1-28-2015

Error Assessment in FEM Calculations of Flows with Moving Boundaries

Vahid Hatamipourdehnow

Vahid Hatamipourdehnow

Candidate

Mechanical Engineering

Department

This thesis is approved, and it is acceptable in quality and form for publication: *Approved by the Thesis Committee:*

Prof. Razani, Chair

Prof. Heinrich, Member

Dr. Poroseva, Member

Error Assessment in FEM Calculations of Flows with Moving Boundaries

by

Vahid Hatamipourdehnow

B.S., Sharif University of Technology, 2007
M.S., University of Tehran, 2010

THESIS

Submitted in Partial Fulfillment of the
Requirements for the Degree of

Master of Science
Mechanical Engineering

The University of New Mexico

Albuquerque, New Mexico

December, 2014

Dedication

This thesis is dedicated to my wife Zahra. Her love, patience, support and understanding have lightened up my spirit to finish this study.

Also this thesis is dedicated to my parents Mahin and Faramarz for their love, endless support and encouragement.

Acknowledgments

I would like to express my gratitude to my advisor Professor Heinrich, whose expertise, understanding, and patience, added considerably to my graduate experience and made this study possible.

Error Assessment in FEM Calculations of Flows with Moving Boundaries

by

Vahid Hatamipourdehnow

B.S., Sharif University of Technology, 2007

M.S., University of Tehran, 2010

M.S., Mechanical Engineering, University of New Mexico, 2014

Abstract

A Finite Element numerical method has been developed to simulate the fluid flow over two dimensional and time dependent domains with rigid moving objects or boundaries. This method falls under the general category of Arbitrary Lagrangian Eulerian methods. In this method the global mesh is fixed and adaptations are made locally in both space and time to describe interface movement. Therefore, the global mesh is independent of interface movement, and the possibility of mesh entanglement is eliminated.

During the simulations, very small elements or elements with very large aspect ratios as compared with the elements of the fixed mesh may be generated to correctly describe the position and shape of the interfaces, these elements are then combined with the adjacent mesh elements which are much larger and used together in the calculations. The question of how these large abrupt changes in the mesh affect the accuracy of the calculations is examined through local truncation error analysis and numerical experiments.

The two-dimensional flow between two plates separating at a prescribed speed, which admits an analytical solution, is used to verify and illustrate the results. It is determined that the accuracy of the calculations is not adversely affected by the large and abrupt changes in the size of the elements and that the convergence rate of the method is of second order. The behavior of the local error next to the interfaces is shown to be of the same order as in the rest of the computational domain.

Contents

List of Figures

List of Tables

Glossary

i,j	node numbers
n	total number of nodes
n	outward unit vector normal to the boundary
$N(x, y, z)$	shape function
p	pressure
q	weighting function
Re	Reynolds number; real
t	time
u	horizontal velocity (x)
v	lateral velocity (y)
w	vertical velocity (z)
$w(x, y, z)$	weighting function
x	horizontal Cartesian coordinate
y	lateral Cartesian coordinate

Glossary

z	vertical Cartesian coordinate
Γ	boundary
Δ	interval (time or space)
θ	relaxation parameter
ν	kinematic viscosity
ρ	density
Ω	domain
Σ	summation
∇	divergence operator

Chapter 1

Introduction

1.1 Motivation

The importance of Computational Fluid Dynamics (CFD) in engineering analysis and design is no longer in question these days and has become a standard tool for designers in all sorts of fields. When the models are based on finite element or finite volume formulations, calculating in domains that are time dependent becomes challenging due to the discrete nature of the methods which require a spatial discretization of a domain that changes shape with time. The practical difficulties are not easy to overcome and can render the methodologies expensive and difficult to use [1, 2]. In many areas of technological importance, models based on the finite element method (FEM) are preferred because of their flexibility and the ease with which they can be applied to domains with irregular geometry [3]. This work is motivated by the need to simulate the processes encountered in internal combustion engines when the fluid inside a cylinder interacts with the motion of a piston. The goal is to generate an accurate and robust procedure to calculate in domains with continuously changing geometry and incorporate it in the KIVA internal combustion simulator developed at Los Alamos National Laboratory [4,5]. A variety of numerical methods have been developed to address these and other similar types of simulations over the years, and the literature in the subject is quite extensive, a few representative references [1, 2, 6–9] can give a good summary of the work done. In this work only ALE formulations based on the FEM are considered, other methods will not be discussed except when necessary for comparison with the present formulation.

FEM models based on the ALE formulation have relied heavily on adaptive mesh methods to discretize the evolving spatial domain geometry. This can have practical disadvantages because the continuous mesh deformation often leads to a state where the mesh has severely degraded and it can no longer be used, which is known as mesh entanglement. At this point a new mesh must be generated and the dependent variables must be interpolated from the old mesh to the new one; this process can lead to instability and loss of accuracy [10, 11] and it extracts a significant cost to the user. A certain amount of checks and measures can be introduced together with criteria to have the code automatically make the decision to re-mesh, however these are not always effective. In this work a local ALE-FEM method is considered based on bilinear and trilinear isoparametric elements in two and three dimensions respectively [12, 13]. This method is very similar to the one introduced in [14] based on triangular elements. It uses a fixed computational grid laid down over the totality of the spatial domain considered over the entire simulation, denoted by Ω_R. The moving interfaces are defined independently using sets of marker points that define them, and are superimposed over the mesh. At each time step in the simulation, in that portion of the region containing fluid where the velocity and pressure will be calculated, the mesh is locally adapted to fit the interfaces independently of the adaptation used in the previous time step. As a result, the method requires no interpolation and the mesh can never become entangled, but as can be expected different types of difficulties arise; however, these are implementation problems that once resolved are no longer an issue and have been addressed in [12, 13].

1.2 Moving Boundaries in the Fluid Domain

In many engineering subjects, the numerical solution of moving boundary problems in fluids is an important field of study. Though many different methods to deal with their challenges have been introduced, this field of research is continually developing. New numerical developments have made the simulations not only more accurate and more applicable to a wider range of problems but also less computationally expensive in some cases. According to all of these factors, developments of ALE (Arbitrary Lagrangian Eulerian) methods used in research [15–18] have been boosted. The ALE methods as a classification of FEA (Finite Element Analysis) formulations are used to conquer the associated challenges of the analysis of the moving boundaries problems. Two steps that are taken in these formulations. At each time step, the beginning of the process is dealing with the moving boundaries motion in the Lagrangian frame work. In the second step, the equations for the fluid domain are solved in the Eulerian (stationary) framework using the geometry obtained form the first step. These methods have been applied with moving mesh schemes in prior research [19–22]. In these schemes, the mesh is attached to the moving boundary, and the whole mesh is deformed during the simulation. According to the mesh deformation, the mesh usually becomes dislocated past the point it could be used in the simulation. At these situations, the simulating program must pause and re-mesh, or by using a routine automate the process. These difficulties make moving mesh schemes troublesome from a practical point of view. The newly developed ALE method [12] eliminates these obstacles by calculating on a locally changing mesh, and leaving the global mesh outside of this undeformed area.

As a result of the complexity of existing ALE methods based on adaptive meshing, and the fact that the entire mesh changes with time, assessing their accuracy becomes very difficult. Few attempts have been made to obtain accurate error measurements and because the flow solvers are based on a projection formulation, the emphasis is placed on achieving second order time accurate convergence rates [9, 11, 23]. In [24,25] the accuracy was assessed by comparison with experimental data and previous numerical simulations. One advantage of the present method is that it can be readily applied to assess both the temporal and spatial errors and formal convergence studies can be performed using cases with known analytical solution. This work concentrates in the spatial discretization error, the time integration method is first order and the size of the time step is chosen so as to not reduce the order of the spatial convergence rate.

The discussion centers on the two and three-dimensional cases. The incompress-ible Navier-Stokes equations are solved in two dimensions using the basic pressure correction projection formulation [26] which is first order in time, and using equal order interpolation for velocity and pressure. In the next chapter, the ALE-FEM method is described; in chapter 3 the local mesh adaptation method is presented; in chapter 4 the results of the local error analysis are given; in chapter 5 the bench-mark problem of flow on a fluid layer between two parallel plates separating at a prescribed speed is introduced and in chapter 6 the numerical results are presented and discussed.

Chapter 2

Background Information

2.1 Governing Equations

Assuming that body forces are zero, the Navier-Stokes equations for viscous incompressible flow are written in non-dimensional vector form along with continuity equation as

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} = -\nabla p + \frac{1}{\mathrm{Re}} \nabla^2 \mathbf{u} \tag{2.1}$$

$$\nabla \cdot \mathbf{u} = 0 \tag{2.2}$$

Where $\mathbf{u} = (u\,\mathbf{i} + v\,\mathbf{j} + w\,\mathbf{k}) \equiv \sum_{i=1}^{3} u_i \mathbf{e}_i$ is the velocity;$\nabla = (\frac{\partial}{\partial x}\mathbf{i} + \frac{\partial}{\partial y}\mathbf{j} + \frac{\partial}{\partial z}\mathbf{k}) \equiv \sum_{i=1}^{3} \frac{\partial}{\partial x_i}\mathbf{e}_i$ is the gradient operator, t is time, p is the pressure and $\mathrm{Re} = \frac{UL}{\nu}$ is the Reynolds number. U is a characteristic velocity, L is a characteristic length, ν is the kinematic viscosity of the fluid, $\tau = \frac{L}{U}$ is reference time, and $P = \rho U^2$ is the reference pressure. Equations 2.1 and 2.2 are defined over the domain $[0, T] \times \Omega(t)$ where T is a real number, and $\Omega(t)$ is a connected time dependent domain in $\mathbb{R}^3$ with a sufficiently smooth boundary $\Gamma(t)$. At time $t_0 = 0$, $\Omega(t_0) = \Omega_0$ and the initial condition is $\mathbf{u}(\mathbf{x}, 0) = \mathbf{u_0}$.

2.2 ALE Formulation Domain

Understanding of the domain and associated conditions used to set up a problem correctly is essential to develop the ALE Finite Element Scheme.

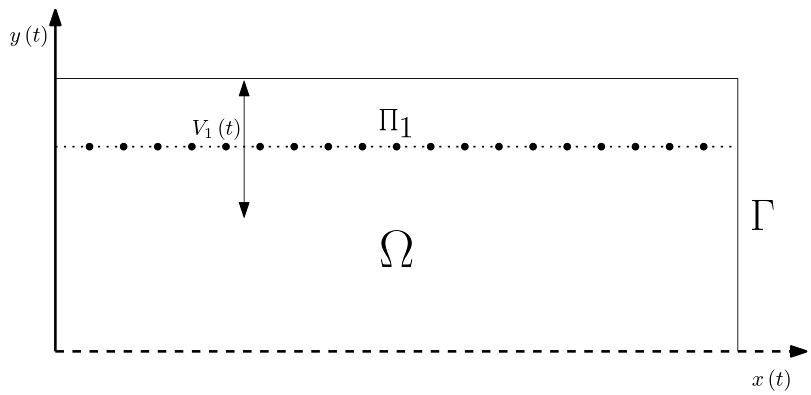

Figure 2.1: Sketch of domain Ω with boundary Γ. Marker set Π_1 defines the moving interface (piston) with a velocity equal to $V_1(t)$

The boundary Γ consists of two types of conditions, Dirichlet and Neumann. The Dirichlet boundary conditions specify a dependent variable value on that boundary, Γ_D. As an example, a Dirichlet boundary condition may specify a velocity or pressure value at the boundary ($u_d = u \; or \; p_d = p$). On the other hand, the Neumann boundary conditions specify gradients of a variable on the boundary, Γ_N. Like $\frac{\partial u}{\partial \mathbf{n}}$ where $\frac{\partial u}{\partial \mathbf{n}}$ means the normal derivative of velocity u in the unit normal direction vector to the boundary $\mathbf{n}$. In Figure 2.1 the boundary Γ is composed of the Dirichlet boundary conditions Γ_D and the Neumann boundary conditions Γ_N. The marker sets Π_1 contains the marker points that define the moving object or boundary during the calculations. The marker set has specified velocity $V_1(t)$ in Figure 2.1. Though marker sets do not necessarily have to have specified velocity such as the case of falling spheres in a fluid [24].

The figure 2.1 can also be used to illustrate the ALE process. In the problem shown by figure 2.1, the marker Π_1 is involved with the Lagrangian part of the formulation. For instance, if there were equations that describe the motion of the marker sets, these equations could be solved to find the updated velocity and location of the marker sets. In the next step, the updated properties for the marker sets could be applied as the known conditions for the Eulerian part of the calculation over the rest of the domain Ω; Therefore, the Eulerian equations could be solved by using the calculated values from the Lagrangian step and the domain boundary conditions Γ_N and Γ_D. These steps are repeated during each time step of an ALE simulation.

2.3 Discretization using the Weak Formulation

By using the domain Ω, boundaries Γ, and marker sets Π_i, the Navier-Stokes equations have to be discretized in a way to make them solvable by FEA. In order to do this, the equation sets 2.1 and 2.2 must be contained in a connected domain $\Omega(t)$ with sufficiently smooth boundaries $\Gamma(t)$, where $t \in [0, T]$. Denoting $\Omega(t) \equiv \Omega_t$ at each time t, the space $H^1(\Omega_t)$ is defined as the space of functions defined in such that the function and its first partial derivatives are square integrable in Ω_t, and the space $L^2(\Omega_t)$, which is shown as $L^2(\Omega) \equiv \left\{ f(x) \mid \int_\Omega (f(x))^2 \Omega < \infty \right\}$ [27], is defined as the space of functions defined in Ω_t that are square integrable in Ω_t. Finally, let $S_k(t) = \left\{ \mathbf{x}_i, i = 1, n_k / \mathbf{x}_i \in \bar{\Omega}(t) \right\}$ be finite sets points that define interfaces/boundaries contained in the reference domain that move within the domain with prescribed velocity $\mathbf{v}_k$.

The weighted residuals formulation of equation 2.1 is stated as follows. At a prescribed time t find a velocity field $\mathbf{u}(\mathbf{x}, t)$ in $H^1(\Omega_t)$ among those functions $\mathbf{u}$ that satisfy the Dirichlet boundary conditions, and a pressure field $p(\mathbf{x}, t)$ in $L^2(\Omega_t)$.

$$\int_\Omega \mathbf{w} \cdot \left(\nabla^2 \mathbf{u}\right) d\Omega = \int_\Gamma \mathbf{w} \cdot \frac{d\mathbf{u}}{d\mathbf{n}} d\Gamma - \int_\Omega \left(\nabla \mathbf{w} : \nabla \mathbf{u}\right) d\Omega \tag{2.3}$$

The weighted residuals formulation is stated as below by using the Gauss theorem, equation 2.3, for the viscous term

$$\int_{\Omega_t} \left\{ \mathbf{w} \cdot \left[\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla)\mathbf{u} + \nabla p \right] + \frac{1}{\mathrm{Re}} (\nabla \mathbf{w} : \nabla \mathbf{u}) \right\} d\Omega = \frac{1}{\mathrm{Re}} \int_{\Gamma_N} \mathbf{w} \cdot \frac{d\mathbf{u}}{d\mathbf{n}} d\Gamma \tag{2.4}$$

For all weighting functions, $\mathbf{w} = (w_x\mathbf{i} + w_y\mathbf{j} + w_z\mathbf{k}) \equiv \sum_{i=1}^{3} w_i \mathbf{e}_i$, in the space $H^1(\Omega_t)$ that satisfy homogeneous Dirichlet boundary conditions in Γ_D, and a pressure field, $p(\mathbf{x}, t)$, in $Q(\Omega_t)$ that satisfies

$$\int_{\Omega_t} q \nabla \cdot \mathbf{u} \, d\Omega = 0 \tag{2.5}$$

for all functions $q(\mathbf{x}, t)$ in $Q(\Omega_t)$. Where $Q(\Omega_t) = L^2(\Omega_t)/\mathbb{R}$, the space "$L^2(\Omega_t)$ modulo constants" [26].

In equation 2.4, the dyadic notation $\nabla \mathbf{w} : \nabla \mathbf{u} \equiv \sum_{i=1}^{3} \sum_{j=1}^{3} \frac{\partial u_i}{\partial x_j} \frac{\partial w_i}{\partial x_j}$ has been used, and the expression $\frac{\partial \mathbf{u}}{\partial \mathbf{n}}$ denotes the normal derivative of the components of $\mathbf{u}$ at the boundary.

The ALE formulation requires that at each time step a mapping be defined between the current domain configuration and a fixed reference domain (that can be for example the initial configuration Ω_0 or the computational reference domain Ω_R) where the problem is solved. This and other theoretical aspects of the method are very well analyzed in [11, 26, 28].

The computational algorithm is defined in two steps:

1. The Lagrangian step consists in updating the position of the interfaces $S_k(t)$ from time $t = t_n$ to time $t = t_{n+1} = t_n + \Delta t$ according to the prescribed velocity $\mathbf{v}_k(t)$ of each interface. How this is done in this finite element algorithm is explained in [12, 13].

