$, $\Delta y_b = \Delta y_a$, and $\Delta y_c = \Delta y_d$. The invariant finite difference equation for the cross type of interface is

$$\begin{aligned}
&-\left[\frac{p_d D_d \alpha_d}{\mathrm{Sinh}(p_d \alpha_d \Delta x_d)} + \frac{p_a D_a \alpha_a}{\mathrm{Sinh}(p_a \alpha_a \Delta x_d)}\right] \phi_{i+1,j} - \left[\frac{p_b D_b \alpha_b}{\mathrm{Sinh}(p_b \alpha_b \Delta x_c)} + \frac{p_c D_c \alpha_c}{\mathrm{Sinh}(p_c \alpha_c \Delta x_c)}\right] \phi_{i-1,j} \\
&+ \left[\begin{array}{l} \dfrac{p_a D_a \alpha_a}{\mathrm{Sinh}(p_a \alpha_a \Delta x_d)}\left(1 + \dfrac{\mathrm{Sinh}^2(p_a \alpha_a \Delta x_d/2)}{p_a^2}\right) + \dfrac{p_b D_b \alpha_b}{\mathrm{Sinh}(p_b \alpha_b \Delta x_c)}\left(1 + \dfrac{\mathrm{Sinh}^2(p_b \alpha_b \Delta x_c/2)}{p_b^2}\right) \\ + \dfrac{p_c D_c \alpha_c}{\mathrm{Sinh}(p_c \alpha_c \Delta x_c)}\left(1 + \dfrac{\mathrm{Sinh}^2(p_c \alpha_c \Delta x_c/2)}{p_c^2}\right) + \dfrac{p_d D_d \alpha_d}{\mathrm{Sinh}(p_d \alpha_d \Delta x_d)}\left(1 + \dfrac{\mathrm{Sinh}^2(p_d \alpha_d \Delta x_d/2)}{p_d^2}\right) \end{array}\right] \phi_{i,j} \\
&-\left[\frac{q_c D_c \alpha_c}{\mathrm{Sinh}(q_c \alpha_c \Delta y_c)} + \frac{q_d D_d \alpha_d}{\mathrm{Sinh}(q_d \alpha_d \Delta y_c)}\right] \phi_{i,j-1} - \left[\frac{q_b D_b \alpha_b}{\mathrm{Sinh}(q_b \alpha_b \Delta y_a)} + \frac{q_a D_a \alpha_a}{\mathrm{Sinh}(q_a \alpha_a \Delta y_a)}\right] \phi_{i,j+1} \\
&+ \left[\begin{array}{l} \dfrac{q_a D_a \alpha_a}{\mathrm{Sinh}(q_a \alpha_a \Delta y_a)}\left(1 + \dfrac{\mathrm{Sinh}^2(q_a \alpha_a \Delta y_a/2)}{q_a^2}\right) + \dfrac{q_b D_b \alpha_b}{\mathrm{Sinh}(q_b \alpha_b \Delta y_a)}\left(1 + \dfrac{\mathrm{Sinh}^2(q_b \alpha_b \Delta y_a/2)}{q_b^2}\right) \\ + \dfrac{q_c D_c \alpha_c}{\mathrm{Sinh}(q_c \alpha_c \Delta y_c)}\left(1 + \dfrac{\mathrm{Sinh}^2(q_c \alpha_c \Delta y_c/2)}{q_c^2}\right) + \dfrac{q_d D_d \alpha_d}{\mathrm{Sinh}(q_d \alpha_d \Delta y_c)}\left(1 + \dfrac{\mathrm{Sinh}^2(q_d \alpha_d \Delta y_c/2)}{q_d^2}\right) \end{array}\right] \phi_{i,j} \\
&= Q\,, \qquad (6.52)
\end{aligned}$$

where $q_r = \sqrt{1 - p_r^2}$ and Q is given by

$$\begin{aligned}
Q = {} & Q_{a,i,j} \frac{\mathrm{Tanh}(p_a \alpha_a \Delta x_d/2)}{\alpha_a p_a} + Q_{b,i,j} \frac{\mathrm{Tanh}(p_b \alpha_b \Delta x_c/2)}{\alpha_b p_b} \\
& + Q_{c,i,j} \frac{\mathrm{Tanh}(p_c \alpha_c \Delta x_c/2)}{\alpha_c p_c} + Q_{d,i,j} \frac{\mathrm{Tanh}(p_d \alpha_d \Delta x_d/2)}{\alpha_d p_d} \qquad (6.53) \\
& QX_a + QX_d - QX_b - QX_c + QY_b + QY_a - QY_c - QY_d\,.
\end{aligned}$$

One interesting result of this operation, is that there is a condition on Δx_r, Δy_r, and p_r that must be satisfied in order to determine an invariant difference equation for the cross-type of interface. This condition is

$$\frac{p_r}{\sqrt{1-p_r^2}} \frac{\mathrm{Tanh}\left[\sqrt{1-p_r^2}\ \alpha_r\,\Delta y_r/2\right]}{\mathrm{Tanh}\left[p_r\alpha_r\Delta x_r/2\right]} = 1, \tag{6.54}$$

which must be satisfied for each of the four regions. Thus if Δx_r, and Δy_r are specified, equation (6.52) must be used to determine an acceptable value of p_r. If $\Delta x_r = \Delta y_r$, an obvious acceptable value of p_r is $1/\sqrt{2}$. However, in general Δx_r is not equal to Δy_r; it would therefore be of use to know if there are other acceptable values of Δx and Δy that permit $0 < p_r < 1$. Since equation (6.54) is a transcendental equation, p_r can not be directly solved for; therefore, one can use a method such as Newton's method to determine p_r. If we define $f = \Delta y_r/\Delta x_r$, we can rewrite equation (6.54) as

$$\frac{p_r}{\sqrt{1-p_r^2}} \frac{\mathrm{Tanh}\left[\sqrt{1-p_r^2}\ f\alpha_r\Delta x_r/2\right]}{\mathrm{Tanh}\left[p_r\alpha_r\Delta x_r/2\right]} = 1\,. \tag{6.55}$$

Using Newton's method, equation (6.55) was used to determine acceptable values of p_r for a range of values of both f and $\alpha_r\Delta x_r$, the results of which are shown in figure 6.5. As can be seen from Figure 6.5, there are two extremes: if $\alpha_r\Delta x_r$ is greater than 0.5, then there are a wide variety of values that $\alpha_r\Delta y_r$ can acquire and there will still be a valid p_r; however, as $\alpha_r\Delta x_r$ becomes small, then $\alpha_r\Delta y_r$ must take on the value of $\alpha_r\Delta x_r$ for p_r to be valid.

We now turn our attention to determining the particular solutions and the corresponding invariant source terms for both the constant and quadratic source approximations. For the constant source approximation, we again assume that the source is constant in the neighborhood of x_i,y_j; therefore, the constant source approximation is

$$S_r(x,y) = S_{r,i,j}\,, \tag{6.56}$$

for a given region, where r equals a, b, c, or d. The particular solution of equation (6.1) for each region is readily found to be

$$\phi_{P,r}(x,y) = \frac{1}{\Sigma_{R,r}} S_{r,i,j} \,. \tag{6.57}$$

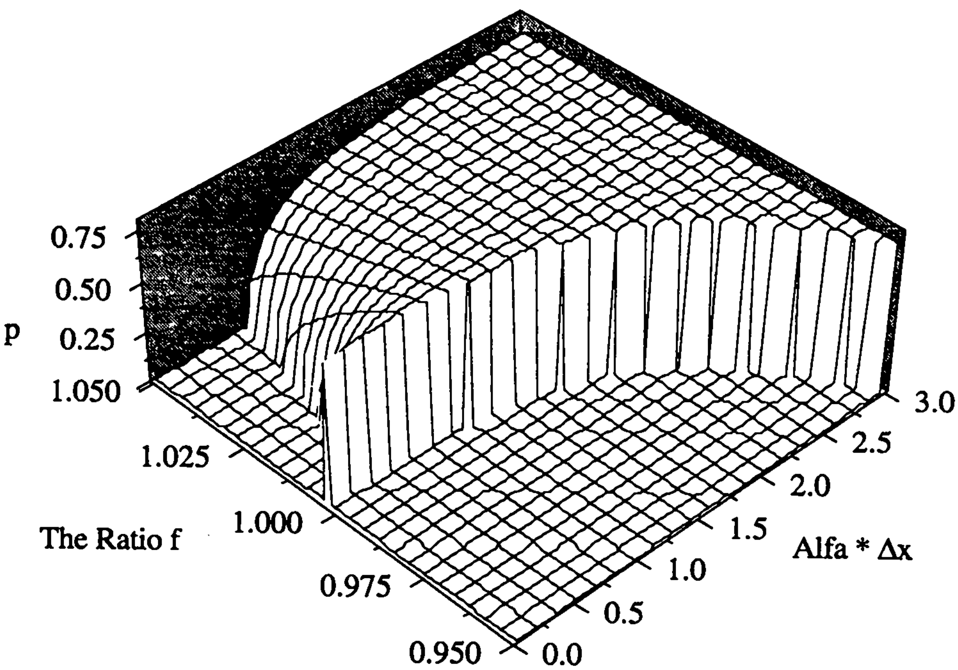

Figure 6.5 The Parameter p_r as a Function of $\alpha_r \Delta x_r$ and the Ratio f