2. Solve the Navier-Stokes equations to find $\mathbf{u}(\mathbf{x}, t_{n+1})$ and $p(\mathbf{x}, t_{n+1})$. This is done using a first order in time projection method [29]. Let $\mathbf{u}^n(\mathbf{x}) \equiv \mathbf{u}(\mathbf{x}, t_n)$

be known. At time $t = t_{n+1}$ the velocity is decomposed as $\mathbf{u}^{n+1} = \mathbf{u}^* + \mathbf{u}'$ where $\mathbf{u}^*$ is an intermediate (viscous) velocity that does not satisfy continuity and $\mathbf{u}'$ is a correction (inviscid) that enforces continuity.

By using a forward difference to approximate the time derivative of the Navier-Stokes equations, and treating convective terms explicitly, the discrete Navier-Stokes equations 2.1 become

$$\frac{\mathbf{u}^{n+1} - \mathbf{u}^n}{\Delta t} + \mathbf{u} \cdot \nabla \mathbf{u}^n = -\nabla p^{n+1} + \frac{1}{\mathrm{Re}} \nabla^2 \mathbf{u}^{n+1} \tag{2.6}$$

Intermediate velocity $\mathbf{u}^*$ is used to define the velocity at t^{n+1}, $\mathbf{u}^{n+1}$, as

$$\mathbf{u}^{n+1} = \mathbf{u}^* + \left(\mathbf{u}^{n+1} - \mathbf{u}^*\right) \tag{2.7}$$

With equation 2.7, the forward difference equation 2.6 can now be written as

$$\frac{\mathbf{u}^* - \mathbf{u}^n}{\Delta t} + \frac{\mathbf{u}^{n+1} - \mathbf{u}^*}{\Delta t} + \mathbf{u}^n \cdot \nabla \mathbf{u}^n = -\nabla p^{n+1} + \frac{1}{\mathrm{Re}} \nabla^2 \mathbf{u}^{n+1} \tag{2.8}$$

Equation 2.8 represents a momentum equation with two distinct parts, viscous and inviscid. The viscous part of the momentum equation is shown as

$$\frac{\mathbf{u}^* - \mathbf{u}^n}{\Delta t} + \mathbf{u}^n \cdot \nabla \mathbf{u}^n = + \frac{1}{\mathrm{Re}} \nabla^2 \mathbf{u}^{n+1} \tag{2.9}$$

The remaining terms of equation 2.8 are

$$\frac{\mathbf{u}^{n+1} - \mathbf{u}^*}{\Delta t} = -\nabla p^{n+1} \tag{2.10}$$

The divergence of equation 2.10 is

$$\frac{\nabla . \mathbf{u}^{n+1} - \nabla . \mathbf{u}^*}{\Delta t} = \nabla . \left(-\nabla p^{n+1}\right) \tag{2.11}$$

Imposing the continuity equation for the $(n+1)$ step, $\nabla . \mathbf{u}^{n+1} = 0$, the pressure can be solved as

$$\nabla^2 p^{n+1} = \frac{1}{\Delta t} \nabla . \mathbf{u}^* \tag{2.12}$$

The pressure p^{n+1} is found using the pressure Poisson equation 2.12. Applying the equation 2.10 and the pressure p^{n+1}, the velocity at time t^{n+1} is

$$\mathbf{u}^{n+1} = \mathbf{u}^* - \Delta t \nabla p^{n+1} \tag{2.13}$$

On the other hand, using the weak form, The intermediate velocity satisfies

$$\int_{\Omega_t} \left\{ \mathbf{w} \cdot \left[\frac{\partial \mathbf{u}^*}{\partial t} + (\mathbf{u} \cdot \nabla)\mathbf{u} \right] + \frac{1}{Re} \nabla \mathbf{w} : \nabla \mathbf{u} \right\} d\Omega = \int_{\Gamma_t} \mathbf{w} \cdot \frac{\partial \mathbf{u}}{\partial \mathbf{n}} d\Gamma \tag{2.14}$$

In the cases addressed here the line integral always vanishes, hence it will be neglected in the rest of this paper. Also, in equation 2.14 the computation of the time derivative term requires the application of the Reynolds transport theorem [30], that is

$$\int_{\Omega_t} \mathbf{w} \cdot \frac{\partial \mathbf{u}^*}{\partial t} d\Omega = \frac{\partial}{\partial t} \int_{\Omega_t} \mathbf{w} \cdot \mathbf{u}^* d\Omega - \int_{\Gamma_t} (\mathbf{w} \cdot \mathbf{u})(\mathbf{v}_k \cdot \mathbf{n})\, d\Gamma \tag{2.15}$$

If the interface velocity is known, as is the case here, the integral over the interface vanishes and equation 2.14 becomes

$$\frac{\partial}{\partial t} \int_{\Omega_t} \mathbf{w} \cdot \mathbf{u}^* d\Omega + \int_{\Omega_t} \left\{ \mathbf{w} \cdot (\mathbf{u} \cdot \nabla)\mathbf{u} + \frac{1}{\mathrm{Re}} \nabla \mathbf{w} : \nabla \mathbf{u} \right\} d\Omega = 0 \tag{2.16}$$

To simplify the expressions the fractional step formulation is written for the x-component of velocity, u only, the equations for the other two components being similar. Discretizing the time derivative using a first order backward Euler difference, the intermediate velocity component u^* is given by

$$\int_{\Omega_{t_{n+1}}} \left\{ \frac{1}{\Delta t} w_u\, u^* + \frac{1}{\mathrm{Re}} \nabla w_u \cdot \nabla u^* \right\} d\Omega = \int_{\Omega_{t_n}} \left\{ w_u (\mathbf{u}^n \cdot \nabla) u^n + \frac{1}{\Delta t} w_u\, u^n \right\} d\Omega \tag{2.17}$$

The convective term is kept explicit, therefore the algorithm is subject to the CFL stability condition, $c \leq 1$, where c is the local Courant number.

The pressure is obtained from the solution to the pressure Poisson equation (PPE)

$$\int_{\Omega_{t_{n+1}}} \nabla q \cdot \nabla p^{n+1}\, d\Omega = -\frac{1}{\Delta t} \int_{\Omega_{t_{n+1}}} q\, \nabla \cdot \mathbf{u}^* d\Omega \tag{2.18}$$

And the final corrected velocity is obtained from

$$\int_{\Omega_{t_{n+1}}} w_u \, u^{n+1} \, d\Omega = \int_{\Omega_{t_{n+1}}} w_u (u^* - \Delta t \, \nabla p^{n+1}) d\Omega \tag{2.19}$$

The same process is repeated to obtain the y- and z-components of velocity.

The final Galerkin discretization is done using a combination of bilinear isoparametric rectangles and linear triangles in two dimensions and trilinear isoparametric hexahedra, linear pyramids and isoparametric prismatic triangular cylinders in three dimensions. The resulting systems of equations have been solved using a direct skyline solver [31], and stabilization has been achieved by means of a Petrov Galerkin formulation of the SUPG type [27].

Chapter 3

Local Mesh Adaptation

The mesh adaptation process has been fully described in [12, 13]. Here we will illustrate it briefly in two dimensions. Consider the situation depicted in Figure 3.1(a) below, where a uniform mesh of 12 elements is intersected by a superimposed interface

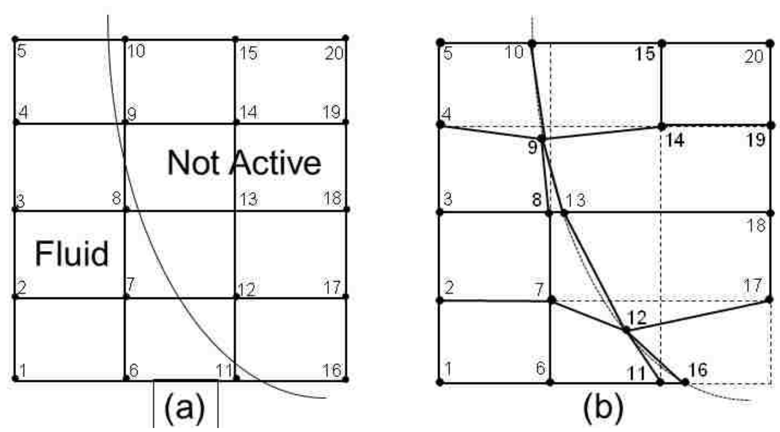

Figure 3.1: Mesh adaptation in a rectangular domain with moving interface

(a) Rectangular domain discretized using 12 rectangular elements with an interface superimposed. The region to the left side of the interface is assumed to contain fluid, the region to the right of the interface will not enter the flow calculation and is labeled “not active”.

(b) The mesh locally adapted to the interface on the fluid side. 4 irregular quadrilateral elements and 2 triangular elements have been generated. The flow calculation on the right hand side will involve only nodes 1-13 and 16. The rest will be inactive.

The adapted mesh is shown in Figure 3.1(b), where the active elements on the fluid side are shown with a full line, there are two types of active elements adjacent to the interface; linear triangles and isoparametric bilinear elements, it is also possible to use higher order elements. In Figure 3.1(b) nodes 1-8 and 11 are fluid, nodes 9, 10, 12, 13 and 16 are on the interface and therefore have a prescribed velocity and nodes 14, 15 and 17-20 are inactive.

The adaptation is not unique, the position of the nodes in the interface can be chosen to some extent, but the final meshes will be always similar. Elements that do not contain any nodes in the fluid are not assembled, and nodes that are not active are treated as having prescribed homogeneous Dirichlet boundary conditions. Because the interface velocity is known, the degrees of freedom lie strictly on nodes in the fixed mesh.

The adaptation is fully automatic, and keeps the total number of nodes constant throughout the simulation. At each time step, the velocity is calculated in the adapted mesh using only the mesh nodes that lie in the fluid. For the next time step, the adaptation is discarded and a new one is performed. It should be stressed that the active degrees of freedom are strictly on mesh nodes that do not change position. The nodes that are moved all lie on the interface.

Chapter 4

Error Analysis

The questions of stability, convergence and (lack of) satisfaction of the consistency condition in the present algorithm are not an issue, these have already been properly answered [11, 26, 28]. It is also well known that the convergence rate in the finite element spatial approximation of second order parabolic equations using linear triangles and bilinear quadrilaterals is of second order [32, 33]; However, questions have been raised about the local accuracy and the actual convergence rate of the methodology used here to simulate the moving interfaces due to the interaction of the mesh adaptation method and the numerical algorithm. The reason is that during the calculation very small elements and elements with very large aspect ratios are generated that are adjacent to the much larger elements of the fixed basic mesh. This mixture of large and small elements is traditionally viewed as poor practice that compromises the accuracy of the FEM calculations. In this chapter, the results of a (admittedly limited) local truncation error analysis is presented to understand the practical effect of this aspect of the method.

The approximation error has two main sources, one is the solution of the convection-diffusion equation 2.9, and the second source of error is the solution of the pressure Poisson equation 2.12. The second equation involves the gradients of the intermediate velocity calculated in equation 2.17 as the forcing term, therefore error in the solution of equation 2.9 affects the accuracy of the solution to equation 2.12.

4.1 Error in the Convection-Diffusion Equation

First the local error in the approximation of the convection diffusion equation

$$\frac{\partial \phi}{\partial t} + \mathbf{u} \cdot \nabla \phi - D \nabla^2 \phi = 0 \tag{4.1}$$

where $D = \frac{1}{Re}$ is considered. Bilinear quadrilateral elements are used on a non-

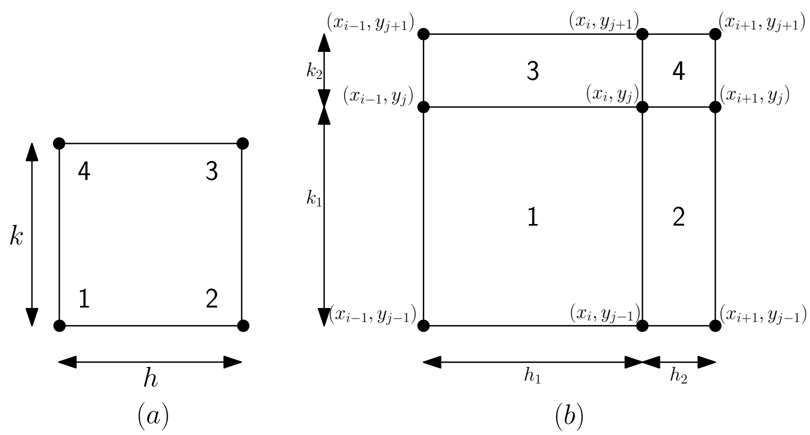

Figure 4.1: (a) Nodal numbering in a bilinear element (b) Four elements assembly around node (x_i, y_i) in an irregular rectangular mesh.

uniform mesh.

Figure 4.1(a) shows the nodal notation used for a single bilinear element and figure 4.1(b) shows the notation in a general two-dimensional irregular rectangular mesh.

ϕ is transport quantity.

Assume that the convective velocity field $\mathbf{u} = (u, v)^T$ is known and constant.

The weak weighted residuals formulation of equation 4.1 gives

$$\int_{\Omega\ t} \left\{ \mathbf{w} \cdot \left[\frac{\partial \phi}{\partial t} + (\mathbf{u} \cdot \nabla)\phi^{n} \right] + D \left(\nabla \mathbf{w} . \nabla \phi^{n+1} \right) \right\} d\Omega = 0 \tag{4.2}$$

Where $\mathbf{w}$ denotes the weighting functions.

The ϕ function is discretized over the space as:

$$\phi\left(x, y, t\right) \cong \sum_{i=1}^{n} N_i \left(x, y, t\right) \phi_i \left(t\right) \tag{4.3}$$

Where N_i are the shape functions over each element, and n is the number of nodes in an element, in this two dimensional case $n = 4$. The weighting functions w_i are set to be equal to shape functions N_i. the final form of the equation 4.2 is

$$\begin{aligned} &\int_0^{\Delta y} \int_0^{\Delta x} N_i \sum_{j=1}^{4} N_j \frac{\partial \phi_j}{\partial t} dxdy \\ &+ \int_0^{\Delta y} \int_0^{\Delta x} \left(uN_i \sum_{j=1}^{4} \left(\frac{\partial N_j}{\partial x} \phi_j^n \right) + vN_i \sum_{j=1}^{4} \left(\frac{\partial N_j}{\partial y} \phi_j^n \right) \right) dxdy \\ &+ \int_0^{\Delta y} \int_0^{\Delta x} D \left(\frac{\partial N_i}{\partial x} \sum_{j=1}^{4} \left(\frac{\partial N_j}{\partial x} \phi_j^{n+1} \right) + \frac{\partial N_i}{\partial y} \sum_{j=1}^{4} \left(\frac{\partial N_j}{\partial y} \phi_j^{n+1} \right) \right) dxdy = 0 \end{aligned} \tag{4.4}$$

The shape functions according to figure 4.1(a) are

$$\begin{cases} N_1 = \left(1 - \frac{x}{h}\right)\left(1 - \frac{y}{k}\right) \\ N_2 = \left(\frac{x}{h}\right)\left(1 - \frac{y}{k}\right) \\ N_3 = \left(1 - \frac{x}{h}\right)\left(\frac{y}{k}\right) \\ N_4 = \left(\frac{x}{h}\right)\left(\frac{y}{k}\right) \end{cases} \tag{4.5}$$

The next task is to calculate the stiffness matrix of an element. By calculating the stiffness matrices the equation 4.4 can be written as

$$S_{ij}^{11} \dot{\phi}_j + S_{ij}^{22} \phi_j^n + S_{ij}^{33} \phi_j^n + S_{ij}^{44} \phi_j^{n+1} + S_{ij}^{55} \phi_j^{n+1} = 0 \tag{4.6}$$

Where S^{mm} are stiffness matrices calculated as

$$S_{ij}^{11} = \frac{\Delta x \Delta y}{36}\begin{bmatrix} 4 & 2 & 1 & 2 \\ 2 & 4 & 2 & 1 \\ 1 & 2 & 4 & 2 \\ 2 & 1 & 2 & 4 \end{bmatrix},\ S_{ij}^{22} = \frac{\mathbf{u}\Delta y}{12}\begin{bmatrix} -2 & 2 & 1 & -1 \\ -2 & 2 & 1 & -1 \\ -1 & 1 & 2 & -2 \\ -1 & 1 & 2 & -2 \end{bmatrix},$$

$$S_{ij}^{33} = \frac{\mathbf{v}\Delta x}{12}\begin{bmatrix} -2 & -1 & 1 & 2 \\ -1 & -2 & 2 & 1 \\ -1 & -2 & 2 & 1 \\ -2 & -1 & 1 & 2 \end{bmatrix},\ S_{ij}^{44} = D\frac{\Delta y}{6\Delta x}\begin{bmatrix} 2 & -2 & -1 & 1 \\ -2 & 2 & 1 & -1 \\ -1 & 1 & 2 & -2 \\ 1 & -1 & -2 & 2 \end{bmatrix},\ \text{and}$$

$$S_{ij}^{55} = D\frac{\Delta x}{6\Delta y}\begin{bmatrix} 2 & 1 & -1 & -2 \\ 1 & 2 & -2 & -1 \\ -1 & -2 & 2 & 1 \\ -2 & -1 & 1 & 2 \end{bmatrix}$$

The most commonly time integration algorithm normally referring to as the θ method is used. It consists in approximating the time derivative by the backward difference

$$\dot{\phi} \cong \frac{1}{\Delta t}\left(\phi^{n+1} - \phi^{n}\right) \tag{4.7}$$

The parameter ϕ is then defined by

$$\phi = \theta\,\phi^{n+1} + (1-\theta)\,\phi^{n} \tag{4.8}$$

in this analysis the relaxation parameter is $\theta = 1$, and the result is $\phi = \phi^{n+1}$.

The element equations written for an element using the notation in figure 4.1(a) are used and $\Delta x = h$ and $\Delta y = k$ are replaced

$$\left\{\frac{hk}{36\Delta t}\begin{bmatrix}4&2&1&2\\2&4&2&1\\1&2&4&2\\2&1&2&4\end{bmatrix}+\frac{Dk}{6h}\begin{bmatrix}2&-2&-1&1\\-2&2&1&-1\\-1&1&2&-2\\1&-1&-2&2\end{bmatrix}+\frac{Dh}{6k}\begin{bmatrix}2&1&-1&-2\\1&2&-2&-1\\-1&-2&2&1\\-2&-1&1&2\end{bmatrix}\right\}\begin{bmatrix}\phi_1^{n+1}\\\phi_2^{n+1}\\\phi_3^{n+1}\\\phi_4^{n+1}\end{bmatrix}=$$
$$\left\{-\frac{\mathbf{u}k}{12}\begin{bmatrix}-2&2&1&-1\\-2&2&1&-1\\-1&1&2&-2\\-1&1&2&-2\end{bmatrix}-\frac{\mathbf{v}h}{12}\begin{bmatrix}-2&-1&1&2\\-1&-2&2&1\\-1&-2&2&1\\-2&-1&1&2\end{bmatrix}+\frac{hk}{36\Delta t}\begin{bmatrix}4&2&1&2\\2&4&2&1\\1&2&4&2\\2&1&2&4\end{bmatrix}\right\}\begin{bmatrix}\phi_1^{n}\\\phi_2^{n}\\\phi_3^{n}\\\phi_4^{n}\end{bmatrix} \tag{4.9}$$

The detailed two dimensional truncation error analysis of convection-diffusion equation can be found in Appendix B.1. Assembling the element equation contributions to node (x_i, y_i) results in the difference equation (DE)

$$DE \equiv DE_{time\ derivation} + DE_{convection} + DE_{diffusion} \tag{4.10}$$

where

$$\begin{aligned}
&DE_{time\ derivation} \equiv \\
&+\frac{k_1}{36\Delta t}\left(h_1\phi_{i-1j-1}^{n+1} + 2\left(h_1+h_2\right)\phi_{ij-1}^{n+1} + h_2\phi_{i+1j-1}^{n+1}\right)\\
&-\frac{k_1}{36\Delta t}\left(h_1\phi_{i-1j-1}^{n} + 2\left(h_1+h_2\right)\phi_{ij-1}^{n} + h_2\phi_{i+1j-1}^{n}\right)\\
&+\frac{(k_1+k_2)}{36\Delta t}\left(2h_1\phi_{i-1j}^{n+1} + 4\left(h_1+h_2\right)\phi_{ij}^{n+1} + 2h_2\phi_{i+1j}^{n+1}\right)\\
&-\frac{(k_1+k_2)}{36\Delta t}\left(2h_1\phi_{i-1j}^{n} + 4\left(h_1+h_2\right)\phi_{ij}^{n} + 2h_2\phi_{i+1j}^{n}\right)\\
&+\frac{k_2}{36\Delta t}\left(h_1\phi_{i-1j+1}^{n+1} + 2\left(h_1+h_2\right)\phi_{ij+1}^{n+1} + h_2\phi_{i+1j+1}^{n+1}\right)\\
&-\frac{k_2}{36\Delta t}\left(h_1\phi_{i-1j+1}^{n} + 2\left(h_1+h_2\right)\phi_{ij+1}^{n} + h_2\phi_{i+1j+1}^{n}\right)
\end{aligned} \tag{4.11}$$

$$
\begin{aligned}
&DE_{convection} \equiv \\
&+\frac{vh_1}{12}\left(2\phi^n_{ij+1}+\phi^n_{i-1j+1}-\phi^n_{i-1j-1}-2\phi^n_{ij-1}\right) \\
&+\frac{vh_2}{12}\left(\phi^n_{i+1j+1}+2\phi^n_{ij+1}-2\phi^n_{ij-1}-\phi^n_{i+1j-1}\right) \\
&+\frac{uk_2}{12}\left(\phi^n_{i+1j+1}+2\phi^n_{i+1j}-2\phi^n_{i-1j}-\phi^n_{i-1j+1}\right) \\
&+\frac{uk_1}{12}\left(2\phi^n_{i+1j}+\phi^n_{i+1j-1}-\phi^n_{i-1j-1}-2\phi^n_{i-1j}\right)
\end{aligned}
\tag{4.12}
$$

and

$$
\begin{aligned}
&DE_{diffusion} \equiv \\
&+\frac{D}{6h_1}\left(k_1\left(\phi^{n+1}_{ij-1}-\phi^{n+1}_{i-1j-1}\right)+2\left(k_1+k_2\right)\left(\phi^{n+1}_{ij}-\phi^{n+1}_{i-1j}\right)+k_2\left(\phi^{n+1}_{ij+1}-\phi^{n+1}_{i-1j+1}\right)\right) \\
&+\frac{D}{6h_2}\left(k_1\left(\phi^{n+1}_{ij-1}-\phi^{n+1}_{i+1j-1}\right)+2\left(k_1+k_2\right)\left(\phi^{n+1}_{ij}-\phi^{n+1}_{i+1j}\right)+k_2\left(\phi^{n+1}_{ij+1}-\phi^{n+1}_{i+1j+1}\right)\right) \\
&+\frac{D}{6k_1}\left(h_1\left(\phi^{n+1}_{i-1j}-\phi^{n+1}_{i-1j-1}\right)+2\left(h_1+h_2\right)\left(\phi^{n+1}_{ij}-\phi^{n+1}_{ij-1}\right)+h_2\left(\phi^{n+1}_{i+1j}-\phi^{n+1}_{i+1j-1}\right)\right) \\
&+\frac{D}{6k_2}\left(h_1\left(\phi^{n+1}_{i-1j}-\phi^{n+1}_{i-1j+1}\right)+2\left(h_1+h_2\right)\left(\phi^{n+1}_{ij}-\phi^{n+1}_{ij+1}\right)+h_2\left(\phi^{n+1}_{i+1j}-\phi^{n+1}_{i+1j+1}\right)\right)
\end{aligned}
\tag{4.13}
$$

A local truncation error analysis can show the deviation between an exact differential equation and its finite difference representation at a point in space and time. There are more information about truncation error analysis in appendix A.

All the terms in DE are expanded in Taylor series about ϕ^{n+1}_{ij}. The DE about

ϕ_{ij}^{n+1} is

$$DE = \frac{(h_1+h_2)(k_1+k_2)}{4} \times \left\{ \begin{array}{l} \dfrac{\partial \phi}{\partial t} - D\left(\dfrac{\partial^2 \phi}{\partial x^2} + \dfrac{\partial^2 \phi}{\partial x^2}\right) + u\dfrac{\partial \phi}{\partial x} + v\dfrac{\partial \phi}{\partial y} \\ +\dfrac{1}{3}\left((h_2-h_1)\dfrac{\partial^2 \phi}{\partial x \partial t} + (k_2-k_1)\dfrac{\partial^2 \phi}{\partial y \partial t}\right) \\ +\dfrac{1}{3}\left((k_2-k_1)\left(-\dfrac{\partial^3 \phi}{\partial y^3} - \dfrac{\partial^3 \phi}{\partial x^2 \partial y}\right) + (h_2-h_1)\left(-\dfrac{\partial^3 \phi}{\partial x^3} - \dfrac{\partial^3 \phi}{\partial x \partial y^2}\right)\right) \\ +u\left(\dfrac{1}{2}(h_2-h_1)\dfrac{\partial^2 \phi}{\partial x^2} + \dfrac{1}{3}(k_2-k_1)\dfrac{\partial^2 \phi}{\partial x \partial y}\right) \\ +v\left(\dfrac{1}{2}(k_2-k_1)\dfrac{\partial^2 \phi}{\partial y^2} + \dfrac{1}{3}(h_2-h_1)\dfrac{\partial^2 \phi}{\partial x \partial y}\right) \\ +O(h^2, k^2, hk, h\Delta t, k\Delta t, \Delta t) \end{array} \right\} \tag{4.14}$$

All terms on the right hand side of equation 4.14 are evaluated at (x_i, y_j, t_{n+1}). Rewriting the first order term of the truncation error as

$$\begin{array}{l} \dfrac{1}{3}\left((k_2-k_1)\dfrac{\partial}{\partial y}\left(\dfrac{\partial \phi}{\partial t} - \dfrac{\partial^2 \phi}{\partial x^2} - \dfrac{\partial^2 \phi}{\partial y^2} + u\dfrac{\partial \phi}{\partial x} + v\dfrac{\partial \phi}{\partial y}\right)\right) + \dfrac{u}{6}(h_2-h_1)\dfrac{\partial^2 \phi}{\partial x^2} \\ +\dfrac{1}{3}\left((h_2-h_1)\dfrac{\partial}{\partial x}\left(\dfrac{\partial \phi}{\partial t} - \dfrac{\partial^2 \phi}{\partial x^2} - \dfrac{\partial^2 \phi}{\partial y^2} + u\dfrac{\partial \phi}{\partial x} + v\dfrac{\partial \phi}{\partial y}\right)\right) + \dfrac{v}{6}(k_2-k_1)\dfrac{\partial^2 \phi}{\partial y^2} \end{array}$$

the leading terms on the left must vanish hence the changes in the mesh introduce a spatial first order local error (FOE) equal to

$$FOE = \frac{1}{6}\left(u(h_2-h_1)\left(\frac{\partial^2 \phi}{\partial x^2}\right)_{ij}^{n+1} + v(k_2-k_1)\left(\frac{\partial^2 \phi}{\partial y^2}\right)_{ij}^{n+1}\right) \tag{4.15}$$

This is of the form of an anisotropic artificial diffusion similar to that arising in stabilizing formulations of the upwind type, and is readily eliminated by the addition of an artificial balancing diffusion in the intersected elements [27], which restores the local second order accuracy in the approximation.

In three dimensions, the first order truncation error terms in the Taylor expansion are

$$DE = \frac{(h_1 + h_2)(k_1 + k_2)(l_2 - l_1)}{8} \times \left(\begin{array}{l} \frac{1}{3}\left((h_2 - h_1)\frac{\partial^2 \phi}{\partial x \partial t} + (k_2 - k_1)\frac{\partial^2 \phi}{\partial y \partial t} + (l_2 - l_1)\frac{\partial^2 \phi}{\partial z \partial t} \right) \\ +\frac{1}{3} D \left(\begin{array}{c} (h_2 - h_1)\left(-\frac{\partial^3 \phi}{\partial x^3} - \frac{\partial^3 \phi}{\partial x \partial y^2} - \frac{\partial^3 \phi}{\partial x \partial z^2} \right) \\ + (k_2 - k_1)\left(-\frac{\partial^3 \phi}{\partial y^3} - \frac{\partial^3 \phi}{\partial x^2 \partial y} - \frac{\partial^3 \phi}{\partial y \partial z^2} \right) \\ + (l_2 - l_1)\left(-\frac{\partial^3 \phi}{\partial z^3} - \frac{\partial^3 \phi}{\partial y^2 \partial z} - \frac{\partial^3 \phi}{\partial x^2 \partial z} \right) \end{array} \right) \\ +u \left(\frac{1}{2}(h_2 - h_1)\frac{\partial^2 \phi}{\partial x^2} + \frac{1}{3}(k_2 - k_1)\frac{\partial^2 \phi}{\partial x\, \partial y} + \frac{1}{3}(l_2 - l_1)\frac{\partial^2 \phi}{\partial x\, \partial z} \right) \\ +v \left(\frac{1}{2}(k_2 - k_1)\frac{\partial^2 \phi}{\partial y^2} + \frac{1}{3}(h_2 - h_1)\frac{\partial^2 \phi}{\partial x\, \partial y} + \frac{1}{3}(l_2 - l_1)\frac{\partial^2 \phi}{\partial y \partial z} \right) \\ +w \left(\frac{1}{2}(l_2 - l_1)\frac{\partial^2 \phi}{\partial z^2} + \frac{1}{3}(h_2 - h_1)\frac{\partial^2 \phi}{\partial x\, \partial z} + \frac{1}{3}(k_2 - k_1)\frac{\partial^2 \phi}{\partial y\, \partial z} \right) \end{array} \right) \tag{4.16}$$

where l_1 and l_2 are the different mesh sizes in the z-direction. The same manipulations as in two dimensions show that the local first order error introduced by the mesh changes is

$$FOE = \frac{1}{6} \left(\begin{array}{c} u\,(h_2 - h_1)\left(\frac{\partial^2 \phi}{\partial x^2} \right)_{i\,j\,k}^{n+1} \\ +v\,(k_2 - k_1)\left(\frac{\partial^2 \phi}{\partial y^2} \right)_{i\,j\,k}^{n+1} \\ +w\,(l_2 - l_1)\left(\frac{\partial^2 \phi}{\partial z^2} \right)_{i\,j\,k}^{n+1} \end{array} \right) \tag{4.17}$$

Therefore the approximation to the convection-diffusion equation requires a correction to eliminate the artificial diffusion introduced by the changes in the mesh. This is readily accomplished by means of any of the procedures already known to eliminate artificial numerical diffusion, and can be implemented in a variety of ways. In particular this correction is similar to the stabilization of SUPG type required for highly convective flows. However, in the present case the additional error is strictly localized next to the interfaces and does not have the global effect of a stabilized Petrov-Galerkin formulation. Moreover, so far numerical experiments have shown that this error is small in the sense that it only increases the relative error at nodes adjacent to the boundary by two or three percent, but this conclusion is based on a limited number of measurements.

Like the two dimensional analysis, the detailed three dimensional truncation error analysis for convection-diffusion equation can be found in Appendix B.2.

4.2 Error in the Pressure Poisson Equation

The second source of approximation error in need of analysis is the solution of the pressure Poisson equation

$$-\nabla^2 p = f \tag{4.18}$$

where

$$f = -\frac{1}{\Delta t}\nabla \cdot \mathbf{u}^* \tag{4.19}$$

Detailed two dimensional truncation error analysis of Poisson equation can be found in Appendix C.1.

In the two-dimensional case, using the notation of Figure 4.1(a) the element equations are

$$\left(\frac{k}{6h}\begin{bmatrix} 2 & -2 & -1 & 1 \\ -2 & 2 & 1 & -1 \\ -1 & 1 & 2 & -2 \\ 1 & -1 & -2 & 2 \end{bmatrix} + \frac{h}{6k}\begin{bmatrix} 2 & 1 & -1 & -2 \\ 1 & 2 & -2 & -1 \\ -1 & -2 & 2 & 1 \\ -2 & -1 & 1 & 2 \end{bmatrix}\right)\begin{bmatrix} p_1 \\ p_2 \\ p_3 \\ p_4 \end{bmatrix} = \frac{hk}{36}\begin{bmatrix} 4 & 2 & 1 & 2 \\ 2 & 4 & 2 & 1 \\ 1 & 2 & 4 & 2 \\ 2 & 1 & 2 & 4 \end{bmatrix}\begin{bmatrix} f_1 \\ f_2 \\ f_3 \\ f_4 \end{bmatrix} \tag{4.20}$$

and assembling the difference equation for node (x_i, y_i) yields

$$\begin{aligned} DE \equiv\ & \frac{1}{6h_1}\left(k_1\left(p_{i\,j-1} - p_{i-1\,j-1}\right) + 2\left(k_1 + k_2\right)\left(p_{i\,j} - p_{i-1\,j}\right) + k_2\left(p_{i\,j+1} - p_{i-1\,j+1}\right)\right) \\ & + \frac{1}{6h_2}\left(k_1\left(p_{i\,j-1} - p_{i+1\,j-1}\right) + 2\left(k_1 + k_2\right)\left(p_{i\,j} - p_{i+1\,j}\right) + k_2\left(p_{i\,j+1} - p_{i+1\,j+1}\right)\right) \\ & + \frac{1}{6k_1}\left(h_1\left(p_{i-1\,j} - p_{i-1\,j-1}\right) + 2\left(h_1 + h_2\right)\left(p_{i\,j} - p_{i\,j-1}\right) + h_2\left(p_{i+1\,j} - p_{i+1\,j-1}\right)\right) \\ & + \frac{1}{6k_2}\left(h_1\left(p_{i-1\,j} - p_{i-1\,j+1}\right) + 2\left(h_1 + h_2\right)\left(p_{i\,j} - p_{i\,j+1}\right) + h_2\left(p_{i+1\,j} - p_{i+1\,j+1}\right)\right) \\ & - \left(\begin{array}{l} \frac{h_1}{36}\left(k_1 f_{i-1\,j-1} + k_2 f_{i-1\,j+1}\right) + \frac{h_2}{36}\left(k_1 f_{i+1\,j-1} + k_2 f_{i+1\,j+1}\right) \\ + \frac{k_1\left(h_1 + h_2\right)}{18} f_{i\,j-1} + \frac{h_1\left(k_1 + k_2\right)}{18} f_{i-1\,j} + \frac{h_2\left(k_1 + k_2\right)}{18} f_{i+1\,j} \\ + \frac{k_2\left(h_1 + h_2\right)}{18} f_{i\,j+1} + \frac{\left(k_1 + k_2\right)\left(h_1 + h_2\right)}{9} f_{i\,j} \end{array}\right) = 0 \end{aligned} \tag{4.21}$$

The Taylor series expansion about $p_{i\,j}$ gives

$$\begin{aligned} DE = & \frac{(h_1 + h_2)(k_1 + k_2)}{4} \times \\ & \left(\begin{array}{l} \left(-\frac{\partial^2 p}{\partial x^2} - \frac{\partial^2 p}{\partial x^2} - f\right) + \frac{1}{3}\left(\begin{array}{c} (k_2 - k_1)\left(-\frac{\partial^3 p}{\partial y^3} - \frac{\partial^3 p}{\partial x^2 \partial y}\right) \\ + (h_2 - h_1)\left(-\frac{\partial^3 p}{\partial y^3} - \frac{\partial^3 p}{\partial x \partial y^2}\right) \end{array}\right) \\ -\frac{1}{3}\left[(k_2 - k_1) f_y + (h_2 - h_1) f_x\right] + O(h^2, k^2, hk) \end{array}\right) \end{aligned} \tag{4.22}$$

Note that the leading first order term in the truncation error is equal to

$$\frac{1}{3}\begin{pmatrix} (k_2-k_1)\dfrac{\partial}{\partial y}\left(-\dfrac{\partial^2 p}{\partial x^2}-\dfrac{\partial^2 p}{\partial y^2}-f\right) \\ +(h_2-h_1)\dfrac{\partial}{\partial x}\left(-\dfrac{\partial^2 p}{\partial x^2}-\dfrac{\partial^2 p}{\partial y^2}-f\right) \end{pmatrix} \equiv 0 \tag{4.23}$$

Provided that the finite element discretization of the right hand side is fully consistent; Therefore, this error vanishes and the method is locally second order accurate regardless of abrupt changes in the mesh. However, if the formulation is not fully consistent, such as the case reduced integration is used to evaluate the pressure gradients in , then a first order error is introduced.