Operating upon the particular solution, (6.57), with the invariant difference operator, (6.28) as modified to

$$\hat{\Omega}_r = \frac{\Sigma_{R,r} p_r^2 \left[\hat{E}^{\,i+1,0} - 2\hat{E}^{\,0,0} + \hat{E}^{\,i+1,0}\right]}{4\mathrm{Sinh}^2(\alpha_r p_r \Delta x/2)} + \frac{\Sigma_{R,r}(1-p_r^2)\left[\hat{E}^{\,0,j-1} - 2\hat{E}^{\,0,0} + \hat{E}^{\,0,j+1}\right]}{4\mathrm{Sinh}^2(\alpha_r \sqrt{1-p_r^2}\,\Delta y/2)} - \Sigma_{R,r}\hat{E}^{\,0,0} \,, \tag{6.58}$$

we find that the invariant source terms, $Q_{r,i,j}$, are

$$Q_{r,i,j} = S_{r,i,j} \,. \tag{6.59}$$

All that remains to be determined is the invariant source terms for the neutron currents, QX_r and QY_r. Using the particular solution, (6.57), QX_r and QY_r are determined, using (6.43) and its y-direction counterpart, to both be zero for all four regions. Therefore, the invariant source term, Q, as given in equation (5.53) has the explicit form

$$\begin{aligned} Q = S_{a,i,j}\frac{\mathrm{Tanh}(p_a\alpha_a\Delta x_d/2)}{\alpha_a p_a} + S_{b,i,j}\frac{\mathrm{Tanh}(p_b\alpha_b\Delta x_c/2)}{\alpha_b p_b} \\ + S_{c,i,j}\frac{\mathrm{Tanh}(p_c\alpha_c\Delta x_c/2)}{\alpha_c p_c} + S_{d,i,j}\frac{\mathrm{Tanh}(p_d\alpha_d\Delta x_d/2)}{\alpha_d p_d} \,. \end{aligned} \tag{6.60}$$

We now turn our attention to the case where we use a quadratic curve fit to approximate the source distribution. The curve fit has in general the form

$$S_r(x,y) = A_r(x - x_i)^2 + B_r(y - y_j)^2 + C_r(x - x_i) + E_r(y - y_j) + S_{r,i,j} \,, \tag{6.61}$$

for each region. The coefficients of (6.61) are given by: region a

$$\begin{aligned} A_a = \frac{S_{a,i,j} - 2S_{a,i+1,j} + S_{a,i+2,j}}{2\Delta x_d^2} \quad B_a = \frac{S_{a,i,j} - 2S_{a,i,j+1} + S_{a,i,j+2}}{2\Delta y_b^2} \\ C_a = \frac{-3S_{a,i,j} + 4S_{a,i+1,j} - S_{a,i+2,j}}{2\Delta x_d} \quad E_a = \frac{-3S_{a,i,j} + 4S_{a,i,j+1} - S_{a,i,j+2}}{2\Delta y_b} \,, \end{aligned} \tag{6.61a}$$

region b

$$\begin{aligned} A_b = \frac{S_{b,i,j} - 2S_{b,i-1,j} + S_{b,i-2,j}}{2\Delta x_c^2} \quad B_b = \frac{S_{b,i,j} - 2S_{b,i,j+1} + S_{b,i,j+2}}{2\Delta y_b^2} \\ C_b = \frac{3S_{b,i,j} - 4S_{b,i-1,j} + S_{b,i-2,j}}{2\Delta x_c} \quad E_b = \frac{-3S_{b,i,j} + 4S_{b,i,j+1} - S_{b,i,j+2}}{2\Delta y_b} \,, \end{aligned} \tag{6.61b}$$

region c

$$A_c = \frac{S_{c,i,j} - 2S_{c,i-1,j} + S_{c,i-2,j}}{2\Delta x_c^2} \quad B_b = \frac{S_{c,i,j} - 2S_{c,i,j-1} + S_{c,i,j-2}}{2\Delta y_c^2}$$

$$C_c = \frac{3S_{c,i,j} - 4S_{c,i-1,j} + S_{c,i-2,j}}{2\Delta x_c} \quad E_b = \frac{3S_{c,i,j} - 4S_{c,i,j-1} + S_{c,i,j-2}}{2\Delta y_c}, \tag{6.61c}$$

and finally region d

$$A_d = \frac{S_{d,i,j} - 2S_{d,i-1,j} + S_{d,i-2,j}}{2\Delta x_d^2} \quad B_d = \frac{S_{d,i,j} - 2S_{d,i,j-1} + S_{d,i,j-2}}{2\Delta y_c^2}$$

$$C_d = \frac{-3S_{d,i,j} + 4S_{cd,i-1,j} - S_{d,i-2,j}}{2\Delta x_d} \quad E_d = \frac{3S_{d,i,j} - 4S_{d,i,j-1} + S_{d,i,j-2}}{2\Delta y_c}. \tag{6.61d}$$

The invariant source terms, $Q_{r,i,j}$, were then determined to be

$$Q_{r,i,j} = S_{r,i,j} + 2\Delta x_r A_r\left[\frac{1}{(\alpha_r\Delta x_r)^2} - \frac{p_r^2}{4\mathrm{Sinh}^2(p_r\alpha_r\Delta x_r/2)}\right] + 2\Delta y_r B_r\left[\frac{1}{(\alpha_r\Delta y_r)^2} - \frac{q_r^2}{4\mathrm{Sinh}^2(q_r\alpha_r\Delta y_r/2)}\right], \tag{6.62}$$

where $q_r = \sqrt{1 - p_r^2}$. The invariant source terms due to the net current, QX_r and QY_r, were determined to be

$$QX_r = \frac{C_r}{\alpha_r^2}\left[1 - \frac{p_r\alpha_r\Delta x_r}{\mathrm{Sinh}(p_r\alpha_r\Delta x_r}\right] \tag{6.63}$$

and

$$QY_r = \frac{E_r}{\alpha_r^2}\left[1 - \frac{q_r\alpha_r\Delta y_r}{\mathrm{Sinh}(q_r\alpha_r\Delta y_r}\right]. \tag{6.64}$$

The invariant source term for the cross type of interface using quadratic curve fits of the source is given by equations (6.53), (6.62), (6.63), and (6.64) using the coefficients (6.61a-d).

We now examine the other two types of interfaces, the vertical and the horizontal types. Both types of interfaces can be derived by setting the appropriate data in equation (6.52) and (6.53) equal to each other. To illustrate this process, we consider the horizontal interface as shown in figure 6.6.

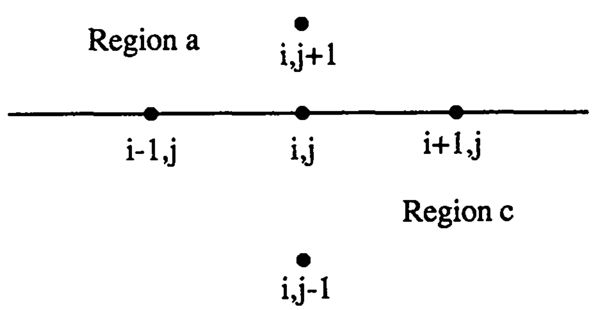

Figure 6.6 A Schematic of the Horizontal Type of Interface

The invariant finite difference equation for the horizontal interface is determined by setting all material properties in regions a and b equal to each other, and the material properties in regions c and d equal to each other. This yields the invariant difference equation as

$$
\begin{aligned}
&-\left(\frac{p_a D_a \alpha_a}{\mathrm{Sinh}(p_a \alpha_a \Delta x)} + \frac{p_c D_c \alpha_c}{\mathrm{Sinh}(p_c \alpha_c \Delta x)}\right)\phi_{i+1,j} - \left(\frac{p_a D_a \alpha_a}{\mathrm{Sinh}(p_a \alpha_a \Delta x)} + \frac{p_c D_c \alpha_c}{\mathrm{Sinh}(p_c \alpha_c \Delta x)}\right)\phi_{i-1,j} \\
&+\left[\frac{2p_a D_a \alpha_a}{\mathrm{Sinh}(p_a \alpha_a \Delta x)}\left(1 + \frac{\mathrm{Sinh}(p_a \alpha_a \Delta x/2)}{p_a^2}\right) + \frac{2p_c D_c \alpha_c}{\mathrm{Sinh}(p_c \alpha_c \Delta x)}\left(1 + \frac{\mathrm{Sinh}(p_c \alpha_c \Delta x/2)}{p_c^2}\right)\right]\phi_{i,j} \\
&+\left[\frac{2q_a D_a \alpha_a}{\mathrm{Sinh}(q_a \alpha_a \Delta y_a)}\left(1 + \frac{\mathrm{Sinh}(q_a \alpha_a \Delta y_a/2)}{q_a^2}\right) + \frac{2q_c D_c \alpha_c}{\mathrm{Sinh}(q_c \alpha_c \Delta y_c)}\left(1 + \frac{\mathrm{Sinh}(q_c \alpha_c \Delta y_c/2)}{q_c^2}\right)\right]\phi_{i,j} \\
&-\frac{2q_a D_a \alpha_a}{\mathrm{Sinh}(q_a \alpha_a \Delta y_a)}\phi_{i,j+1} - \frac{2q_c D_c \alpha_c}{\mathrm{Sinh}(q_c \alpha_c \Delta y_c)}\phi_{i,j-1} = Q\,,
\end{aligned}
\qquad (6.65)
$$

where the invariant source Q is given by

$$Q = \frac{2\mathrm{Tanh}(p_a\alpha_a\Delta x/2)}{p_a\alpha_a} Q_{a,i,j} + \frac{2\mathrm{Tanh}(p_c\alpha_c\Delta x/2)}{p_c\alpha_c} Q_{c,i,j} + 2QY_a - 2QY_c\,, \tag{6.66}$$

or making use of equation (6.54)

$$Q = \frac{2\mathrm{Tanh}(q_a\alpha_a\Delta y_a/2)}{q_a\alpha_a} Q_{a,i,j} + \frac{2\mathrm{Tanh}(q_c\alpha_c\Delta y_c/2)}{q_c\alpha_c} Q_{c,i,j} + 2QY_a - 2QY_c\,. \tag{6.67}$$