In three dimensions the leading term in the truncation error takes the form

$$\begin{aligned} &\frac{1}{3}\begin{pmatrix} (k_2-k_1)\left(-\dfrac{\partial^3 p}{\partial x^2\partial y}-\dfrac{\partial^3 p}{\partial y^3}-\dfrac{\partial^3 p}{\partial y\,\partial z^2}\right) \\ +(h_2-h_1)\left(-\dfrac{\partial^3 p}{\partial x^3}-\dfrac{\partial^3 p}{\partial x\,\partial y^2}-\dfrac{\partial^3 p}{\partial x\,\partial z^2}\right) \\ +(l_2-l_1)\left(-\dfrac{\partial^3 p}{\partial x^2\partial z}-\dfrac{\partial^3 p}{\partial y^2\partial z}-\dfrac{\partial^3 p}{\partial z^3}\right) \end{pmatrix} \\ &-\frac{1}{3}\left((h_2-h_1)\frac{\partial f}{\partial x}+(k_2-k_1)\frac{\partial f}{\partial y}+\ (l_2-l_1)\frac{\partial f}{\partial z}\right)+O(h^2,k^2,l^2) \end{aligned} \tag{4.24}$$

Re-writing equation 4.24 gives

$$FOE=\frac{1}{3}\begin{pmatrix} (h_2-h_1)\,\dfrac{\partial}{\partial x}\left(-\dfrac{\partial^2 p_{ijk}}{\partial x^2}-\dfrac{\partial^2 p_{ijk}}{\partial y^2}-\dfrac{\partial^2 p_{ijk}}{\partial z^2}-f_{ijk}\right) \\ +(k_2-k_1)\,\dfrac{\partial}{\partial y}\left(-\dfrac{\partial^2 p_{ijk}}{\partial x^2}-\dfrac{\partial^2 p_{ijk}}{\partial y^2}-\dfrac{\partial^2 p_{ijk}}{\partial z^2}-f_{ijk}\right) \\ +(l_2-l_1)\,\dfrac{\partial}{\partial z}\left(-\dfrac{\partial^2 p_{ijk}}{\partial x^2}-\dfrac{\partial^2 p_{ijk}}{\partial y^2}-\dfrac{\partial^2 p_{ijk}}{\partial z^2}-f_{ijk}\right) \end{pmatrix}\equiv 0 \tag{4.25}$$

and as expected the same results as in two dimensions are true in three dimensions. Detailed analysis for Poisson equation three dimensional truncation error can be found in appendix C.2.

The results presented in this chapter are easily confirmed through simple numerical examples and indicate that when very small elements or elements with very large aspect ratios next to elements of a standard size are generated next to the moving interfaces the accuracy of the calculations is not significantly affected. Errors introduced in the solution of the convection diffusion equations are localized to the immediate vicinity of the moving interface and can be corrected by existing techniques which results in retaining full second order spatial accuracy in the solution of the intermediate velocity; however, the effect of the correction has shown to have only a marginal improvement in the accuracy. Consequently, the accuracy of the calculations is either not affected by the appearance of very small elements or the additional error introduced by the large ratio between the sizes of adjacent elements is small.

In the implementation of the method, to avoid difficulties stemming from truncation when the size of the intersection of an element turns out to be extremely small, if the element area (in two dimensions) or the volume (in three dimensions) turns out to be less than 0.1% of the size of the original intersected element the small intersection is neglected. This precaution guarantees that the derivatives of the shape functions do not differ by more than four orders of magnitude and prevents truncation errors from becoming a problem.

Chapter 5

Benchmark Problem

To validate the method and the results above and gain further insight into the behavior of the method consider two-dimensional flow of a fluid layer between two parallel plates moving away from each other with time [34]. This flow admits an analytical similarity solution when the velocity at which the plates move has the prescribed form shown below. The domain is a rectangular region of size $2L$ long by $2h(t)$ high where $x = 0$ and $y = 0$ are symmetry planes. The problem set up is depicted in Figure 5.1. Note that using symmetry only a quarter of the domain may be used in the calculations, that is $0 \leq x \leq L$, $0 \leq y \leq h(t)$.

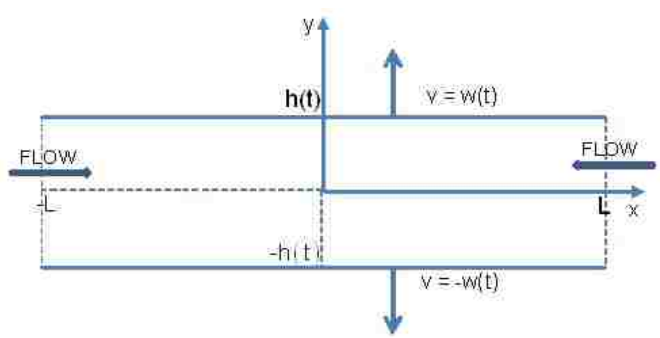

Figure 5.1: Schematic of flow between separating parallel planes.

The maximum allowed separation to be reached between the upper plate and the x-axis is showed by H, and the initial position of the plate is denoted by $y_0 = h(0)$; Therefore, the position , $h\left(t\right)$, of the plate as a function of time is

$$h\left(t\right) = y_0{(1 - \alpha t)}^{1/2} \tag{5.1}$$

and the velocity of the plate is given by

$$w\left(t\right) = \frac{d\left(h\left(t\right)\right)}{dt} = \frac{-\alpha y_0}{2{(1 - \alpha t)}^{1/2}} \tag{5.2}$$

and an analytical similarity solution exists [34] of the form

$$u^*\left(\mathbf{x}, t\right) = \frac{\alpha x}{2\left(1 - \alpha t\right)} f'\left(\eta\right) \tag{5.3}$$

$$\mathrm{v}^*\left(\mathbf{x}, t\right) = \frac{-\alpha y_0}{2{(1 - \alpha t)}^{1/2}} f\left(\eta\right) \tag{5.4}$$

where η is the stretched vertical coordinate $\eta = \frac{y}{h(t)}$, $f'\left(\eta\right)$ is the derivative of f with respect to η and

$$f\left(\eta\right) = \eta + \frac{1}{\pi}\sin\left(\pi\eta\right) \tag{5.5}$$

The value of α is obtained from $\alpha = -\frac{\pi^2\nu}{2h_0^2}$ where ν is the kinematic viscosity of the fluid.

The solution for the pressure p is more involved [35] and is given by

$$p^* = \frac{\rho\left(L^2 - x^2\right)}{2h^2}\left[\mathrm{v}^2{(f')}^2 + \left(\mathrm{v}^2 - \mathrm{v}'\right)f' + \mathrm{v}^2\left(\eta - f\right)f'' + \frac{\nu}{h}\mathrm{v}\,f'''\right] - p\left(L\right) \tag{5.6}$$

where ρ is the fluid density.

In the purpose of this study, an artificial balancing diffusion introduced by change in the mesh and equal to first order error in convection-diffusion equation is added [27] in the intersected elements to a provided numerical simulation to restore the local second order accuracy in the approximation. However, up to now numerical experiments have shown that this error is small in the sense that it only increases the relative error at nodes adjacent to the boundary by two or three percent, but this conclusion is based on a limited number of measurements.

Chapter 6

Numerical Solution to the Benchmark Problem

The problem discussed above is now used to assess the accuracy of the ALE-FEM numerical model under consideration. The computational domain and boundary conditions are shown in figure 6.1

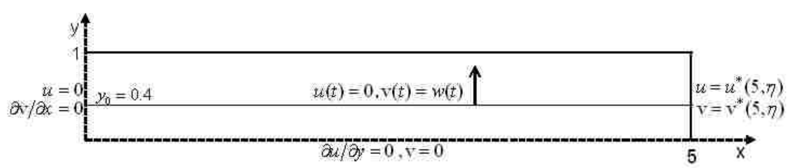

Figure 6.1: Domain and boundary conditions for the separating plates flow solved over one quarter of the complete region

For the set of calculations that follows the density is set to $\rho = 1$ and the kinematic viscosity is $\nu = 0.05$. The maximum height is set as $H = 1$ and the width of one halve of the region is set to $L = 5$. Using H as the characteristic length and a characteristic velocity $U = 1$ this results in a Reynolds number $Re = 20$. The initial position of the upper boundary is chosen at $y_0 = 0.4$. The initial conditions and the boundary conditions for the velocity at $x = 5$ are taken from the analytical solutions 5.3 and 5.4 and the interface position and velocity are given in equations 5.1 and 5.2.

The results of numerical simulations using the parameters given above and three uniform finite element meshes are reported here. The first mesh contains 50 x 10 bilinear elements with $\Delta x = \Delta y = 0.1$; the second mesh has 100 x 20 bilinear elements and $\Delta x = \Delta y = 0.05$; the third mesh has 200 x 40 bilinear elements and $\Delta x = \Delta y = 0.025$. Note that the meshes involve only rectangular elements, therefore the analysis in chapter 4 applies directly to these simulations without any kind of further approximation. For the first mesh the time step was chosen to be $\Delta t = 0.005$, for the second mesh $\Delta t = 0.00125$ and for the third $\Delta t = 0.0003125$; that is, the time step is divided by four every time the mesh is halved to account for the fact that the time stepping scheme is only first order. Calculations were performed for a total of 2 time units in each mesh, the top plate starts at $y_0 = 0.4$ and ends at $h(2) = 0.8038$. Figure 6.2 shows the flow and pressure fields at the end of the simulation when $t = 2$.

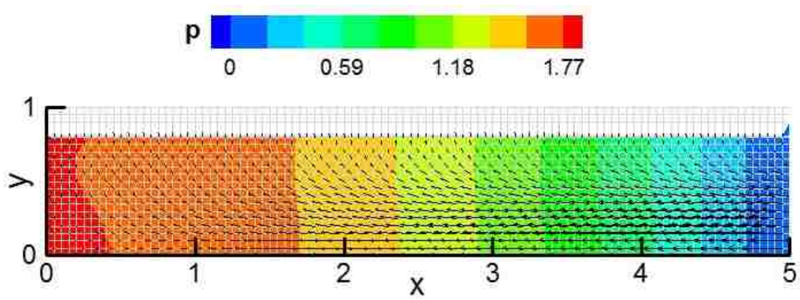

Figure 6.2: Flow and pressure fields for the benchmark problem at $t = 2$

Establishment of a meaningful comparison between the analytical and numerical solutions can be somewhat tricky. The objective here is to present a realistic picture of the accuracy of the method without claiming that the conclusions are absolute but that this is a viable method that exhibits appropriate accuracy and rate of convergence. To this purpose several decisions were made in an attempt to present a clear picture of the behavior of the algorithm without becoming entangled in a lengthy and overly detailed discussion. First the choice was made to calculate the average relative error in the velocity magnitude and the pressure for all active nodes located at $x = 2.5$, that is the vertical cross section located in the middle of the domain. Hence, at each time step t_n the average errors

$$EV(t_n) = \left(\frac{\sum_{i=1}^{k} \left[(u_i^* - u_i^a)^2 + (v_i^* - v_i^a)^2 \right]}{\sum_{i=1}^{k} \left[(u_i^*)^2 + (v_i^*)^2 \right]} \right)^{\frac{1}{2}} \tag{6.1}$$

and

$$EP(t_n) = \left(\frac{\sum_{i=1}^{k} \left[(p_i^* - p_i^a)^2 \right]}{\sum_{i=1}^{k} \left[(p_i^*)^2 \right]} \right)^{\frac{1}{2}} \tag{6.2}$$

are found. Here the star superscript denotes the analytical solution, the superscript a denotes the approximate finite element solution and k is the number of nodes active in the line $x = 2.5$ at time step t_n.

The error as a function of time for the three meshes is shown in figures 6.3 and 6.4

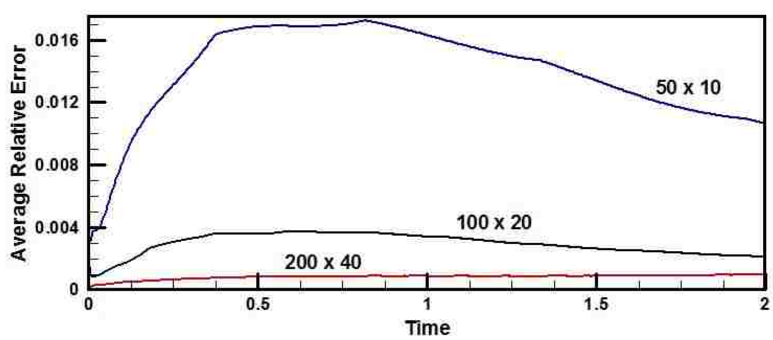

Figure 6.3: Average relative error in the velocity magnitude

Figures 6.3 and 6.4 show that both the velocity magnitude and the pressure converge as the size of the mesh spacing and time step decrease. The individual components of the velocity show the same type of behavior. The pressure error shows an unexpected

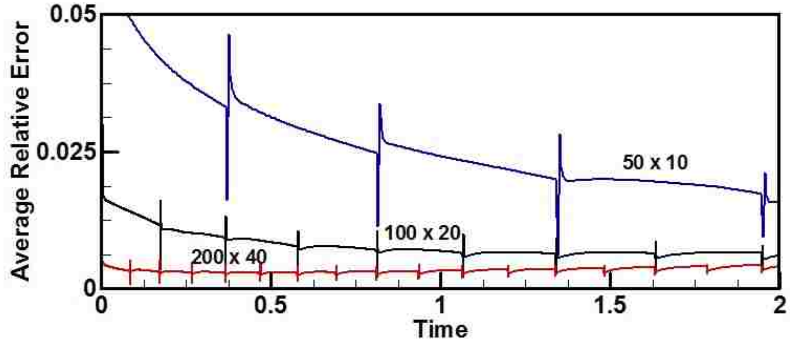

Figure 6.4: Average relative error in the pressure

behavior at the first time step, where the error is very large and decays very rapidly towards its average value; it also exhibits a sharp decay followed by a jump when the interface crosses to a new element in the vertical direction. It has not been possible for us to fully explain this behavior, measures can be taken to reduce and almost eliminate these perturbations, but these modifications complicate the model and are probably not effective for more general cases. The presence of a programming error cannot be ruled out; another possibility is that this problem offers a sort of "worst case scenario" in which all the nodes lying on the interface cross to a new element at the same time therefore compounding the error. However, the jumps in the error are not significant and are rapidly reduced when the mesh size is reduced; the reduction in the error when first adding a new row of elements is more puzzling though. Because these are incompressible flow calculations, any small perturbation in the mass conservation can produce a large change in the pressure, this could be what is observed here.

To get an idea of the rate at which convergence takes place, the average of the above values over a time interval is considered, to obtain one value for each mesh that can be thought of as representative of the error in the simulation. This was done over the whole time interval $0 \leq t \leq 2$ so the effect of the ends of the time interval are included. The values for the error are given by $(EV)_j = \frac{1}{2}\int_0^2 EV(t)\,dt$ and $(EP)_j = \frac{1}{2}\int_0^2 EP(t)\,dt$, $j = 1,\ 3$ where j denotes each of the three meshes.

Figures 6.5 and 6.6 show the rates of convergence obtained for the velocity magnitude and the pressure respectively, for the velocity the calculated convergence rate is 2.05 and for the pressure 1.50.

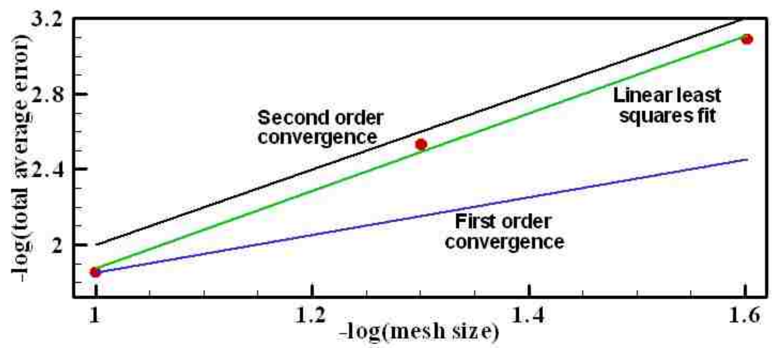

Figure 6.5: Convergence rate for the velocity magnitude

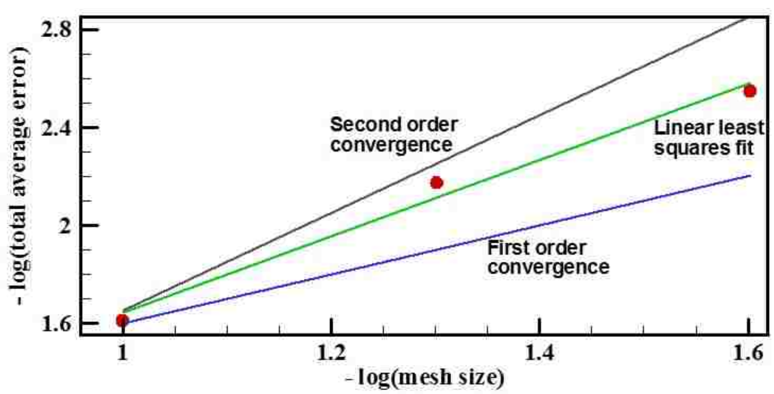

Figure 6.6: Convergence rate for the pressure

The actual calculated values for the errors $(EV)_j$ and $(EP)_j$ are given in Table 1.

j	h_j	$(EV)_j$	$(EP)_j$
1	0.1	0.0140	0.0272
2	0.05	0.0029	0.0079
3	0.025	0.0008	0.0034

Table 6.1: Averaged error for expanding channel problem with uniform meshes

The above results with the criterion used here to measure the error show that the finite element approximation to the velocity converges at a second order rate, and that the average relative error in the approximation of the velocity is reasonably small even for coarse meshes, as can be seen in figure 6.3 and table 6.1. Evidently, if different kinds of averaging are chosen or if different time intervals are chosen to average over, the results will be slightly different but always very similar. The same conclusion is reached when different parameters are used in the example. Examination of the error at each node shows that the relative error in a velocity component can be quite large depending on the location of the node and the magnitude of the velocity component relative to the maximum magnitude of that component in the whole domain; this can be the situation for the u component of velocity at nodes next to the moving interface where the magnitude of this component is very small compared to its maximum. However, this is not a deficiency of the present method but a property of finite element approximations that produce an even distribution of the error over the region [32]; the absolute error is relatively uniform and therefore the relative error is large for values of the dependent variable that have a small absolute magnitude. A simple example that illustrates this phenomenon is given by the one dimensional equation $\frac{d^2\phi}{dx^2} = 12x^2,\ \phi(0) = 0,\ \phi(1) = 1$ which has the solution $\phi^* = x^4$. The finite element solution using 10 linear elements produces a relative error of 900% at $x = 0.1$ where $\phi^* = 0.0001$ and a relative error of 0.14% at $x = 0.9$ where $\phi^* = 0.6561$; but the absolute error at both points is 0.03 and is the smallest error at the nodes. As the mesh is refined, the solution converges at the expected second order rate, but the relative error at the first few nodes next to $x = 0$ remains very large; in fact, using 20 linear elements in the same example yields an error of 1900% at $x = 0.05$.

The above discussion illustrates the difficulty in determining a criterion to assess the error and the fact that measuring relative error may not be the best thing to do. It underscores the need to examine the models from various different points of view before reaching conclusions about their accuracy and general behavior.

Chapter 7

Conclusions

To assess the accuracy of ALE finite element CFD simulations in situations that involve time dependent domains can be a complicated task, especially because the methods usually used in these cases are based on adaptive meshes that continuously change with time. A new approach has been developed that utilizes a fixed mesh, and applied to a two-dimensional flow with moving boundaries for which an analytical solution is available where the accuracy of the simulations can be measured directly. At the same time local truncation error analyses have been performed to assess the effect that local changes in the mesh size have in the numerical approximations, especially when these changes generate adjacent elements that have a two or three orders of magnitude difference in area or volume. The conclusion is that the accuracy of this new ALE-FEM method is not adversely affected by the abrupt mesh changes and that it has second order spatial rate of convergence.

References

[1] D. Juric and G. Tryggvasson. A front-tracking method for dendritic solidification. *Journal of Computational Physics*, 123(1):127–148, 1996.

[2] R. Löhner, J. R. Cebral, F. F. Camelli, J. D. Baum, E. L. Mestreau, and O. A. Soto. Adaptive embedded/immersed unstructured grid techniques. *Archives of Computational Methods in Engineering*, 14(3):279–301, 2007.

[3] O. C. Zienkiewicz and R. L. Taylor. The finite element method 4th edn, vol 2 solid and fluid mechanics/dynamics and non-linearity, 1991.

[4] D. J. Torres and M. F. Trujillo. KIVA-4: An unstructured ALE code for compressible gas flow with sprays. *Journal of Computational Physics*, 219(2):943–975, 2006.

[5] D. B. Carrington. A fractional step h-p adaptive finite element method for turbulent reactive flows. Los Alamos Report LA-UR-11-00466, Los Alamos National Laboratory, 2011.

[6] A. A. Johnson and T. E. Tezduyar. Mesh update strategies in parallel finite element computations of flow problems with moving boundaries and interfaces. *Computer methods in applied mechanics and engineering*, 119(1):73–94, 1994.

[7] W. Shyy, R. W. Smith, H. S. Udaykumar, and M. M. Rao. Computational fluid dynamics with moving boundaries. 1996.

[8] T. E. Tezduyar. Finite element methods for flow problems with moving boundaries and interfaces. *Archives of Computational Methods in Engineering*, 8(2):83–130, 2001.

[9] C. Farhatl and P. Geuzaine. Design and analysis of robust ALE time-integrators for the solution of unsteady flow problems on moving grids. *Computer Methods in Applied Mechanics and Engineering*, 193(39):4073–4095, 2004.

[10] C. Farhat and P. Geuzaine. On the significance of the geometric conservation law for flow computations on moving meshes. *Computer Methods in Applied Mechanics and Engineering*, 190(11):1467–1482, 2000.

[11] L. Formaggia and F. Nobile. Stability analysis of second-order time accurate schemes for ALE - FEM. *Computer methods in applied mechanics and engineering*, 193(39):4097–4116, 2004.

[12] D. B. Carrington, D. A. Muoz, and J. C. Heinrich. Modelling fluid flow in domains containing moving interfaces. *Progress in Computational Fluid Dynamics*, 14(3):193–150, 2014.

[13] D. B. Carrington, A. K. M. Monayem H. Mazumder, and J. C. Heinrich. Simulation of fluid flow in three-dimensional domains containing moving interfaces with a fixed mesh ALE-FEM method. *Submitted*.

[14] R. Codina, G. Houzeaux, H. Coppola-Owen, and J. Baiges. The fixed-mesh ALE approach for the numerical approximation of flows in moving domains. *Journal of Computational Physics*, 228(5):1591–1611, 2009.

[15] C. Hirt, A. Amsden, and J. Cook. An arbitrary lagrangian-eulerian computing method for all flow speeds. *Journal of Computational Physics*, 14(3):227–253, 1974.

[16] J. Donea, S. Giuliani, and J. P. Halleux. An arbitrary lagrangian-eulerian finite element method for transient dynamic fluid-structure interactions. *Computer methods in applied mechanics and engineering*, 33(1):689–723, 1982.

[17] W. Dettmer and D. Perić. A fully implicit computational strategy for strongly coupled fluid–solid interaction. *Archives of Computational Methods in Engineering*, 14(3):205–247, 2007.

[18] M. S. Gadala. Recent trends in ALE formulation and its applications in solid mechanics. *Computer methods in applied mechanics and engineering*, 193(39):4247–4275, 2004.

[19] J. Brackbill and J. Saltzman. Adaptive zoning for singular problems in two dimensions. *Journal of Computational Physics*, 46(3):342–368, 1982.

[20] J. L. Steger and J. A. Benek. On the use of composite grid schemes in computational aerodynamics. *Computer Methods in Applied Mechanics and Engineering*, 64(1):301–320, 1987.

[21] H. Askes and L. J. Sluys. Remeshing strategies for adaptive ALE analysis of strain localisation. *European Journal of Mechanics-A/Solids*, 19(3):447–467, 2000.

[22] P. H. Saksono, W. G. Dettmer, , and D. Perić. An adaptive remeshing strategy for flows with moving boundaries and fluid–structure interaction. *International Journal for Numerical Methods in Engineering*, 71(9):1009–1050, 2007.

[23] D. Boffi and L. Gastaldi. Stability and geometric conservation laws for ALE formulations. *Computer methods in applied mechanics and engineering*, 193(42):4717–4739, 2004.

[24] A. A. Johnson and T. E. Tezduyar. Simulation of multiple spheres falling in a liquid-filled tube. *Computer Methods in Applied Mechanics and Engineering*, 134(3):351–373, 1996.

[25] P. Zhao, J. C. Heinrich, and D. R. Poirier. Numerical modeling of fluid–particle interactions. *Computer methods in applied mechanics and engineering*, 195(41):5780–5796, 2006.

[26] J. L. Guermond, P. Minev, and J. Shen. An overview of projection methods for incompressible flows. *Computer methods in applied mechanics and engineering*, 195(44):6011–6045, 2006.

[27] J. C. Heinrich and D. W. Pepper. *Intermediate Finite Element Methods: Heat Transfer and Fluid Flow Applications*. Taylor and Francis, Philadelphia, USA, 1999.

[28] S. Badia and R. Codina. Analysis of a stabilized finite element approximation of the transient convection-diffusion equation using an ALE framework. *SIAM Journal on Numerical Analysis*, 44(5):2159–2197, 2006.

[29] L. Quartapellei. *Numerical solution of the incompressible Navier-Stokes equations*, volume 113. Springer, Birkhauser, Basel, 1993.

[30] R. Aris. *Vectors, tensors and the basic equations of fluid mechanics*. Courier Dover Publications, New York, USA, 1962.

[31] K-J Bathe. *Finite Element Procedures in Engineering Analysis*. Prentice-Hall, Englewood Cliffs, New Jersey, USA, 1982.

[32] G. Strang and G. J. Fix. *An Analysis of the Finite Element Method*. Prentice-Hall, Englewood Cliffs, New Jersey, USA, 1973.

[33] G. F. Carey and J. T. Oden. *Finite Elements, Vol. VI, Fluid Mechanics.* Prentice-Hall, Englewood Cliffs, New Jersey, USA, 1986.

[34] P. Drazin and N. Riley. *The Navier-Stokes equations: a classification of flows and exact solutions.* Number 334. Cambridge University Press, 2006.

[35] D. Muoz. A fixed mesh ALE method for flow calculations in fluid domains containing moving boundaries. M.S. report, University of New Mexico, Department of Mechanical Engineering, Albuquerque, NM, USA, 2010.

Appendices

Appendix A

Truncation Error

A.1 Trncation Error

Local truncation error represents the difference between an exact differential equation and its Finite Difference representation at a point in space and time. Local truncation error provides a basis for comparing local accuracies of various difference schemes.

As an example, the local truncation error of a forward in time and central in space approach to equation

$$\frac{\partial U}{\partial t} - \frac{\partial^2 U}{\partial x^2} = 0 \tag{A.1}$$

with

$$FD = \frac{u_i^{n+1} - u_i^n}{\Delta t} - \frac{u_{i-1}^n - 2u_i^n + u_{i+1}^n}{(\Delta x)^2} = 0 \tag{A.2}$$

where u_{ij} denotes the numerical approximation of exact value U at (x_i, y_j) is

$$LTE = \frac{U_i^{n+1} - U_i^n}{\Delta t} - \frac{U_{i-1}^n - 2U_i^n + U_{i+1}^n}{(\Delta x)^2} = 0 \tag{A.3}$$

Using Taylor expansions, the expression for LTE is

$$\begin{aligned} LTE = &\left(\frac{\partial U}{\partial t} - \frac{\partial^2 U}{\partial x^2}\right)_i^n + \frac{\Delta t}{2}\left(\frac{\partial^2 U}{\partial t^2}\right)_i^n - \frac{(\Delta x)^2}{12}\left(\frac{\partial^4 U}{\partial x^4}\right)_i^n \\ &+ \frac{(\Delta t)^2}{6}\left(\frac{\partial^3 U}{\partial t^3}\right)_i^n - \frac{(\Delta x)^4}{360}\left(\frac{\partial^4 U}{\partial x^6}\right)_i^n + \cdots \end{aligned} \tag{A.4}$$

As U is the solution to the differential equation

$$\left(\frac{\partial U}{\partial t} - \frac{\partial^2 U}{\partial x^2}\right)_i^n = 0 \tag{A.5}$$

the local truncation error is

$$LTE = \frac{\Delta t}{2}\left(\frac{\partial^2 U}{\partial t^2}\right)_i^n - \frac{(\Delta x)^2}{12}\left(\frac{\partial^4 U}{\partial x^4}\right)_i^n + \cdots \tag{A.6}$$

A.2 Taylor Expansions

The general Taylor expansions used in this study are given as:

Two dimensional expansions are

$$\begin{aligned} \phi_{i+1j+1} = \phi_{ij} &+ \left(\Delta x(\phi_{ij})_x + \Delta y(\phi_{ij})_y\right) + \frac{1}{2!}\left(\Delta x^2(\phi_{ij})_{xx} + 2\Delta x\Delta y(\phi_{ij})_{xy} + \Delta y^2(\phi_{ij})_{yy}\right) \\ &+ \frac{1}{3!}\left(\Delta x^3(\phi_{ij})_{xxx} + 3\Delta x^2\Delta y(\phi_{ij})_{xxy} + 3\Delta x\Delta y^2(\phi_{ij})_{xyy} + \Delta y^3(\phi_{ij})_{yyy}\right) \\ &+ O\left(\Delta x^4,\ \Delta x^3\Delta y,\ \Delta x^2\Delta y^2,\ \Delta x\Delta y^3,\ \Delta y^4\right) \end{aligned} \tag{A.7}$$

and

$$\begin{aligned} \phi_{i-1j-1} = \phi_{ij} &- \left(\Delta x(\phi_{ij})_x + \Delta y(\phi_{ij})_y\right) + \frac{1}{2!}\left(\Delta x^2(\phi_{ij})_{xx} + 2\Delta x\Delta y(\phi_{ij})_{xy} + \Delta y^2(\phi_{ij})_{yy}\right) \\ &- \frac{1}{3!}\left(\Delta x^3(\phi_{ij})_{xxx} + 3\Delta x^2\Delta y(\phi_{ij})_{xxy} + 3\Delta x\Delta y^2(\phi_{ij})_{xyy} + \Delta y^3(\phi_{ij})_{yyy}\right) \\ &+ O\left(\Delta x^4,\ \Delta x^3\Delta y,\ \Delta x^2\Delta y^2,\ \Delta x\Delta y^3,\ \Delta y^4\right) \end{aligned} \tag{A.8}$$

Three dimensional expansions are

$$\begin{aligned}
\phi_{i-1j-1k-1} &= \phi_{ijk} - \Big(h_1(\phi_{ijk})_x + k_1(\phi_{ijk})_y + l_1(\phi_{ijk})_z\Big) \\
&+\frac{1}{2!}\begin{pmatrix} h_1{}^2(\phi_{ijk})_{xx} + 2h_1k_1(\phi_{ijk})_{xy} + 2h_1l_1(\phi_{ijk})_{xz} \\ +k_1{}^2(\phi_{ijk})_{yy} + 2k_1l_1(\phi_{ijk})_{yz} + l_1{}^2(\phi_{ijk})_{zz} \end{pmatrix} \\
&-\frac{1}{3!}\begin{pmatrix} h_1{}^3(\phi_{ijk})_{xxx} + 3h_1{}^2k_1(\phi_{ijk})_{xxy} + 3h_1{}^2l_1(\phi_{ijk})_{xxz} \\ +3h_1k_1{}^2(\phi_{ijk})_{xyy} + 6h_1k_1l_1(\phi_{ijk})_{xyz} + 3h_1l_1{}^2(\phi_{ijk})_{xzz} \\ +k_1{}^3(\phi_{ijk})_{yyy} + 3k_1{}^2l_1(\phi_{ijk})_{yyz} + 3k_1l_1{}^2(\phi_{ijk})_{yzz} + l_1{}^3(\phi_{ijk})_{zzz} \end{pmatrix}
\end{aligned} \tag{A.9}$$

and

$$\begin{aligned}
\phi_{i+1j+1k+1} &= \phi_{ijk} + \Big(h_2(\phi_{ijk})_x + k_2(\phi_{ijk})_y + l_2(\phi_{ijk})_z\Big) \\
&+\frac{1}{2!}\begin{pmatrix} h_2{}^2(\phi_{ijk})_{xx} + 2h_2k_2(\phi_{ijk})_{xy} + 2h_2l_2(\phi_{ijk})_{xz} \\ +k_2{}^2(\phi_{ijk})_{yy} + 2k_2l_2(\phi_{ijk})_{yz} + l_2{}^2(\phi_{ijk})_{zz} \end{pmatrix} \\
&+\frac{1}{3!}\begin{pmatrix} h_2{}^3(\phi_{ijk})_{xxx} + 3h_2{}^2k_2(\phi_{ijk})_{xxy} + 3h_2{}^2l_2(\phi_{ijk})_{xxz} \\ +3h_2k_2{}^2(\phi_{ijk})_{xyy} + 6h_2k_2l_2(\phi_{ijk})_{xyz} + 3h_2l_2{}^2(\phi_{ijk})_{xzz} \\ +k_2{}^3(\phi_{ijk})_{yyy} + 3k_2{}^2l_2(\phi_{ijk})_{yyz} + 3k_2l_2{}^2(\phi_{ijk})_{yzz} + l_2{}^3(\phi_{ijk})_{zzz} \end{pmatrix}
\end{aligned} \tag{A.10}$$

These are general Taylor expansions. The rest of the Taylor expansions can be calculated by using these equations and setting the proper value for $\Delta x, \Delta y or \Delta z$ depends on the problem.