Using the constant source approximation, $S_r(x,y) = S_{r,i,j}$, we find that the particular solution of equation (6.1) is $\phi_{P,r}(x,y) = S_{r,i,j}/\Sigma_{R,r}$, and that the invariant source term, Q, is given by

$$Q = \frac{2\mathrm{Tanh}(q_a\alpha_a\Delta y_a/2)}{q_a\alpha_a} S_{a,i,j} + \frac{2\mathrm{Tanh}(q_c\alpha_c\Delta y_c/2)}{q_c\alpha_c} S_{c,i,j}\,. \tag{6.68}$$

Using a quadratic curve fit of the source distribution, as given by equation (6.61), where the coefficients are

$$A_a = \frac{S_{a,i-1,j} - 2S_{a,i,j} + S_{a,i+1,j}}{2\Delta x^2} \quad B_a = \frac{S_{a,i,j} - 2S_{a,i,j+1} + S_{a,i,j+2}}{2\Delta y_a^2}$$
$$C_a = \frac{S_{a,i+1,j} - S_{a,i-1,j}}{2\Delta x} \quad E_a = \frac{-3S_{a,i,j} + 4S_{a,i,j+1} - S_{a,i,j+2}}{2\Delta y_a} \tag{6.69a}$$

and

$$A_a = \frac{S_{a,i-1,j} - 2S_{a,i,j} + S_{a,i+1,j}}{2\Delta x^2} \quad B_a = \frac{S_{a,i,j} - 2S_{a,i,j+1} + S_{a,i,j+2}}{2\Delta y_b^2}$$
$$C_a = \frac{S_{a,i+1,j} - S_{c,i-1,j}}{2\Delta x} \quad E_a = \frac{3S_{a,i,j} + 4S_{a,i,j+1} - S_{a,i,j+2}}{2\Delta y_b}\,, \tag{6.69b}$$

we find that the invariant source term, Q, is

$$Q = S_{a,i,j} + S_{c,i,j} + 2\Delta x^2 A_a\left[\frac{1}{(\alpha_a \Delta x)^2} - \frac{p_a^2}{4\mathrm{Sinh}^2(p_a\alpha_a\Delta x/2)}\right]$$

$$+ 2\Delta y_a^2 B_a\left[\frac{1}{(\alpha_a \Delta y_a)^2} - \frac{q_a^2}{4\mathrm{Sinh}^2(q_a\alpha_a\Delta y_a/2)}\right] + 2\Delta x^2 A_c\left[\frac{1}{(\alpha_c \Delta x)^2} - \frac{p_c^2}{4\mathrm{Sinh}^2(p_c\alpha_c\Delta x/2)}\right] \tag{6.70}$$

$$+ 2\Delta y_a^2 B_a\left[\frac{1}{(\alpha_a \Delta y_a)^2} - \frac{q_a^2}{4\mathrm{Sinh}^2(q_a\alpha_a\Delta y_a/2)}\right]$$

$$+ 2\frac{E_a}{\alpha_a^2}\left[1 - \frac{q_a\alpha_a\Delta y_a}{\mathrm{Sinh}(q_a\alpha_a\Delta y_a)}\right] - 2\frac{E_c}{\alpha_c^2}\left[1 - \frac{q_c\alpha_c\Delta y_c}{\mathrm{Sinh}(q_c\alpha_c\Delta y_c)}\right].$$

In a very similar manner the invariant difference equations for the vertical interface, shown in figure 6.7, may be derived. Since the processes of deriving such equations has already been illustrated, we will only present the results of the derivation. The invariant difference equation for a vertical interface was determined to be

$$- \frac{2p_aD_a\alpha_a}{\mathrm{Sinh}(p_a\alpha_a\Delta x_a)}\phi_{i+1,j} - \frac{2p_bD_b\alpha_b}{\mathrm{Sinh}(p_b\alpha_b\Delta x_b)}\phi_{i-1,j}$$

$$+\left[\frac{2p_aD_a\alpha_a}{\mathrm{Sinh}(p_a\alpha_a\Delta x_a)}\left(1+\frac{\mathrm{Sinh}^2(p_a\alpha_a\Delta x_a/2)}{p_a^2}\right)+\frac{2p_bD_b\alpha_b}{\mathrm{Sinh}(p_b\alpha_b\Delta x_b)}\left(1+\frac{\mathrm{Sinh}^2(p_b\alpha_b\Delta x_b/2)}{p_b^2}\right)\right]\phi_{i,j} \tag{6.71}$$

$$+\left[\frac{2q_aD_a\alpha_a}{\mathrm{Sinh}(q_a\alpha_a\Delta y)}\left(1+\frac{\mathrm{Sinh}^2(q_a\alpha_a\Delta y/2)}{q_a^2}\right)+\frac{2q_bD_b\alpha_b}{\mathrm{Sinh}(q_b\alpha_b\Delta y)}\left(1+\frac{\mathrm{Sinh}^2(q_b\alpha_b\Delta y/2)}{q_b^2}\right)\right]\phi_{i,j}$$

$$-\left(\frac{2q_aD_a\alpha_a}{\mathrm{Sinh}(q_a\alpha_a\Delta y)}+\frac{2q_bD_b\alpha_b}{\mathrm{Sinh}(q_b\alpha_b\Delta y)}\right)\phi_{i,j+1} - \left(\frac{2q_aD_a\alpha_a}{\mathrm{Sinh}(q_a\alpha_a\Delta y)}+\frac{2q_bD_b\alpha_b}{\mathrm{Sinh}(q_b\alpha_b\Delta y)}\right)\phi_{i,j-1} = Q,$$

where the invariant source term, Q, was found as

$$Q = \frac{2\mathrm{Tanh}(p_a\alpha_a\Delta x/2)}{p_a\alpha_a}Q_{a,i,j} + \frac{2\mathrm{Tanh}(p_b\alpha_b\Delta x/2)}{p_b\alpha_b}Q_{b,i,j} + 2QX_a - 2QX_b. \tag{6.72}$$

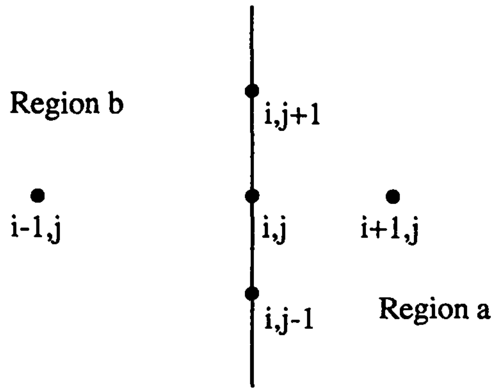

Figure 6.7 Schematic of the Vertical Interface

For the constant source approximation of the source distribution, $S_r(x,y) = S_{r,i,j}$, the invariant source term was found to be

$$Q = \frac{2\text{Tanh}(p_a\alpha_a\Delta x/2)}{p_a\alpha_a} S_{a,i,j} + \frac{2\text{Tanh}(p_b\alpha_b\Delta x/2)}{p_b\alpha_b} S_{b,i,j} \,. \qquad (6.73)$$

Finally, for the quadratic curve fit of the source distribution, equation (6.61), where the coefficients are

$$A_a = \frac{S_{a,i,j} - 2S_{a,i+1,j} + S_{a,i+2,j}}{2\Delta x_a^2} \quad B_a = \frac{S_{a,i,j-1} - 2S_{a,i,j} + S_{a,i,j+1}}{2\Delta y^2}$$
$$C_a = \frac{-3S_{a,i,j} + 4S_{a,i+1,j} - S_{a,i+2,j}}{2\Delta x_s} \quad E_a = \frac{S_{a,i,j+1} - S_{a,i,j-1}}{2\Delta y} \qquad (6.74a)$$

and

$$A_b = \frac{S_{b,i,j} - 2S_{b,i-1,j} + S_{b,i-2,j}}{2\Delta x_b^2} \quad B_b = \frac{S_{b,i,j-1} - 2S_{b,i,j} + S_{b,i,j+1}}{2\Delta y^2}$$
$$C_b = \frac{3S_{b,i,j} - 4S_{b,i-1,j} + S_{b,i-2,j}}{2\Delta x_b} \quad E_b = \frac{S_{b,i,j+1} - S_{b,i,j-1}}{2\Delta y} \qquad (6.74b)$$

the invariant source term, Q, was determined as

$$
\begin{aligned}
Q = S_{a,i,j} + S_{b,i,j} &+ 2\Delta x_a^2 A_a\left[\frac{1}{(\alpha_a \Delta x_a)^2} - \frac{p_a^2}{4\mathrm{Sinh}^2(p_a\alpha_a\Delta x_a/2)}\right] \\
&+ 2\Delta x_b^2 A_b\left[\frac{1}{(\alpha_b \Delta x_b)^2} - \frac{p_b^2}{4\mathrm{Sinh}^2(p_b\alpha_b\Delta x_b/2)}\right] \\
&+ 2\Delta y^2 B_a\left[\frac{1}{(\alpha_a \Delta y)^2} - \frac{q_a^2}{4\mathrm{Sinh}^2(q_a\alpha_a\Delta y/2)}\right] + 2\Delta y^2 B_a\left[\frac{1}{(\alpha_a \Delta y)^2} - \frac{q_a^2}{4\mathrm{Sinh}^2(q_a\alpha_a\Delta y/2)}\right] \\
&+ 2\frac{C_a}{\alpha_a^2}\left[1 - \frac{p_a\alpha_a\Delta x_a}{\mathrm{Sinh}(p_a\alpha_a\Delta x_a)}\right] - 2\frac{C_b}{\alpha_b^2}\left[1 - \frac{p_b\alpha_b\Delta x_b}{\mathrm{Sinh}(p_b\alpha_b\Delta x_b)}\right].
\end{aligned}
\tag{6.75}
$$

This is by no means the only way to derive the horizontal and vertical type interface equations. One could equally start with two in-region invariant difference equations and the discrete forms of the interface equations, then proceed to eliminate the two unknown fluxes from the equations, in a manner akin to that employed in Chapter 5, to obtain the same results as presented here.