Appendix B

Convection-Diffusion Truncation Error Analysis

B.1 2-D Domain

Assume that the convective velocity field $\mathbf{u} = (u, v)^T$ is known and constant.

The weak weighted residuals formulation of equation 4.1 gives

$$\int_{\Omega\ t} \left\{ \mathbf{w} \cdot \left[\frac{\partial \phi}{\partial t} + (\mathbf{u} \cdot \nabla)\phi^n \right] + D \left(\nabla \mathbf{w} . \nabla \phi^{n+1} \right) \right\} d\Omega = 0 \tag{B.1}$$

Where $\mathbf{w}$ denotes the weighting functions.
The ϕ is discretized over the space as:

$$\phi\left(x, y, t\right) \cong \sum_{i=1}^{n} N_i\left(x, y\right) \phi_i\left(t\right) \tag{B.2}$$

Where N_i are the shape functions over each element, and n is the number of nodes in an element, in this two dimensional case $n = 4$. The weighting functions w_i are set to be equal to shape functions N_i. the final form of the equation B.1 is

$$\begin{aligned}
&\int_0^{\Delta y}\int_0^{\Delta x} N_i \sum_{j=1}^{4} N_j \frac{\partial \phi_j}{\partial t} dxdy \\
&+\int_0^{\Delta y}\int_0^{\Delta x}\left(uN_i\sum_{j=1}^{4}\left(\frac{\partial N_j}{\partial x}\phi_j^n\right)+vN_i\sum_{j=1}^{4}\left(\frac{\partial N_j}{\partial y}\phi_j^n\right)\right)dxdy \\
&+\int_0^{\Delta y}\int_0^{\Delta x} D\left(\frac{\partial N_i}{\partial x}\sum_{j=1}^{4}\left(\frac{\partial N_j}{\partial x}\phi_j^{n+1}\right)+\frac{\partial N_i}{\partial y}\sum_{j=1}^{4}\left(\frac{\partial N_j}{\partial y}\phi_j^{n+1}\right)\right)dxdy = 0
\end{aligned} \tag{B.3}$$

Another representation of equation B.3 is

$$\begin{aligned}
&\sum_{j=1}^{4}\int_0^{\Delta y}\int_0^{\Delta x} N_i N_j \frac{\partial \phi_j}{\partial t} dxdy \\
&+u\sum_{j=1}^{4}\int_0^{\Delta y}\int_0^{\Delta x} N_i \frac{\partial N_j}{\partial x}\phi_j^n dxdy + v\sum_{j=1}^{4}\int_0^{\Delta y}\int_0^{\Delta x} N_i \frac{\partial N_j}{\partial y}\phi_j^n dxdy \\
&+D\sum_{j=1}^{4}\int_0^{\Delta y}\int_0^{\Delta x}\frac{\partial N_i}{\partial x}\frac{\partial N_j}{\partial x}\phi_j^{n+1}dxdy + D\sum_{j=1}^{4}\int_0^{\Delta y}\int_0^{\Delta x}\frac{\partial N_i}{\partial y}\frac{\partial N_j}{\partial y}\phi_j^{n+1}dxdy = 0
\end{aligned}$$

(B.4)

The shape functions according to figure 4.1(a) are

$$\begin{cases}
N_1 = \left(1-\frac{x}{h}\right)\left(1-\frac{y}{k}\right) \\
N_2 = \left(\frac{x}{h}\right)\left(1-\frac{y}{k}\right) \\
N_3 = \left(1-\frac{x}{h}\right)\left(\frac{y}{k}\right) \\
N_4 = \left(\frac{x}{h}\right)\left(\frac{y}{k}\right)
\end{cases} \tag{B.5}$$

The next task is to calculate the stiffness matrix of an element. By calculating the stiffness matrices the equation B.4 can be written as:

$$S_{ij}^{11}\dot{\phi}_j + S_{ij}^{22}\phi_j^n + S_{ij}^{33}\phi_j^n + S_{ij}^{44}\phi_j^{n+1} + S_{ij}^{55}\phi_j^{n+1} = 0 \tag{B.6}$$

Where S^{mm} are stiffness matrices calculated as

$$S^{11}_{ij} = \frac{\Delta x \Delta y}{36}\begin{bmatrix} 4 & 2 & 1 & 2 \\ 2 & 4 & 2 & 1 \\ 1 & 2 & 4 & 2 \\ 2 & 1 & 2 & 4 \end{bmatrix},\ S^{22}_{ij} = \frac{\mathbf{u}\Delta y}{12}\begin{bmatrix} -2 & 2 & 1 & -1 \\ -2 & 2 & 1 & -1 \\ -1 & 1 & 2 & -2 \\ -1 & 1 & 2 & -2 \end{bmatrix},$$

$$S^{33}_{ij} = \frac{\mathbf{v}\Delta x}{12}\begin{bmatrix} -2 & -1 & 1 & 2 \\ -1 & -2 & 2 & 1 \\ -1 & -2 & 2 & 1 \\ -2 & -1 & 1 & 2 \end{bmatrix},\ S^{44}_{ij} = D\frac{\Delta y}{6\Delta x}\begin{bmatrix} 2 & -2 & -1 & 1 \\ -2 & 2 & 1 & -1 \\ -1 & 1 & 2 & -2 \\ 1 & -1 & -2 & 2 \end{bmatrix},\text{ and}$$

$$S^{55}_{ij} = D\frac{\Delta x}{6\Delta y}\begin{bmatrix} 2 & 1 & -1 & -2 \\ 1 & 2 & -2 & -1 \\ -1 & -2 & 2 & 1 \\ -2 & -1 & 1 & 2 \end{bmatrix}$$

The most commonly time integration algorithm normally referring to as the θ method is used. It consists in approximating the time derivative by the backward difference

$$\dot{\phi} \cong \frac{1}{\Delta t}\left(\phi^{n+1} - \phi^{n}\right) \tag{B.7}$$

The transport quantity, ϕ, is then defined by

$$\phi = \theta\,\phi^{n+1} + (1-\theta)\,\phi^{n} \tag{B.8}$$

in this analysis the relaxation parameter is $\theta = 1$ and, as a result, $\phi = \phi^{n+1}$.

The element equation written for the first element using the notation in figure

4.1 is

$$
\begin{aligned}
&\left\{ \frac{h_1 k_1}{36\Delta t} \begin{bmatrix} 4 & 2 & 1 & 2 \\ 2 & 4 & 2 & 1 \\ 1 & 2 & 4 & 2 \\ 2 & 1 & 2 & 4 \end{bmatrix} + \frac{D k_1}{6 h_1} \begin{bmatrix} 2 & -2 & -1 & 1 \\ -2 & 2 & 1 & -1 \\ -1 & 1 & 2 & -2 \\ 1 & -1 & -2 & 2 \end{bmatrix} + \frac{D h_1}{6 k_1} \begin{bmatrix} 2 & 1 & -1 & -2 \\ 1 & 2 & -2 & -1 \\ -1 & -2 & 2 & 1 \\ -2 & -1 & 1 & 2 \end{bmatrix} \right\} \begin{bmatrix} \phi^{n+1}_{i-1j-1} \\ \phi^{n+1}_{ij-1} \\ \phi^{n+1}_{ij} \\ \phi^{n+1}_{i-1j} \end{bmatrix} = \\
&\left\{ -\frac{u k_1}{12} \begin{bmatrix} -2 & 2 & 1 & -1 \\ -2 & 2 & 1 & -1 \\ -1 & 1 & 2 & -2 \\ -1 & 1 & 2 & -2 \end{bmatrix} - \frac{v h_1}{12} \begin{bmatrix} -2 & -1 & 1 & 2 \\ -1 & -2 & 2 & 1 \\ -1 & -2 & 2 & 1 \\ -2 & -1 & 1 & 2 \end{bmatrix} + \frac{h_1 k_1}{36\Delta t} \begin{bmatrix} 4 & 2 & 1 & 2 \\ 2 & 4 & 2 & 1 \\ 1 & 2 & 4 & 2 \\ 2 & 1 & 2 & 4 \end{bmatrix} \right\} \begin{bmatrix} \phi^{n}_{i-1j-1} \\ \phi^{n}_{ij-1} \\ \phi^{n}_{ij} \\ \phi^{n}_{i-1j} \end{bmatrix}
\end{aligned}
\tag{B.9}
$$

for the second element the equation is

$$
\begin{aligned}
&\left\{ \frac{h_2 k_1}{36\Delta t} \begin{bmatrix} 4 & 2 & 1 & 2 \\ 2 & 4 & 2 & 1 \\ 1 & 2 & 4 & 2 \\ 2 & 1 & 2 & 4 \end{bmatrix} + \frac{D k_1}{6 h_2} \begin{bmatrix} 2 & -2 & -1 & 1 \\ -2 & 2 & 1 & -1 \\ -1 & 1 & 2 & -2 \\ 1 & -1 & -2 & 2 \end{bmatrix} + \frac{D h_2}{6 k_1} \begin{bmatrix} 2 & 1 & -1 & -2 \\ 1 & 2 & -2 & -1 \\ -1 & -2 & 2 & 1 \\ -2 & -1 & 1 & 2 \end{bmatrix} \right\} \begin{bmatrix} \phi^{n+1}_{ij-1} \\ \phi^{n+1}_{i+1j-1} \\ \phi^{n+1}_{i+1j} \\ \phi^{n+1}_{ij} \end{bmatrix} = \\
&\left\{ -\frac{u k_1}{12} \begin{bmatrix} -2 & 2 & 1 & -1 \\ -2 & 2 & 1 & -1 \\ -1 & 1 & 2 & -2 \\ -1 & 1 & 2 & -2 \end{bmatrix} - \frac{v h_2}{12} \begin{bmatrix} -2 & -1 & 1 & 2 \\ -1 & -2 & 2 & 1 \\ -1 & -2 & 2 & 1 \\ -2 & -1 & 1 & 2 \end{bmatrix} + \frac{h_2 k_1}{36\Delta t} \begin{bmatrix} 4 & 2 & 1 & 2 \\ 2 & 4 & 2 & 1 \\ 1 & 2 & 4 & 2 \\ 2 & 1 & 2 & 4 \end{bmatrix} \right\} \begin{bmatrix} \phi^{n}_{ij-1} \\ \phi^{n}_{i+1j-1} \\ \phi^{n}_{i+1j} \\ \phi^{n}_{ij} \end{bmatrix}
\end{aligned}
\tag{B.10}
$$

the equation for the third element is

$$
\begin{aligned}
&\left\{ \frac{h_1 k_2}{36\Delta t} \begin{bmatrix} 4 & 2 & 1 & 2 \\ 2 & 4 & 2 & 1 \\ 1 & 2 & 4 & 2 \\ 2 & 1 & 2 & 4 \end{bmatrix} + \frac{D k_2}{6 h_1} \begin{bmatrix} 2 & -2 & -1 & 1 \\ -2 & 2 & 1 & -1 \\ -1 & 1 & 2 & -2 \\ 1 & -1 & -2 & 2 \end{bmatrix} + \frac{D h_1}{6 k_2} \begin{bmatrix} 2 & 1 & -1 & -2 \\ 1 & 2 & -2 & -1 \\ -1 & -2 & 2 & 1 \\ -2 & -1 & 1 & 2 \end{bmatrix} \right\} \begin{bmatrix} \phi^{n+1}_{i-1j} \\ \phi^{n+1}_{ij} \\ \phi^{n+1}_{ij+1} \\ \phi^{n+1}_{i-1j+1} \end{bmatrix} = \\
&\left\{ -\frac{u k_2}{12} \begin{bmatrix} -2 & 2 & 1 & -1 \\ -2 & 2 & 1 & -1 \\ -1 & 1 & 2 & -2 \\ -1 & 1 & 2 & -2 \end{bmatrix} - \frac{v h_1}{12} \begin{bmatrix} -2 & -1 & 1 & 2 \\ -1 & -2 & 2 & 1 \\ -1 & -2 & 2 & 1 \\ -2 & -1 & 1 & 2 \end{bmatrix} + \frac{h_1 k_2}{36\Delta t} \begin{bmatrix} 4 & 2 & 1 & 2 \\ 2 & 4 & 2 & 1 \\ 1 & 2 & 4 & 2 \\ 2 & 1 & 2 & 4 \end{bmatrix} \right\} \begin{bmatrix} \phi^{n}_{i-1j} \\ \phi^{n}_{ij} \\ \phi^{n}_{ij+1} \\ \phi^{n}_{i-1j+1} \end{bmatrix}
\end{aligned}
\tag{B.11}
$$

and the equation for the final element is

$$
\begin{aligned}
&\left\{ \frac{h_2 k_2}{36\Delta t} \begin{bmatrix} 4 & 2 & 1 & 2 \\ 2 & 4 & 2 & 1 \\ 1 & 2 & 4 & 2 \\ 2 & 1 & 2 & 4 \end{bmatrix} + \frac{D k_2}{6 h_2} \begin{bmatrix} 2 & -2 & -1 & 1 \\ -2 & 2 & 1 & -1 \\ -1 & 1 & 2 & -2 \\ 1 & -1 & -2 & 2 \end{bmatrix} + \frac{D h_2}{6 k_2} \begin{bmatrix} 2 & 1 & -1 & -2 \\ 1 & 2 & -2 & -1 \\ -1 & -2 & 2 & 1 \\ -2 & -1 & 1 & 2 \end{bmatrix} \right\} \begin{bmatrix} \phi^{n+1}_{ij} \\ \phi^{n+1}_{i+1j} \\ \phi^{n+1}_{i+1j+1} \\ \phi^{n+1}_{ij+1} \end{bmatrix} = \\
&\left\{ -\frac{u k_2}{12} \begin{bmatrix} -2 & 2 & 1 & -1 \\ -2 & 2 & 1 & -1 \\ -1 & 1 & 2 & -2 \\ -1 & 1 & 2 & -2 \end{bmatrix} - \frac{v h_2}{12} \begin{bmatrix} -2 & -1 & 1 & 2 \\ -1 & -2 & 2 & 1 \\ -1 & -2 & 2 & 1 \\ -2 & -1 & 1 & 2 \end{bmatrix} + \frac{h_2 k_2}{36\Delta t} \begin{bmatrix} 4 & 2 & 1 & 2 \\ 2 & 4 & 2 & 1 \\ 1 & 2 & 4 & 2 \\ 2 & 1 & 2 & 4 \end{bmatrix} \right\} \begin{bmatrix} \phi^{n}_{ij} \\ \phi^{n}_{i+1j} \\ \phi^{n}_{i+1j+1} \\ \phi^{n}_{ij+1} \end{bmatrix}
\end{aligned}
\tag{B.12}
$$

Assembling the element equation contributions to node (x_i, y_i) results in the difference equation (DE)

$$
\begin{aligned}
DE \equiv &+\frac{k_1}{36\Delta t}\left(h_1\phi^{n+1}_{i-1\,j-1} + 2\left(h_1+h_2\right)\phi^{n+1}_{i\,j-1} + h_2\phi^{n+1}_{i+1\,j-1}\right)\\
&-\frac{k_1}{36\Delta t}\left(h_1\phi^{n}_{i-1\,j-1} + 2\left(h_1+h_2\right)\phi^{n}_{i\,j-1} + h_2\phi^{n}_{i+1\,j-1}\right)\\
&+\frac{(k_1+k_2)}{36\Delta t}\left(2h_1\phi^{n+1}_{i-1\,j} + 4\left(h_1+h_2\right)\phi^{n+1}_{i\,j} + 2h_2\phi^{n+1}_{i+1\,j}\right)\\
&-\frac{(k_1+k_2)}{36\Delta t}\left(2h_1\phi^{n}_{i-1\,j} + 4\left(h_1+h_2\right)\phi^{n}_{i\,j} + 2h_2\phi^{n}_{i+1\,j}\right)\\
&+\frac{k_2}{36\Delta t}\left(h_1\phi^{n+1}_{i-1\,j+1} + 2\left(h_1+h_2\right)\phi^{n+1}_{i\,j+1} + h_2\phi^{n+1}_{i+1\,j+1}\right)\\
&-\frac{k_2}{36\Delta t}\left(h_1\phi^{n}_{i-1\,j+1} + 2\left(h_1+h_2\right)\phi^{n}_{i\,j+1} + h_2\phi^{n}_{i+1\,j+1}\right)\\
&+\frac{vh_1}{12}\left(2\phi^n_{ij+1} + \phi^n_{i-1j+1} - \phi^n_{i-1j-1} - 2\phi^n_{ij-1}\right)\\
&+\frac{vh_2}{12}\left(\phi^n_{i+1j+1} + 2\phi^n_{ij+1} - 2\phi^n_{ij-1} - \phi^n_{i+1j-1}\right)\\
&+\frac{uk_2}{12}\left(\phi^n_{i+1j+1} + 2\phi^n_{i+1j} - 2\phi^n_{i-1j} - \phi^n_{i-1j+1}\right)\\
&+\frac{uk_1}{12}\left(2\phi^n_{i+1j} + \phi^n_{i+1j-1} - \phi^n_{i-1j-1} - 2\phi^n_{i-1j}\right)\\
&+\frac{D}{6h_1}\left(k_1\left(\phi^{n+1}_{i\,j-1} - \phi^{n+1}_{i-1\,j-1}\right) + 2\left(k_1+k_2\right)\left(\phi^{n+1}_{i\,j} - \phi^{n+1}_{i-1\,j}\right) + k_2\left(\phi^{n+1}_{i\,j+1} - \phi^{n+1}_{i-1\,j+1}\right)\right)\\
&+\frac{D}{6h_2}\left(k_1\left(\phi^{n+1}_{i\,j-1} - \phi^{n+1}_{i+1\,j-1}\right) + 2\left(k_1+k_2\right)\left(\phi^{n+1}_{i\,j} - \phi^{n+1}_{i+1\,j}\right) + k_2\left(\phi^{n+1}_{i\,j+1} - \phi^{n+1}_{i+1\,j+1}\right)\right)\\
&+\frac{D}{6k_1}\left(h_1\left(\phi^{n+1}_{i-1\,j} - \phi^{n+1}_{i-1\,j-1}\right) + 2\left(h_1+h_2\right)\left(\phi^{n+1}_{i\,j} - \phi^{n+1}_{i\,j-1}\right) + h_2\left(\phi^{n+1}_{i+1\,j} - \phi^{n+1}_{i+1\,j-1}\right)\right)\\
&+\frac{D}{6k_2}\left(h_1\left(\phi^{n+1}_{i-1\,j} - \phi^{n+1}_{i-1\,j+1}\right) + 2\left(h_1+h_2\right)\left(\phi^{n+1}_{i\,j} - \phi^{n+1}_{i\,j+1}\right) + h_2\left(\phi^{n+1}_{i+1\,j} - \phi^{n+1}_{i+1\,j+1}\right)\right)
\end{aligned}
\tag{B.13}
$$

All the terms in DE are expanded in Taylor series about $\phi^{n+1}_{i\,j}$. For example:

$$
\begin{aligned}
\phi_{i+1j+1} = \phi_{ij} &+ \left(\Delta x(\phi_{ij})_x + \Delta y(\phi_{ij})_y\right) + \frac{1}{2!}\left(\Delta x^2(\phi_{ij})_{xx} + 2\Delta x\Delta y(\phi_{ij})_{xy} + \Delta y^2(\phi_{ij})_{yy}\right)\\
&+\frac{1}{3!}\left(\Delta x^3(\phi_{ij})_{xxx} + 3\Delta x^2\Delta y(\phi_{ij})_{xxy} + 3\Delta x\Delta y^2(\phi_{ij})_{xyy} + \Delta y^3(\phi_{ij})_{yyy}\right)\\
&+O\left(\Delta x^4,\ \Delta x^3\Delta y,\ \Delta x^2\Delta y^2,\ \Delta x\Delta y^3,\ \Delta y^4\right)
\end{aligned}
$$

and

$$\begin{aligned}\phi_{i-1j-1} = \phi_{ij} &- \Big(\Delta x(\phi_{ij})_x + \Delta y(\phi_{ij})_y\Big) + \frac{1}{2!}\Big(\Delta x^2(\phi_{ij})_{xx} + 2\Delta x\Delta y(\phi_{ij})_{xy} + \Delta y^2(\phi_{ij})_{yy}\Big)\\ &- \frac{1}{3!}\Big(\Delta x^3(\phi_{ij})_{xxx} + 3\Delta x^2\Delta y(\phi_{ij})_{xxy} + 3\Delta x\Delta y^2(\phi_{ij})_{xyy} + \Delta y^3(\phi_{ij})_{yyy}\Big)\\ &+O\left(\Delta x^4,\ \Delta x^3\Delta y,\ \Delta x^2\Delta y^2,\ \Delta x\Delta y^3,\ \Delta y^4\right)\end{aligned}$$

The diffusion terms, convection terms, and time derivative terms in equation B.13 are shown respectively on the following pages. First, the diffusion parts have been shown in two parts about ϕ_{ij}^{n+1} are

$$\begin{aligned}&\frac{Dk_2}{6h_1}\left(-2\phi_{i-1j}^{n+1} + 2\phi_{ij}^{n+1} + \phi_{ij+1}^{n+1} - \phi_{i-1j+1}^{n+1}\right)\\ +&\frac{Dk_2}{6h_2}\left(2\phi_{ij}^{n+1} - 2\phi_{i+1j}^{n+1} - \phi_{i+1j+1}^{n+1} + \phi_{ij+1}^{n+1}\right)\\ +&\frac{Dk_1}{6h_1}\left(-\phi_{i-1j-1}^{n+1} + \phi_{ij-1}^{n+1} + 2\phi_{ij}^{n+1} - 2\phi_{i-1j}^{n+1}\right)\\ +&\frac{Dk_1}{6h_2}\left(\phi_{ij-1}^{n+1} - \phi_{i+1j-1}^{n+1} - 2\phi_{i+1j}^{n+1} + 2\phi_{ij}^{n+1}\right) =\\ -D&\left(\begin{array}{l} -\frac{k_2}{2}\left(\phi_{ij}^{n+1}\right)_x + \frac{k_2}{2}\left(\phi_{ij}^{n+1}\right)_x - \frac{k_1}{2}\left(\phi_{ij}^{n+1}\right)_x + \frac{k_1}{2}\left(\phi_{ij}^{n+1}\right)_x\\ + \left(\begin{array}{l} \frac{k_2h_1}{4}\left(\phi_{ij}^{n+1}\right)_{xx} - \frac{{k_2}^2}{6}\left(\phi_{ij}^{n+1}\right)_{xy} + \frac{k_2h_2}{4}\left(\phi_{ij}^{n+1}\right)_{xx} + \frac{{k_2}^2}{6}\left(\phi_{ij}^{n+1}\right)_{xy}\\ +\frac{k_1h_1}{4}\left(\phi_{ij}^{n+1}\right)_{xx} + \frac{{k_1}^2}{6}\left(\phi_{ij}^{n+1}\right)_{xy} + \frac{k_1h_2}{4}\left(\phi_{ij}^{n+1}\right)_{xx} - \frac{{k_1}^2}{6}\left(\phi_{ij}^{n+1}\right)_{xy} \end{array}\right)\\ + \left(\begin{array}{l} -\frac{1}{2}\frac{k_2{h_1}^2}{3!}\left(\phi_{ij}^{n+1}\right)_{xxx} + \frac{1}{2}\frac{h_1{k_2}^2}{3!}\left(\phi_{ij}^{n+1}\right)_{xxy} - \frac{1}{2}\frac{{k_2}^3}{3!}\left(\phi_{ij}^{n+1}\right)_{xyy}\\ +\frac{1}{2}\frac{k_2{h_2}^2}{3!}\left(\phi_{ij}^{n+1}\right)_{xxx} + \frac{1}{2}\frac{h_2{k_2}^2}{3!}\left(\phi_{ij}^{n+1}\right)_{xxy} + \frac{1}{2}\frac{{k_2}^3}{3!}\left(\phi_{ij}^{n+1}\right)_{xyy}\\ -\frac{1}{2}\frac{k_1{h_1}^2}{3!}\left(\phi_{ij}^{n+1}\right)_{xxx} - \frac{1}{2}\frac{h_1{k_1}^2}{3!}\left(\phi_{ij}^{n+1}\right)_{xxy} - \frac{1}{2}\frac{{k_1}^3}{3!}\left(\phi_{ij}^{n+1}\right)_{xyy}\\ +\frac{1}{2}\frac{k_1{h_2}^2}{3!}\left(\phi_{ij}^{n+1}\right)_{xxx} - \frac{1}{2}\frac{h_2{k_1}^2}{3!}\left(\phi_{ij}^{n+1}\right)_{xxy} + \frac{1}{2}\frac{{k_1}^3}{3!}\left(\phi_{ij}^{n+1}\right)_{xyy} \end{array}\right) \end{array}\right)\end{aligned} \tag{B.14}$$

and

$$
\begin{aligned}
&\frac{Dh_1}{6k_2}\left(\phi^{n+1}_{i-1j} + 2\phi^{n+1}_{ij} - 2\phi^{n+1}_{ij+1} - \phi^{n+1}_{i-1j+1}\right)\\
&+\frac{Dh_2}{6k_2}\left(2\phi^{n+1}_{ij} + \phi^{n+1}_{i+1j} - \phi^{n+1}_{i+1j+1} - 2\phi^{n+1}_{ij+1}\right)\\
&+\frac{Dh_1}{6k_1}\left(-\phi^{n+1}_{i-1j-1} - 2\phi^{n+1}_{ij-1} + 2\phi^{n+1}_{ij} + \phi^{n+1}_{i-1j}\right)\\
&+\frac{Dh_2}{6k_1}\left(-2\phi^{n+1}_{ij-1} - \phi^{n+1}_{i+1j-1} + \phi^{n+1}_{i+1j} + 2\phi^{n+1}_{ij}\right) =\\
&-D\begin{pmatrix}
+\frac{h_1}{2}\left(\phi^{n+1}_{ij}\right)_y + \frac{h_2}{2}\left(\phi^{n+1}_{ij}\right)_y - \frac{h_1}{2}\left(\phi^{n+1}_{ij}\right)_y - \frac{h_2}{2}\left(\phi^{n+1}_{ij}\right)_y\\
+\begin{pmatrix}
\frac{h_1k_2}{4}\left(\phi^{n+1}_{ij}\right)_{yy} - \frac{h_1^2}{6}\left(\phi^{n+1}_{ij}\right)_{xy} + \frac{h_2k_2}{4}\left(\phi^{n+1}_{ij}\right)_{yy} + \frac{h_2^2}{6}\left(\phi^{n+1}_{ij}\right)_{xy}\\
+\frac{h_1k_1}{4}\left(\phi^{n+1}_{ij}\right)_{yy} + \frac{h_1^2}{6}\left(\phi^{n+1}_{ij}\right)_{xy} + \frac{h_2k_1}{4}\left(\phi^{n+1}_{ij}\right)_{yy} - \frac{h_2^2}{6}\left(\phi^{n+1}_{ij}\right)_{xy}
\end{pmatrix}\\
+\begin{pmatrix}
+\frac{1}{2}\frac{h_1k_2^2}{3!}\left(\phi^{n+1}_{ij}\right)_{yyy} + \frac{1}{2}\frac{h_1^3}{3!}\left(\phi^{n+1}_{ij}\right)_{xxy} - \frac{1}{2}\frac{h_1^2k_2}{3!}\left(\phi^{n+1}_{ij}\right)_{xyy}\\
+\frac{1}{2}\frac{h_2k_2^2}{3!}\left(\phi^{n+1}_{ij}\right)_{yyy} + \frac{1}{2}\frac{h_2^3}{3!}\left(\phi^{n+1}_{ij}\right)_{xxy} + \frac{1}{2}\frac{h_2^2k_2}{3!}\left(\phi^{n+1}_{ij}\right)_{xyy}\\
-\frac{1}{2}\frac{h_1k_1^2}{3!}\left(\phi^{n+1}_{ij}\right)_{yyy} - \frac{1}{2}\frac{h_1^3}{3!}\left(\phi^{n+1}_{ij}\right)_{xxy} - \frac{1}{2}\frac{h_1^2k_1}{3!}\left(\phi^{n+1}_{ij}\right)_{xyy}\\
-\frac{1}{2}\frac{h_2k_1^2}{3!}\left(\phi^{n+1}_{ij}\right)_{yyy} - \frac{1}{2}\frac{h_2^3}{3!}\left(\phi^{n+1}_{ij}\right)_{xxy} + \frac{1}{2}\frac{h_2^2k_1}{3!}\left(\phi^{n+1}_{ij}\right)_{xyy}
\end{pmatrix}
\end{pmatrix}
\end{aligned}
\tag{B.15}
$$