These results for three types of interfaces, cross, vertical and horizontal, are valid for each energy group, $1 \le g \le G$. In Section 6.5, numerical results will be presented that utilize these invariant difference equations. Two cases will be presented; Case 1 will consist of the invariant difference equations in which the constant source approximation was used. Case 2 consists of the invariant difference equations in which a two-dimensional quadratic curve fit was used to model the source distribution. Before we go onto the discussion of the solution process and the presentation of the numerical results, we will discuss the local truncation error of the invariant finite difference equations; additionally we will demonstrate that the standard cell edged finite difference equations can be recovered from the invariant finite difference equations.

6.3 The Local Truncation Error and Consistency of the Invariant Finite Difference Equations

Here we will discuss the local truncation error of the Lie group invariant finite difference equations. We will also show that the invariant finite difference approximations of the two dimensional neutron diffusion equation are consistent with the original differential equations. Along the way we will show that a standard finite difference approximation of the neutron diffusion equation, namely the cell edged finite difference equations, can be recovered from the invariant finite difference equations.

We begin by considering the in-region invariant finite difference equation as given by

$$\frac{\Sigma_{R,g}p_g^2\left[\phi_{g,i-1,j} - 2\phi_{g,i,j} + \phi_{g,i+1,j}\right]}{4\mathrm{Sinh}^2(\alpha_g p_g \Delta x/2)} + \frac{\Sigma_{R,g}(1-p_g^2)\left[\phi_{g,i,j-1} - 2\phi_{g,i,j} + \phi_{g,i,j+1}\right]}{4\mathrm{Sinh}^2(\alpha_g\sqrt{1-p_g^2}\Delta y/2)} - \Sigma_{R,g}\phi_{g,i,j} + S_{g,i,j} = 0 . \tag{6.76}$$

We will first demonstrate that the standard finite difference approximation of the neutron diffusion equation can be recovered from the invariant finite difference equations. Expanding the hyperbolic-sines in a series expansion as

$$4\mathrm{Sinh}^2(\delta/2) = \delta^2 + \frac{\delta^4}{12} + \frac{\delta^6}{360} + \cdots , \tag{6.77}$$

and truncating the series in terms δ^4 and greater, equation (6.76) becomes

$$\frac{\Sigma_{R,g}p_g^2\left[\phi_{g,i-1,j} - 2\phi_{g,i,j} + \phi_{g,i+1,j}\right]}{4(\alpha_g p_g \Delta x/2)^2} + \frac{\Sigma_{R,g}(1-p_g^2)\left[\phi_{g,i,j-1} - 2\phi_{g,i,j} + \phi_{g,i,j+1}\right]}{4(\alpha_g\sqrt{1-p_g^2}\Delta y/2)^2} - \Sigma_{R,g}\phi_{g,i,j} + S_{g,i,j} = 0 . \tag{6.78}$$

Upon canceling like terms and using $\alpha_g^2 = \Sigma_{R,g}/D_g$, we obtain

$$\frac{D_g\left[\phi_{g,i-1,j} - 2\phi_{g,i,j} + \phi_{g,i+1,j}\right]}{\Delta x^2} + \frac{D_g\left[\phi_{g,i,j-1} - 2\phi_{g,i,j} + \phi_{g,i,j+1}\right]}{\Delta y^2}$$

$$- \Sigma_{R,g}\phi_{g,i,j} + S_{g,i,j} = 0\,, \tag{6.79}$$

which is the standard finite difference approximation of the neutron diffusion equation. The local truncation error for equation (6.76) is determined by expanding terms in (6.76) about the point x_i,y_j as both Δx and Δy become small. This yields upon the elimination of the original differential equation (6.1)

$$\tau_\varepsilon = \frac{\Delta x^2}{12}\left[D_g\frac{\partial^4\phi_g(x,y)}{\partial x^4} - p_g^2\Sigma_{R,g}\frac{\partial^2\phi(x,y)}{\partial x^2}\right]_{\substack{x = x_i\\ y = y_j}}$$

$$+ \frac{\Delta y^2}{12}\left[D_g\frac{\partial^4\phi_g(x,y)}{\partial y^4} - \sqrt{1 - p_g^2}\Sigma_{R,g}\frac{\partial^2\phi(x,y)}{\partial y^2}\right]_{\substack{x = x_i\\ y = y_j}} + O(\Delta x^3,\Delta y^3)\,. \tag{6.80}$$

As can be seen from equation (6.80), the local truncation error is second order in both Δx and Δy. One can also see that as both Δx and Δy go to zero, the local truncation error goes to zero; hence the invariant finite difference equation is consistent with the original differential equation.

We now turn our attention to the interface equations. We consider the cross type of interface first as given by equation (6.52). The invariant source term for the constant source distribution approximation is

$$Q = S_{a,i,j}\frac{\mathrm{Tanh}(p_a\alpha_a\Delta x_d/2)}{\alpha_a p_a} + S_{b,i,j}\frac{\mathrm{Tanh}(p_b\alpha_b\Delta x_c/2)}{\alpha_b p_b}$$

$$+ S_{c,i,j}\frac{\mathrm{Tanh}(p_c\alpha_c\Delta x_c/2)}{\alpha_c p_c} + S_{d,i,j}\frac{\mathrm{Tanh}(p_d\alpha_d\Delta x_d/2)}{\alpha_d p_d}\,, \tag{6.81}$$

which may be rewritten as

$$
\begin{aligned}
Q = {} & S_{a,i,j}\left(\frac{\mathrm{Tanh}(p_a\alpha_a\Delta x_d/2)}{2\alpha_a p_a} + \frac{\mathrm{Tanh}(q_a\alpha_a\Delta y_b/2)}{2\alpha_a q_a}\right) \\
& + S_{b,i,j}\left(\frac{\mathrm{Tanh}(p_b\alpha_b\Delta x_c/2)}{2\alpha_b p_b} + \frac{\mathrm{Tanh}(q_b\alpha_b\Delta y_b/2)}{2\alpha_b q_b}\right) \\
& + S_{c,i,j}\left(\frac{\mathrm{Tanh}(p_c\alpha_c\Delta x_c/2)}{2\alpha_c p_c} + \frac{\mathrm{Tanh}(q_c\alpha_c\Delta y_c/2)}{2\alpha_c q_c}\right) \\
& + S_{d,i,j}\left(\frac{\mathrm{Tanh}(p_d\alpha_d\Delta x_d/2)}{2\alpha_d p_d} + \frac{\mathrm{Tanh}(q_d\alpha_d\Delta y_c/2)}{2\alpha_d q_d}\right).
\end{aligned}
\tag{6.81}
$$

Expanding the hyperbolic-sines and tangents in a series and keeping only the first terms in the series, we obtain the standard difference formulation as

$$
\begin{aligned}
& -\left(\frac{D_{g,a}}{\Delta x_d} + \frac{D_{g,d}}{\Delta x_d}\right)\phi_{g,i+1,j} - \left(\frac{D_{g,b}}{\Delta x_c} + \frac{D_{g,c}}{\Delta x_c}\right)\phi_{g,i-1,j} \\
& + \left[\frac{D_{g,a}}{\Delta x_d} + \frac{\Sigma_{R,g,a}\Delta x_d}{4} + \frac{D_{g,b}}{\Delta x_c} + \frac{\Sigma_{R,g,b}\Delta x_c}{4} + \frac{D_{g,c}}{\Delta x_c} + \frac{\Sigma_{R,g,c}\Delta x_c}{4} + \frac{D_{g,c}}{\Delta x_d} + \frac{\Sigma_{R,g,c}\Delta x_d}{4}\right]\phi_{g,i,j} \\
& + \left[\frac{D_{g,a}}{\Delta y_b} + \frac{\Sigma_{R,g,a}\Delta y_b}{4} + \frac{D_{g,b}}{\Delta y_b} + \frac{\Sigma_{R,g,b}\Delta y_b}{4} + \frac{D_{g,c}}{\Delta y_c} + \frac{\Sigma_{R,g,c}\Delta y_c}{4} + \frac{D_{g,d}}{\Delta y_c} + \frac{\Sigma_{R,g,d}\Delta y_c}{4}\right]\phi_{g,i,j} \\
& -\left(\frac{D_{g,c}}{\Delta y_c} + \frac{D_{g,d}}{\Delta y_c}\right)\phi_{g,i,j-1} - \left(\frac{D_{g,a}}{\Delta y_b} + \frac{D_{g,b}}{\Delta y_b}\right)\phi_{g,i,j+1} \\
& = \frac{S_{g,a,i,j}}{4}(\Delta x_d + \Delta y_b) + \frac{S_{g,b,i,j}}{4}(\Delta x_c + \Delta y_b) \\
& + \frac{S_{g,c,i,j}}{4}(\Delta x_c + \Delta y_c) + \frac{S_{g,d,i,j}}{4}(\Delta x_d + \Delta y_c).
\end{aligned}
\tag{6.82}
$$

The local truncation error for the cross type interface was determined by expanding the invariant difference equation in a series about the point x_i, y_j as Δx and Δy become small to yield

$$\tau_\varepsilon = \left(2D_{g,a}\frac{\partial^2\phi_g(x,y)}{\partial y^2} + 2D_{g,b}\frac{\partial^2\phi_g(x,y)}{\partial y^2} - (\Sigma_{R,g,a}+\Sigma_{R,g,b})\phi_g(x,y) + S_a + S_b\right)_{\substack{x=x_i\\y=y_j}}\Delta y_b$$

$$+\left(2D_{g,c}\frac{\partial^2\phi_g(x,y)}{\partial y^2} + 2D_{g,d}\frac{\partial^2\phi_g(x,y)}{\partial y^2} - (\Sigma_{R,g,c}+\Sigma_{R,g,d})\phi_g(x,y) + S_c + S_d\right)_{\substack{x=x_i\\y=y_j}}\Delta y_c$$

$$+\left(2D_{g,a}\frac{\partial^2\phi_g(x,y)}{\partial x^2} + 2D_{g,d}\frac{\partial^2\phi_g(x,y)}{\partial x^2} - (\Sigma_{R,g,a}+\Sigma_{R,g,d})\phi_g(x,y) + S_a + S_d\right)_{\substack{x=x_i\\y=y_j}}\Delta x_d \quad (6.83)$$

$$+\left(2D_{g,b}\frac{\partial^2\phi_g(x,y)}{\partial x^2} + 2D_{g,c}\frac{\partial^2\phi_g(x,y)}{\partial x^2} - (\Sigma_{R,g,b}+\Sigma_{R,g,c})\phi_g(x,y) + S_c + S_b\right)_{\substack{x=x_i\\y=y_j}}\Delta x_c$$

$$+ O(\Delta x^2,\Delta y^2)\,.$$

From equation (6.83), we see that as the mesh spacing goes to zero, the local truncation error also goes to zero. Therefore, the invariant finite difference equation for the cross-type of interface is consistent with the original differential equations.

In a similar manner, the local truncation error for the invariant finite difference equation and the standard finite difference approximation for the horizontal type of interface were respectively determined as

$$\tau_\varepsilon = \frac{1}{2}\left(2D_{g,a}\frac{\partial^2\phi_g(x,y)}{\partial y^2} - \Sigma_{R,g,a}\phi_g(x,y) + S_a\right)_{\substack{x=x_i\\y=y_j}}\Delta y_a$$

$$+\frac{1}{2}\left(2D_{g,c}\frac{\partial^2\phi_g(x,y)}{\partial y^2} - \Sigma_{R,g,c}\phi_g(x,y) + S_c\right)_{\substack{x=x_i\\y=y_j}}\Delta y_c \quad (6.84)$$

$$+\frac{1}{2}\left(2D_{g,a}\frac{\partial^2\phi_g(x,y)}{\partial x^2} + 2D_{g,c}\frac{\partial^2\phi_g(x,y)}{\partial x^2} - (\Sigma_{R,g,a}+\Sigma_{R,g,c})\phi_g(x,y) + S_a + S_c\right)_{\substack{x=x_i\\y=y_j}}\Delta x$$

$$+ O(\Delta x^2,\Delta y^2)$$

and

$$-\left(\frac{D_{g,a}}{\Delta x}+\frac{D_{g,c}}{\Delta x}\right)(\phi_{g,i-1,j}+\phi_{g,i+1})+\left(\frac{2D_{g,a}}{\Delta x}+\frac{\Sigma_{R,g,a}\Delta x}{2}+\frac{2D_{g,c}}{\Delta x}+\frac{\Sigma_{R,g,c}\Delta x}{2}\right)\phi_{g,i,j}$$

$$+\left(\frac{2D_{g,a}}{\Delta y_a}+\frac{\Sigma_{R,g,a}\Delta y_a}{2}+\frac{2D_{g,c}}{\Delta y_c}+\frac{\Sigma_{R,g,c}\Delta y_c}{2}\right)\phi_{g,i,j}-\frac{2D_{g,c}}{\Delta y_c}\phi_{g,i,j-1} \quad (6.85)$$

$$-\frac{2D_{g,a}}{\Delta y_a}\phi_{g,i,j+1}=\Delta y_a S_{a,g,i,j}+\Delta y_c S_{c,g,i,j}\ .$$

The local truncation error for the invariant finite difference equation and the cell edged standard finite difference equation for the vertical interface were determined to be, respectively,

$$\tau_\varepsilon=\frac{-1}{2}\left(2D_{g,a}\frac{\partial^2\phi_g(x,y)}{\partial y^2}+2D_{g,b}\frac{\partial^2\phi_g(x,y)}{\partial y^2}-(\Sigma_{R,g,a}+\Sigma_{R,g,b})\phi_g(x,y)+S_a+S_b\right)\Bigg|_{\substack{x=x_i\\y=y_j}}\Delta y$$

$$+\frac{-1}{2}\left(2D_{g,a}\frac{\partial^2\phi_g(x,y)}{\partial x^2}-\Sigma_{R,g,a}\phi_g(x,y)+S_a\right)\Bigg|_{\substack{x=x_i\\y=y_j}}\Delta x_a \quad (6.86)$$

$$+\frac{-1}{2}\left(2D_{g,b}\frac{\partial^2\phi_g(x,y)}{\partial x^2}-\Sigma_{R,g,b}\phi_g(x,y)+S_b\right)\Bigg|_{\substack{x=x_i\\y=y_j}}\Delta x_b+O(\Delta x^2,\Delta y^2)$$

and

$$-\frac{2D_{g,b}}{\Delta x_b}\phi_{g,i-1,j}-\frac{2D_{g,a}}{\Delta x_a}\phi_{g,i+1,j}+\left(\frac{2D_{g,a}}{\Delta x_a}+\frac{\Sigma_{R,g,a}\Delta x_a}{2}+\frac{2D_{g,b}}{\Delta x_b}+\frac{\Sigma_{R,g,b}\Delta x_b}{2}\right)\phi_{g,i,j}$$

$$\left(\frac{2D_{g,a}}{\Delta y}+\frac{\Sigma_{R,g,a}\Delta y}{2}+\frac{2D_{g,b}}{\Delta y}+\frac{\Sigma_{R,g,b}\Delta y}{2}\right)\phi_{g,i,j} \quad (6.87)$$

$$-\left(\frac{D_{g,a}}{\Delta y}+\frac{D_{g,b}}{\Delta y}\right)(\phi_{g,i,j-1}+\phi_{g,i,j+1})=\Delta x_a S_{g,a,i,j}+\Delta x_b S_{g,b,i,j}\ .$$

From equations (6.84) and (6.85), we see that both the horizontal and vertical interface invariant difference equations are consistent with the original differential equations since as Δx and Δy go to zero, the local truncation error goes to zero. Now that the invariant finite difference equations have been shown to be consistent with the original differential equation, we are ready to discuss the solution of these difference equations.

6.4 The Source Iteration Solution Method

The method used to solve the multigroup Lie group invariant finite difference equations is the power method as outlined in Section 5.5.2. The solution method employed is identical to that used in the one-dimensional problems with the exception that the Alternating Direction Implicit (ADI), see references 5, 10, and 18, method was used in the inner iterations to solve for the neutron flux.

Since the direct inversion of the leakage plus removal matrix is impractical, an iterative method is utilized to determine the neutron flux. The ADI method was chosen for this purpose. As a specific example to show how the ADI method is used, we consider the in-region invariant finite difference equation (6.29). Equation (6.29) can be rewritten as

$$A_g\left[\phi_{g,i-1,j} - 2\phi_{g,i,j} + \phi_{g,i+1,j}\right] + B_g\left[\phi_{g,i,j-1} - 2\phi_{g,i,j} + \phi_{g,i,j+1}\right] - \Sigma_{R,g}\phi_{g,i,j} + Q_{g,i,j} = 0\,, \tag{6.88}$$

where

$$A_g = \frac{\Sigma_{R,g}p_g^2}{4\mathrm{Sinh}^2(\alpha_g p_g \Delta x/2)} \text{ and } B_g = \frac{\Sigma_{R,g}(1-p_g^2)}{4\mathrm{Sinh}^2(\alpha_g\sqrt{1-p_g^2}\,\Delta y/2)}\,. \tag{6.89}$$

We begin the solution of the neutron flux, by carrying out a sweep in the x-direction using equation (6.86), rewritten as

$$- A_g\phi_{g,i-1,j}^{n+1/2} + \left(2A_g + \tfrac{1}{2}\Sigma_{R,g} + R\right)\phi_{g,i,j}^{n+1/2} - A_g\phi_{g,i+1,j}^{n+1/2} = Q_{g,i,j} + \left[- B_g\phi_{g,i,j-1}^{n} + \left(2B_g + \tfrac{1}{2}\Sigma_{R,g} - R\right)\phi_{g,i,j}^{n} - B_g\phi_{g,i,j+1}^{n}\right], \tag{6.90}$$

where the superscript n refers to the inner iteration number and R is a real number. We then carry out a sweep in the y-direction using

$$\begin{aligned} - B_g\phi^{n+1}_{g,i,j-1} + \left(2B_g + \frac{1}{2}\Sigma_{R,g} + R\right)\phi^{n+1}_{g,i,j} - B_g\phi^{n+1}_{g,i,j+1} = Q_{g,i,j} \\ + \left[- A_g\phi^{n+1/2}_{g,i-1,j} + \left(2A_g + \frac{1}{2}\Sigma_{R,g} - R\right)\phi^{n+1/2}_{g,i,j} - A_g\phi^{n+1/2}_{g,i+1,j}\right] . \end{aligned} \tag{6.91}$$

This iterative process is carried out until some convergence criterion on the neutron flux is met. The parameter R is chosen, such that this iterative process converges after N iterations. For further information on the use of ADI, the interested reader is referred to references 5, 10, and 18.

6.5 Numerical Results for the Two-Dimensional Neutron Diffusion Equation

We will now present numerical results for the invariant finite difference schemes as outlined above. Additionally, we will present results for the standard cell edged finite difference equations as given by equations (6.79), (6.82), (6.85), and (6.87). We will also present numerical results as obtained for the sample problem by the computer code DIF3D, reference 16, which employs a cell centered finite difference approximation of the multigroup neutron diffusion equation.

There are two invariant finite difference schemes for which results will be presented. Case 1 consists of the invariant finite difference equations, as given by equations (6.33), (6.52), (6.60), (6.65), (6.68), (6.71), and (6.73), in which the source distribution was approximated by a constant source. Case 2 consists of the invariant finite difference scheme, as given by equations (6.37), (6.52), (6.62), (6.63), (6.64), (6.65), (6.70), (6.71), and (6.75), where quadratic curve fits were used to approximate the source distribution.

The two-dimensional sample problem consisted of a two-region reactor that was symmetric about the x and y axis as shown in Figure 6.8. The core region was 50 cm by 50 cm and the reflector region was 100 cm by 100 cm Two energy groups were used in modeling the sample problem; the material properties were those used in the one-dimensional sample problem and are given in Table 5.2.

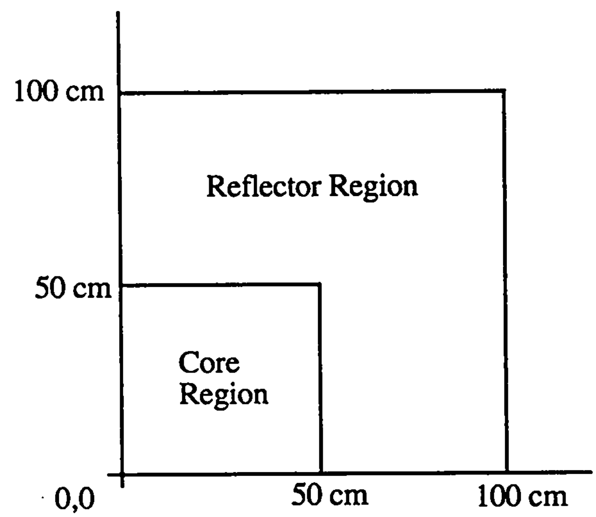

Figure 6.8 Schematic of the Symmetric, Two-Region, Two-Dimensional Sample Problem

Figures 6.9 and 6.10 respectively show the group one and two neutron fluxes that were calculated on a 1.0 cm by 1.0 cm mesh.

To compare the four methods used to calculate the sample problem, we will examine the accuracy of the eigenvalue as a function of mesh spacing. In these calculations, uniform mesh spacing, $\Delta x = \Delta y$, was used. Figure 6.11 shows the eigenvalues as a function of the mesh spacing. Since the eigenvalue, as calculated by the computer code DIF3D, approaches the converged eigenvalue from below it will be more useful to compare the error in the eigenvalue. We again define the error in the eigenvalue as

$$e = \left| \frac{\lambda - \lambda_{convergerd}}{\lambda_{converged}} \right| , \qquad (6.92)$$

where $\lambda_{convergerd}$ is the eigenvalue to which all four computational methods converged, as the mesh spacing went to zero.

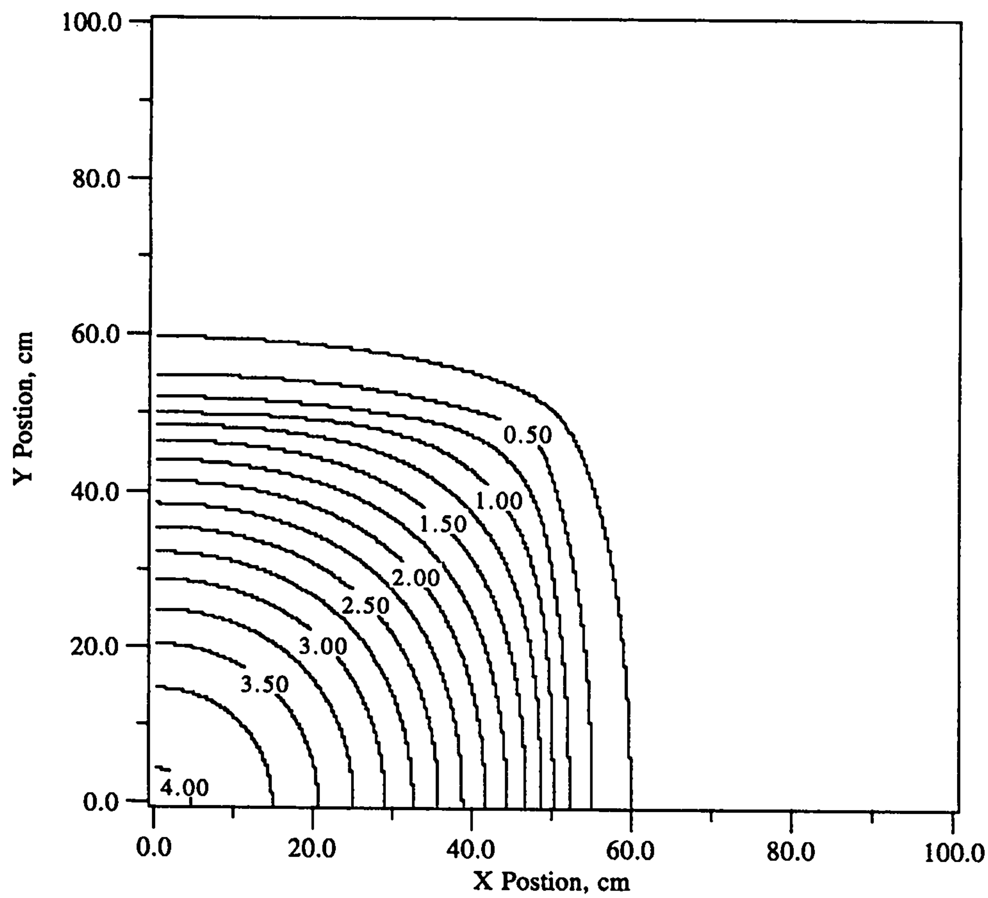

Figure 6.9 Contour Plot of the Group One Neutron Flux for the Two-Dimensional Sample Problem

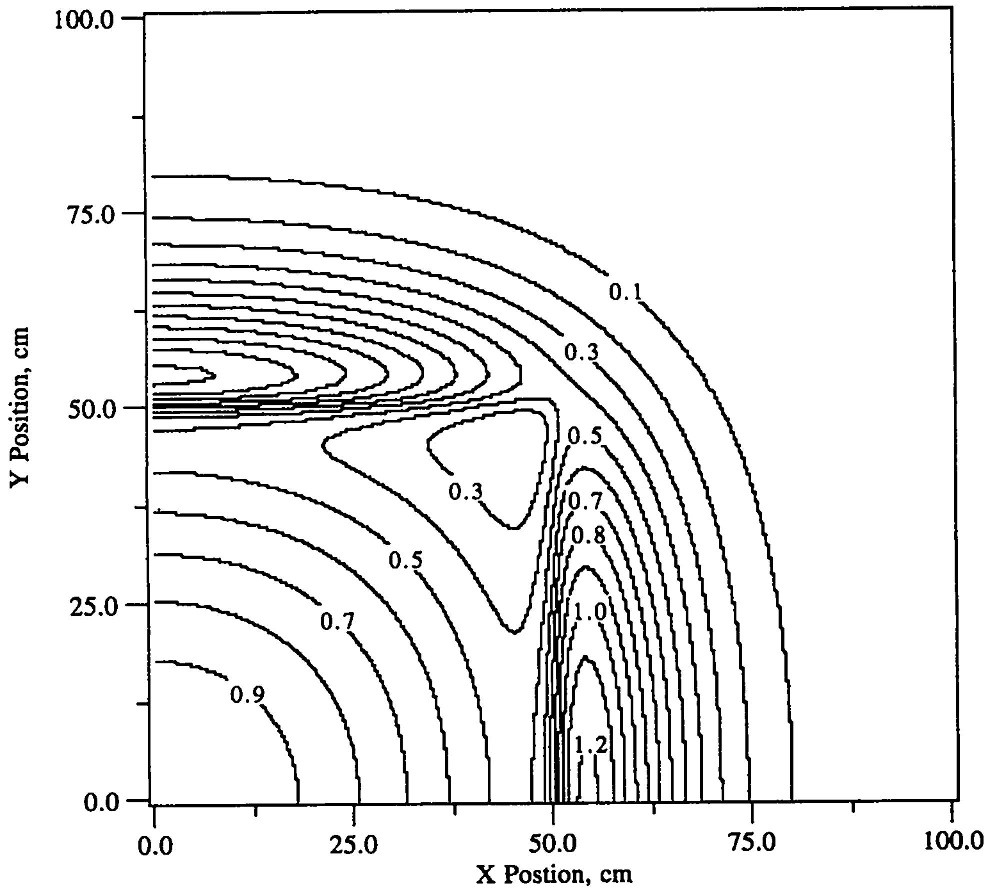

Figure 6.10 Contour Plot of the Group Two Neutron Flux for the Two-Dimensional Sample Problem

Figure 6.12 shows the error in the eigenvalue as a function of the mesh spacing. As is somewhat expected, the Case 1 invariant difference scheme is not as accurate as the three other difference schemes. This is due to the fact that the source distribution was modeled by assuming that sources at points adjacent to the point x_i,y_i were equal to the source at x_i,y_i. As with the one-dimensional problem, this assumption is not very accurate, particularly at interfaces.

We now turn our attention to Figure 6.13, which shows the error in the eigenvalue as a function of the mesh spacing for the three remaining finite difference schemes. As is expected, the cell edged finite difference scheme is not as accurate as the cell centered finite difference scheme. The cell edged finite difference scheme was included merely for interest, since this scheme can be recovered from the invariant finite difference equations. As we can see from Figure 6.13, the computer code DIF3D calculates the eigenvalue better at larger mesh spacings, greater that 2.5 cm, than does the Case 2 invariant difference scheme. However, neither DIF3D or the Case 2 invariant difference scheme could accurately calculate the flux for these large mesh spacings, so the calculations are somewhat suspect. The failure of both DIF3D and the Case 2 invariant difference scheme to calculate accurately the neutron flux can be traced to the fact that the largest diffusion length for the sample problem is 2.236 cm, which is smaller than the mesh spacing of 2.5 cm. Once the mesh spacing is on the order of, or smaller than, the diffusion length, the Case 2 invariant difference scheme calculates the eigenvalue with greater accuracy than does the computer code DIF3D.

Thus, for a desired level in accuracy in the eigenvalue, one can use fewer mesh points when calculating with the Case 2 invariant difference scheme, than with the cell centered standard finite difference scheme.

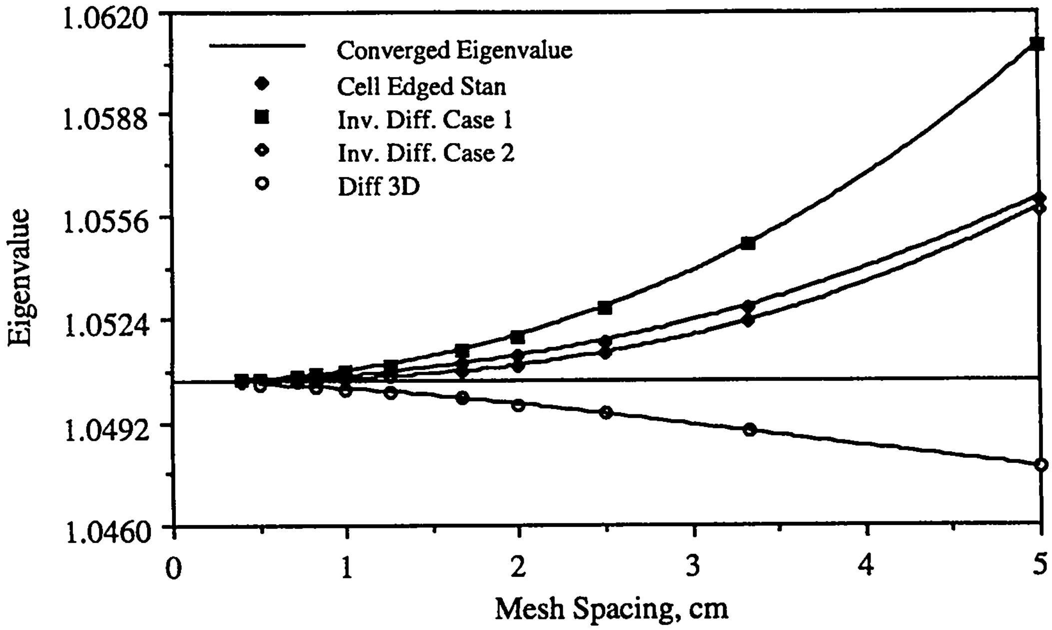

Figure 6.11 The Eigenvalue as a Function of the Mesh Spacing as Calculated by DIF3D, the Standard Cell Edged Scheme, and the Invariant Finite Difference Cases 1 and 2

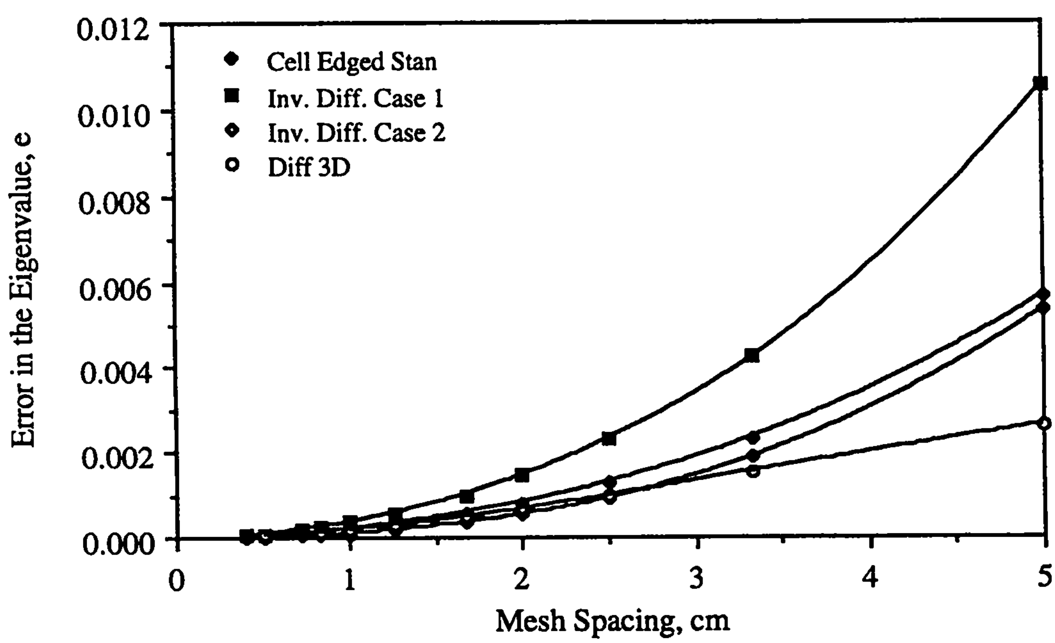

Figure 6.12 The Error in the Eigenvalue as a Function of the Mesh Spacing as Calculated by DIF3D, the Standard Cell Edged Scheme, and the Invariant Finite Difference Cases 1 and 2

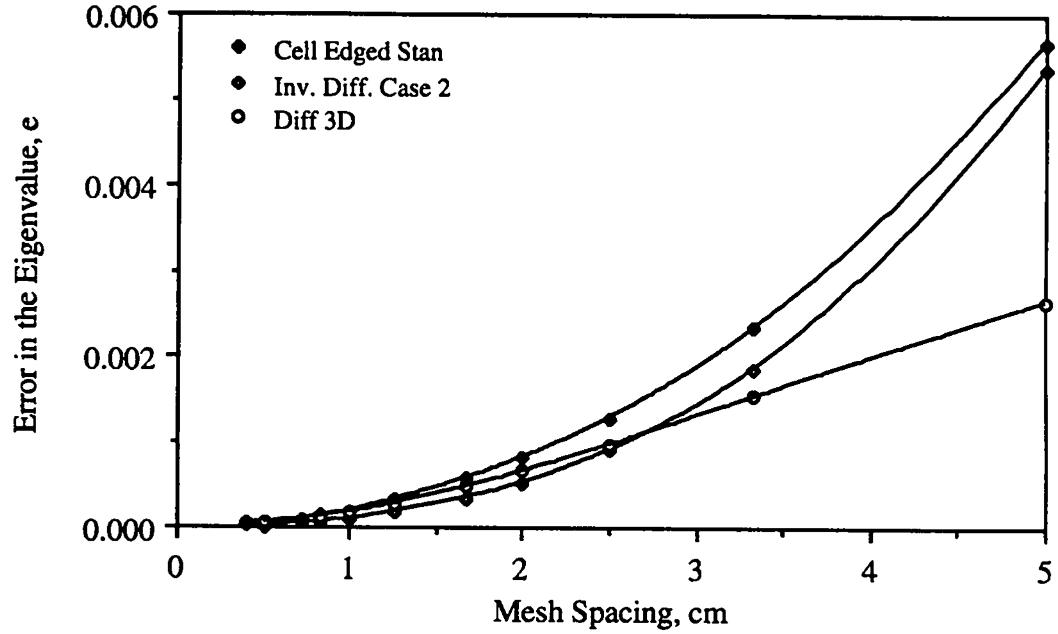

Figure 6.13 The Error in the Eigenvalue as a Function of the Mesh Spacing for the Case 2 Invariant Difference Scheme, the Cell Edged and Cell Centered Standard Difference Schemes

7 CONCLUSIONS AND RECOMMENDATIONS FOR FUTURE RESEARCH

In the course of this research, we have explored the construction of Lie group invariant finite difference equations for the multigroup neutron diffusion equation. Additionally, numerical results were presented which demonstrated that the invariant finite difference equations could determine the eigenvalue with greater accuracy than standard finite difference equations for a given mesh spacing.

We began this study by examining the invariance properties of the one- and two-dimensional diffusion equation in Cartesian coordinates. Here, we found that for a general source distribution both the one and two-dimensional diffusion equations admitted evolutionary vector fields, whose coordinate functions satisfied the homogeneous diffusion equation. Next, we proceeded to use Axford's definition of an invariant finite difference scheme to develop the extensions of the group generators to grid point values. Using the extensions of the group generators extended to grid point values, the invariant difference operators were constructed. The construction process involved operating with the candidate difference operator upon the homogeneous solution, evaluated at a grid point; this result was then made invariant with respect to the action of the group extended to grid points. The invariant source term was determined by operating upon a particular solution of the neutron diffusion equation evaluated at a grid point. The particular solution was obtained by assuming some source distribution, and solving the neutron diffusion equation for the particular solution based upon the assumed source distribution.

In Chapters 5 and 6 respectively, numerical results were presented for the one- and two-dimensional problems. Consider the one-dimensional problems that could be broken down into two classes. The first class of problems consisted of multiple regions in which the source in each region was a constant. It was found for this particular situation that the invariant finite difference equations produced the exact solution of the original differential equations. This fact could be verified by either direct numerical solution of the difference equations or by substituting the analytic solution into the invariant difference equations. It is also of interest to note that the local truncation error for the constant source problem was determined to be zero; this result is not surprising, since the invariant finite difference equations produced the exact result for the solution of the differential equation.

Next we considered the one-dimensional class of problems in which the source was dependent upon the neutron flux. For this class, it was found that the higher the order of the curve fit used to approximate the source distribution, the better the invariant finite difference approximation performed; however, it should be noted that in general this was not the case. An example of where the higher order curve fits of the source distribution did not perform better can be found in the invariant different schemes with a sixth order local truncation error. Two of the sixth order invariant finite difference schemes did not perform as well as the invariant difference scheme with a fourth order local truncation error; thus, we can conclude that the local truncation error does not play as large a role in determining the accuracy of an invariant difference scheme as does the type of curve fit used to approximate the source distribution. The importance of the way in which the source distribution modeling determines the accuracy of the invariant finite difference scheme was demonstrated in particular for the invariant finite difference scheme where the source distribution was assumed to be a constant in the neighborhood of given point; for this difference scheme, the local truncation error was determined to be second order. However, this difference scheme could not calculate the eigenvalue as well as the standard cell centered finite difference scheme, which also has a second order local truncation error.

In Chapter 6, results were presented for a two-dimensional sample problem. These results were similar in nature to those of the one-dimensional problem presented in Chapter 5. As with the one-dimensional problems, we found that the higher the order of the curve fit of the source distribution, the better the invariant finite difference scheme was able to determine the eigenvalue. The invariant finite difference scheme, in which the source distribution was approximated as a constant in the neighborhood of a given point, could not calculate the eigenvalue as well as the cell centered standard difference scheme, even though both schemes had a local truncation error that was second order in Δx and Δy. However, when a second order curve fit of the source distribution was used to approximate the source, the invariant finite difference scheme more accurately calculated the eigenvalue than the cell centered standard difference scheme for a given mesh spacing. Therefore, by building the invariance properties of the original differential equation into the finite difference scheme and using an appropriate approximation of the source distribution, the invariant finite difference schemes calculated the eigenvalue with greater accuracy than the cell centered standard difference scheme.

During this research, we have demonstrated that the accuracy of a difference scheme can be improved by incorporating the invariance properties of the original differential equation into the finite difference equations. Since the purpose of this research was to demonstrate an improvement in accuracy, the scope of our investigation was somewhat limited; thus leaving many areas unexplored.

One particular area which needs exploration is that of problem geometry. In this study, we limited ourselves to one- and two-dimensional Cartesian geometry; this leaves cylindrical, spherical and three-dimensional geometries to be explored. The one-dimensional spherical geometry should be a fairly straight forward problem, since there is a well known transformation, $\phi(r) = r\Psi(r)$, which converts the spherical problem into a slab type problem. Therefore, many of the one-dimensional results that have been presented should apply to the spherical problem, though the effects of this transformation upon the choice of curve fits should be explored. For the one-dimensional cylindrical problem, the solution of the homogeneous diffusion equation will be expressed in terms of Bessel's functions; therefore; the form taken by the invariant difference equations is complicated.

For the two-dimensional problems, the question as to what form the invariant difference equations will take is again of concern, since the solutions of the homogeneous diffusion equations would involve complicated expressions involving Bessel's and trigonometric functions as well as Legendre polynomials. Another question that needs to be explored is what are the conditions which need to be satisfied for the interface equations to be derived. We recall that, in the two-dimensional Cartesian problem, the eigenvalue for the solution of the homogeneous diffusion equation was found to have a range of acceptable values.

Another area which requires further investigation is that of the curve fits used to model the source distribution. For the one-dimensional problems, we found, for a given mesh spacing, that as the order of the curve fit increased the eigenvalue could be determined with greater accuracy; it would therefore be of interest to determine if this trend were to continue for the two-dimensional problems. In this study, we limited ourselves to some rather simple polynomial curve fits of the source distribution. However, other types of curve fits are certainly possible; in fact, there may be an optimal type of curve fit of the source distribution. One can imagine several types of curve fits which could utilize hyperbolic, trigonometric or some other type of function as their bases.

Finally, there is one other area for further research. This study dealt mainly with showing that the accuracy of the finite difference equations could be improved by incorporating the invariance properties of the original differential equations into the difference equations; hence, no attempt was made at either optimizing or accelerating the numerical solution process. As a result, there were no performance measurements, such as the amount of computer time required to run a problem. Acceleration techniques such as source extrapolation or coarse mesh rebalancing could be explored. In addition, since all of the coefficients in the invariant difference equations can be calculated before the source iteration calculation begins, one could also examine the effects of vectorization upon the time required to calculate the problem.

In conclusion, we have demonstrated for the neutron diffusion equation that the accuracy of the finite difference approximation can be improved by incorporating the invariance properties into the finite difference equations. Though there is much work remaining to be done on this subject, many of the results presented have direct application to the nuclear power industry, since current nuclear power reactors can be modeled using a two-dimensional Cartesian coordinate system. While the neutron diffusion equation is a specific example of an elliptic differential equation, many of these results should carry over to other elliptic differential equations.

REFERENCES

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

2. R. A. Axford, "Neutronics Computational Applications of Symmetry Algebras", *Proceedings of the ANS Meeting, Advances in Nuclear Engineering Computation and Radiation Shielding, Santa Fe, New Mexico, April 9-13, 1989*

3. R. A. Axford, "Lectures on Lie Groups and Systems of Ordinary and Partial Differential Equations", *Unpublished Lecture Notes for Nuc. E. 490, 490 N, 490 NN and 495, Department of Nuclear Engineering, University of Illinois at Urbana-Champaign*,(1989, 1990, 1991)

4. G. D. Smith, *Numerical Solutions of Partial Differential Equations: Finite Difference Methods*, (Oxford University Press, New York, 1987)

5. C. A. J. Fletcher, *Computational Techniques for Fluid Dynamics, Vol. I*, (Springer-Verlag, New York, New York, 1991)

6. H. Greenspan, C. N. Kelber, and D. Okrent, (Eds.), *Computing Methods in Reactor Physics*, (Gordon and Breach Science Publishers, New York, New York, 1963)

7. S. Nakamura, *Computational Methods in Engineering and Science*, (Robert E. Krieger Publishing Co., Malabar, Florida, 1986)

8. D. Greenspan, V. Casulli, *Numerical Analysis for Applied Mathematics, Science, and Engineering*, (Addison-Wesley Publishing Co., Redwood City, California, 1988)

9. J. J. Duderstadt, L. J. Hamilton, *Nuclear Reactor Analysis*, (John Wiley & Sons, New York, New York, 1976)

10. J. Stoer and R. Bulirsch, *Introduction to Numerical Analysis*, Translated by R. Bartels, W. Gautschi, and C. Witzgall, (Springer-Verlag, New York, New York, 1980)

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

12. G. W. Bluman, and S. Kumei, *Symmetries and Differential Equations*, (Springer-Verlag, New York, New York, 1989)

13. H. Stephani, *Differential Equations Their Solution Using Symmetries*, Edited by Malcolm MacCallum, (Cambridge University Press, New York, New York, 1989)

14. R. S. Varga, *Matrix Iterative Analysis*, (Prentice-Hall, Englewood Cliffs, New Jersey, 1962)

15. E. L. Wachspress, "The Numerical Solution of Boundary Value Problems", *Mathematical Method for Digital Computers*, Edited by Anthony Ralston and Herbert S. Wilf, (J. Wiley & Sons, New York, New York, 1960)

16. K. L. Dersteine, *DIF3D: A Code to Solve One-, Two-, and Three-Dimensional Finite-Difference Diffusion Theory Problems*, (Argonne National Laboratory report ANL-82-64, 1984)

17. L. A. Hageman, *Numerical Methods and Techniques used in the Two-Dimensional Neutron-Diffusion Program PDQ-5*, (Bettis Atomic Power Laboratory report WAPD-TM-364, 1963)

18. W. H. Press, B. P. Flannery, S. A. Teukolsky, and W. T. Vetterling, *Numerical Recipes, The Art of Scientific Computing*, (Cambridge University Press, New York, New York, 1986)

19. R. A. Axford, Private communication, 1993

*U.S. GOVERNMENT PRINTING OFFICE 1994-0-573-024/7009

Los Alamos
NATIONAL LABORATORY

Los Alamos, New Mexico 87545