The summation of diffusion terms is

$$
\begin{aligned}
&+\frac{D}{6h_1}\left(k_1\left(\phi^{n+1}_{i\,j-1}-\phi^{n+1}_{i-1\,j-1}\right)+2\left(k_1+k_2\right)\left(\phi^{n+1}_{i\,j}-\phi^{n+1}_{i-1\,j}\right)+k_2\left(\phi^{n+1}_{i\,j+1}-\phi^{n+1}_{i-1\,j+1}\right)\right)\\
&+\frac{D}{6h_2}\left(k_1\left(\phi^{n+1}_{i\,j-1}-\phi^{n+1}_{i+1\,j-1}\right)+2\left(k_1+k_2\right)\left(\phi^{n+1}_{i\,j}-\phi^{n+1}_{i+1\,j}\right)+k_2\left(\phi^{n+1}_{i\,j+1}-\phi^{n+1}_{i+1\,j+1}\right)\right)\\
&+\frac{D}{6k_1}\left(h_1\left(\phi^{n+1}_{i-1\,j}-\phi^{n+1}_{i-1\,j-1}\right)+2\left(h_1+h_2\right)\left(\phi^{n+1}_{i\,j}-\phi^{n+1}_{i\,j-1}\right)+h_2\left(\phi^{n+1}_{i+1\,j}-\phi^{n+1}_{i+1\,j-1}\right)\right)\\
&+\frac{D}{6k_2}\left(h_1\left(\phi^{n+1}_{i-1\,j}-\phi^{n+1}_{i-1\,j+1}\right)+2\left(h_1+h_2\right)\left(\phi^{n+1}_{i\,j}-\phi^{n+1}_{i\,j+1}\right)+h_2\left(\phi^{n+1}_{i+1\,j}-\phi^{n+1}_{i+1\,j+1}\right)\right)=\\
&-D\left(\begin{array}{l}
+\frac{h_1}{2}\left(\phi^{n+1}_{ij}\right)_y+\frac{h_2}{2}\left(\phi^{n+1}_{ij}\right)_y-\frac{h_1}{2}\left(\phi^{n+1}_{ij}\right)_y-\frac{h_2}{2}\left(\phi^{n+1}_{ij}\right)_y\\
-\frac{k_2}{2}\left(\phi^{n+1}_{ij}\right)_x+\frac{k_2}{2}\left(\phi^{n+1}_{ij}\right)_x-\frac{k_1}{2}\left(\phi^{n+1}_{ij}\right)_x+\frac{k_1}{2}\left(\phi^{n+1}_{ij}\right)_x\\
+\left(\begin{array}{l}
\frac{h_1k_2}{4}\left(\phi^{n+1}_{ij}\right)_{yy}-\frac{h_1^2}{6}\left(\phi^{n+1}_{ij}\right)_{xy}+\frac{h_2k_2}{4}\left(\phi^{n+1}_{ij}\right)_{yy}+\frac{h_2^2}{6}\left(\phi^{n+1}_{ij}\right)_{xy}\\
+\frac{h_1k_1}{4}\left(\phi^{n+1}_{ij}\right)_{yy}+\frac{h_1^2}{6}\left(\phi^{n+1}_{ij}\right)_{xy}+\frac{h_2k_1}{4}\left(\phi^{n+1}_{ij}\right)_{yy}-\frac{h_2^2}{6}\left(\phi^{n+1}_{ij}\right)_{xy}
\end{array}\right)\\
+\left(\begin{array}{l}
\frac{k_2h_1}{4}\left(\phi^{n+1}_{ij}\right)_{xx}-\frac{{k_2}^2}{6}\left(\phi^{n+1}_{ij}\right)_{xy}+\frac{k_2h_2}{4}\left(\phi^{n+1}_{ij}\right)_{xx}+\frac{{k_2}^2}{6}\left(\phi^{n+1}_{ij}\right)_{xy}\\
+\frac{k_1h_1}{4}\left(\phi^{n+1}_{ij}\right)_{xx}+\frac{{k_1}^2}{6}\left(\phi^{n+1}_{ij}\right)_{xy}+\frac{k_1h_2}{4}\left(\phi^{n+1}_{ij}\right)_{xx}-\frac{{k_1}^2}{6}\left(\phi^{n+1}_{ij}\right)_{xy}
\end{array}\right)\\
+\left(\begin{array}{l}
+\frac{1}{2}\frac{h_1k_2^2}{3!}\left(\phi^{n+1}_{ij}\right)_{yyy}+\frac{1}{2}\frac{h_1^3}{3!}\left(\phi^{n+1}_{ij}\right)_{xxy}-\frac{1}{2}\frac{h_1^2k_2}{3!}\left(\phi^{n+1}_{ij}\right)_{xyy}\\
+\frac{1}{2}\frac{h_2k_2^2}{3!}\left(\phi^{n+1}_{ij}\right)_{yyy}+\frac{1}{2}\frac{h_2^3}{3!}\left(\phi^{n+1}_{ij}\right)_{xxy}+\frac{1}{2}\frac{h_2^2k_2}{3!}\left(\phi^{n+1}_{ij}\right)_{xyy}\\
-\frac{1}{2}\frac{h_1k_1^2}{3!}\left(\phi^{n+1}_{ij}\right)_{yyy}-\frac{1}{2}\frac{h_1^3}{3!}\left(\phi^{n+1}_{ij}\right)_{xxy}-\frac{1}{2}\frac{h_1^2k_1}{3!}\left(\phi^{n+1}_{ij}\right)_{xyy}\\
-\frac{1}{2}\frac{h_2k_1^2}{3!}\left(\phi^{n+1}_{ij}\right)_{yyy}-\frac{1}{2}\frac{h_2^3}{3!}\left(\phi^{n+1}_{ij}\right)_{xxy}+\frac{1}{2}\frac{h_2^2k_1}{3!}\left(\phi^{n+1}_{ij}\right)_{xyy}
\end{array}\right)\\
+\left(\begin{array}{l}
-\frac{1}{2}\frac{k_2{h_1}^2}{3!}\left(\phi^{n+1}_{ij}\right)_{xxx}+\frac{1}{2}\frac{h_1{k_2}^2}{3!}\left(\phi^{n+1}_{ij}\right)_{xxy}-\frac{1}{2}\frac{{k_2}^3}{3!}\left(\phi^{n+1}_{ij}\right)_{xyy}\\
+\frac{1}{2}\frac{k_2{h_2}^2}{3!}\left(\phi^{n+1}_{ij}\right)_{xxx}+\frac{1}{2}\frac{h_2{k_2}^2}{3!}\left(\phi^{n+1}_{ij}\right)_{xxy}+\frac{1}{2}\frac{{k_2}^3}{3!}\left(\phi^{n+1}_{ij}\right)_{xyy}\\
-\frac{1}{2}\frac{k_1{h_1}^2}{3!}\left(\phi^{n+1}_{ij}\right)_{xxx}-\frac{1}{2}\frac{h_1{k_1}^2}{3!}\left(\phi^{n+1}_{ij}\right)_{xxy}-\frac{1}{2}\frac{{k_1}^3}{3!}\left(\phi^{n+1}_{ij}\right)_{xyy}\\
+\frac{1}{2}\frac{k_1{h_2}^2}{3!}\left(\phi^{n+1}_{ij}\right)_{xxx}-\frac{1}{2}\frac{h_2{k_1}^2}{3!}\left(\phi^{n+1}_{ij}\right)_{xxy}+\frac{1}{2}\frac{{k_1}^3}{3!}\left(\phi^{n+1}_{ij}\right)_{xyy}
\end{array}\right)
\end{array}\right)
\end{aligned}
\tag{B.16}
$$

After some mathematical manipulations the diffusion terms are

$$\begin{aligned}
&\frac{D}{6h_1}\left(k_1\left(\phi^{n+1}_{i\,j-1}-\phi^{n+1}_{i-1\,j-1}\right)+2\left(k_1+k_2\right)\left(\phi^{n+1}_{i\,j}-\phi^{n+1}_{i-1\,j}\right)+k_2\left(\phi^{n+1}_{i\,j+1}-\phi^{n+1}_{i-1\,j+1}\right)\right)\\
&+\frac{D}{6h_2}\left(k_1\left(\phi^{n+1}_{i\,j-1}-\phi^{n+1}_{i+1\,j-1}\right)+2\left(k_1+k_2\right)\left(\phi^{n+1}_{i\,j}-\phi^{n+1}_{i+1\,j}\right)+k_2\left(\phi^{n+1}_{i\,j+1}-\phi^{n+1}_{i+1\,j+1}\right)\right)\\
&+\frac{D}{6k_1}\left(h_1\left(\phi^{n+1}_{i-1\,j}-\phi^{n+1}_{i-1\,j-1}\right)+2\left(h_1+h_2\right)\left(\phi^{n+1}_{i\,j}-\phi^{n+1}_{i\,j-1}\right)+h_2\left(\phi^{n+1}_{i+1\,j}-\phi^{n+1}_{i+1\,j-1}\right)\right)\\
&+\frac{D}{6k_2}\left(h_1\left(\phi^{n+1}_{i-1\,j}-\phi^{n+1}_{i-1\,j+1}\right)+2\left(h_1+h_2\right)\left(\phi^{n+1}_{i\,j}-\phi^{n+1}_{i\,j+1}\right)+h_2\left(\phi^{n+1}_{i+1\,j}-\phi^{n+1}_{i+1\,j+1}\right)\right)=\\
&-\frac{D}{4}\left(h_1+h_2\right)\left(k_1+k_2\right)\left(\phi^{n+1}_{ij}\right)_{yy}-\frac{D}{4}\left(h_1+h_2\right)\left(k_1+k_2\right)\left(\phi^{n+1}_{ij}\right)_{xx}\\
&-\frac{D}{2\times 3!}\left(h_1+h_2\right)\left(k_1+k_2\right)\left(k_2-k_1\right)\left(\left(\phi^{n+1}_{ij}\right)_{yyy}+\left(\phi^{n+1}_{ij}\right)_{xxy}\right)\\
&-\frac{D}{2\times 3!}\left(k_1+k_2\right)\left(h_1+h_2\right)\left(h_2-h_1\right)\left(\left(\phi^{n+1}_{ij}\right)_{xxx}+\left(\phi^{n+1}_{ij}\right)_{xyy}\right)
\end{aligned}\tag{B.17}$$

In the next step, all the terms in convection part of equation B.13 are expanded in Taylor series about $\phi^{n+1}_{i\,j}$

$$\begin{aligned}
&\textit{Convection part} =\\
&\frac{uk_2}{6}\left(-\phi^n_{i-1j}+\phi^n_{ij}+\frac{1}{2}\phi^n_{ij+1}-\frac{1}{2}\phi^n_{i-1j+1}\right)+\frac{vh_1}{6}\left(-\frac{1}{2}\phi^n_{i-1j}-\phi^n_{ij}+\phi^n_{ij+1}+\frac{1}{2}\phi^n_{i-1j+1}\right)\\
&+\frac{uk_2}{6}\left(-\phi^n_{ij}+\phi^n_{i+1j}+\frac{1}{2}\phi^n_{i+1j+1}-\frac{1}{2}\phi^n_{ij+1}\right)+\frac{vh_2}{6}\left(-\phi^n_{ij}-\frac{1}{2}\phi^n_{i+1j}+\frac{1}{2}\phi^n_{i+1j+1}+\phi^n_{ij+1}\right)\\
&+\frac{uk_1}{6}\left(-\frac{1}{2}\phi^n_{i-1j-1}+\frac{1}{2}\phi^n_{ij-1}+\phi^n_{ij}-\phi^n_{i-1j}\right)+\frac{vh_1}{6}\left(-\frac{1}{2}\phi^n_{i-1j-1}-\phi^n_{ij-1}+\phi^n_{ij}+\frac{1}{2}\phi^n_{i-1j}\right)\\
&+\frac{uk_1}{6}\left(-\frac{1}{2}\phi^n_{ij-1}+\frac{1}{2}\phi^n_{i+1j-1}+\phi^n_{i+1j}-\phi^n_{ij}\right)+\frac{vh_2}{6}\left(-\phi^n_{ij-1}-\frac{1}{2}\phi^n_{i+1j-1}+\frac{1}{2}\phi^n_{i+1j}+\phi^n_{ij}\right)
\end{aligned}\tag{B.18}$$

the spatial Taylor expansion of equation B.18 about ϕ_{ij}^{n} is

$$
\begin{aligned}
&Convection\ part = \\
&\frac{u}{4}(k_1+k_2)(h_1+h_2)\left(\phi_{ij}^{n}\right)_x + \frac{v}{4}(k_1+k_2)(h_1+h_2)\left(\phi_{ij}^{n}\right)_y \\
&-\frac{u}{8}(k_1+k_2)(h_1+h_2)(h_1-h_2)\left(\phi_{ij}^{n}\right)_{xx} - \frac{v}{8}(k_1+k_2)(k_2-k_1)(h_1+h_2)\left(\phi_{ij}^{n}\right)_{yy} \\
&-\frac{u}{12}(k_1+k_2)(k_2-k_1)(h_1+h_2)\left(\phi_{ij}^{n}\right)_{xy} - \frac{v}{12}(k_1+k_2)(h_1+h_2)(h_1-h_2)\left(\phi_{ij}^{n}\right)_{xy} \\
&+\frac{u}{24}(k_1+k_2)\left({h_1}^3+{h_2}^3\right)\left(\phi_{ij}^{n}\right)_{xxx} + \frac{v}{24}\left({k_1}^3+{k_2}^3\right)(h_1+h_2)\left(\phi_{ij}^{n}\right)_{yyy} \\
&-\frac{u}{24}\left({k_1}^2-{k_2}^2\right)\left({h_1}^2-{h_2}^2\right)\left(\phi_{ij}^{n}\right)_{xxy} + \frac{v}{24}(k_1+k_2)\left({h_1}^3+{h_2}^3\right)\left(\phi_{ij}^{n}\right)_{xxy} \\
&+\frac{u}{24}\left({k_1}^3+{k_2}^3\right)(h_1+h_2)\left(\phi_{ij}^{n}\right)_{xyy} - \frac{v}{24}\left({k_1}^2-{k_2}^2\right)\left({h_1}^2-{h_2}^2\right)\left(\phi_{ij}^{n}\right)_{xyy}
\end{aligned}
\tag{B.19}
$$

after some mathematical manipulations equation B.19 becomes

$$
\begin{aligned}
&Convection\ part = \\
&\frac{1}{4}(k_1+k_2)(h_1+h_2)\Big(u\left(\phi_{ij}^{n}\right)_x + v\left(\phi_{ij}^{n}\right)_y\Big) \\
&-\frac{1}{4}(k_1+k_2)(h_1+h_2)\Big((h_1-h_2)\frac{u}{2}\left(\phi_{ij}^{n}\right)_{xx} + (k_1-k_2)\frac{v}{2}\left(\phi_{ij}^{n}\right)_{yy}\Big) \\
&-\frac{1}{4}(k_1+k_2)(h_1+h_2)\Big((k_1-k_2)\frac{u}{3}\left(\phi_{ij}^{n}\right)_{xy} + (h_1-h_2)\frac{v}{3}\left(\phi_{ij}^{n}\right)_{xy}\Big) \\
&+\frac{1}{4}(k_1+k_2)(h_1+h_2)\Big(\left({h_1}^2-h_1h_2+{h_2}^2\right)\frac{u}{6}\left(\phi_{ij}^{n}\right)_{xxx} + \left({k_1}^2-k_1k_2+{k_2}^2\right)\frac{v}{6}\left(\phi_{ij}^{n}\right)_{yyy}\Big) \\
&-\frac{1}{4}(k_1+k_2)(h_1+h_2)\Big((k_2-k_1)(h_1-h_2)\frac{u}{6}\left(\phi_{ij}^{n}\right)_{xxy} - \left({h_1}^2-h_1h_2+{h_2}^2\right)\frac{v}{24}\left(\phi_{ij}^{n}\right)_{xxy}\Big) \\
&+\frac{1}{4}(k_1+k_2)(h_1+h_2)\Big(\left({k_1}^2-k_1k_2+{k_2}^2\right)\frac{u}{6}\left(\phi_{ij}^{n}\right)_{xyy} - (k_2-k_1)(h_1-h_2)\frac{v}{4}\left(\phi_{ij}^{n}\right)_{xyy}\Big)
\end{aligned}
\tag{B.20}
$$

In this step, all the terms are expanded about ϕ_{ij}^{n+1} by using temporal Taylor expansion

$$
\phi_{ij}^{n} = \phi_{ij}^{n+1} - \Delta t\left(\phi_{ij}^{n+1}\right)_t + \frac{\Delta t^2}{2}\left(\phi_{ij}^{n+1}\right)_{tt} + O\left(\Delta t^3\right)
$$

The convection part about ϕ_{ij}^{n+1} is

$$
\begin{aligned}
&Convection\ part = \\
&\frac{1}{4}(k_1+k_2)(h_1+h_2)\begin{pmatrix} u\left(\phi_{ij}^{n+1}-\Delta t\left(\phi_{ij}^{n+1}\right)_t+\frac{\Delta t^2}{2}\left(\phi_{ij}^{n+1}\right)_{tt}+...\right)_x \\ +v\left(\phi_{ij}^{n+1}-\Delta t\left(\phi_{ij}^{n+1}\right)_t+\frac{\Delta t^2}{2}\left(\phi_{ij}^{n+1}\right)_{tt}+...\right)_y \end{pmatrix} \\
&-\frac{1}{4}(k_1+k_2)(h_1+h_2)\begin{pmatrix} (h_1-h_2)\frac{u}{2}\left(\phi_{ij}^{n+1}-\Delta t\left(\phi_{ij}^{n+1}\right)_t+\frac{\Delta t^2}{2}\left(\phi_{ij}^{n+1}\right)_{tt}+...\right)_{xx} \\ +(k_1-k_2)\frac{v}{2}\left(\phi_{ij}^{n+1}-\Delta t\left(\phi_{ij}^{n+1}\right)_t+\frac{\Delta t^2}{2}\left(\phi_{ij}^{n+1}\right)_{tt}+...\right)_{yy} \end{pmatrix} \\
&-\frac{1}{4}(k_1+k_2)(h_1+h_2)\begin{pmatrix} (k_1-k_2)\frac{u}{3}\left(\phi_{ij}^{n+1}-\Delta t\left(\phi_{ij}^{n+1}\right)_t+\frac{\Delta t^2}{2}\left(\phi_{ij}^{n+1}\right)_{tt}+...\right)_{xy} \\ +(h_1-h_2)\frac{v}{3}\left(\phi_{ij}^{n+1}-\Delta t\left(\phi_{ij}^{n+1}\right)_t+\frac{\Delta t^2}{2}\left(\phi_{ij}^{n+1}\right)_{tt}+...\right)_{xy} \end{pmatrix} \\
&+\frac{1}{4}(k_1+k_2)(h_1+h_2)\begin{pmatrix} \left({h_1}^2-h_1h_2+{h_2}^2\right)\frac{u}{6}\left(\phi_{ij}^{n+1}-\Delta t\left(\phi_{ij}^{n+1}\right)_t+\frac{\Delta t^2}{2}\left(\phi_{ij}^{n+1}\right)_{tt}+...\right)_{xxx} \\ +\left({k_1}^2-k_1k_2+{k_2}^2\right)\frac{v}{6}\left(\phi_{ij}^{n+1}-\Delta t\left(\phi_{ij}^{n+1}\right)_t+\frac{\Delta t^2}{2}\left(\phi_{ij}^{n+1}\right)_{tt}+...\right)_{yyy} \end{pmatrix} \\
&-\frac{1}{4}(k_1+k_2)(h_1+h_2)\begin{pmatrix} (k_2-k_1)(h_1-h_2)\frac{u}{6}\left(\phi_{ij}^{n+1}-\Delta t\left(\phi_{ij}^{n+1}\right)_t+\frac{\Delta t^2}{2}\left(\phi_{ij}^{n+1}\right)_{tt}+...\right)_{xxy} \\ -\left({h_1}^2-h_1h_2+{h_2}^2\right)\frac{v}{24}\left(\phi_{ij}^{n+1}-\Delta t\left(\phi_{ij}^{n+1}\right)_t+\frac{\Delta t^2}{2}\left(\phi_{ij}^{n+1}\right)_{tt}+...\right)_{xxy} \end{pmatrix} \\
&+\frac{1}{4}(k_1+k_2)(h_1+h_2)\begin{pmatrix} \left({k_1}^2-k_1k_2+{k_2}^2\right)\frac{u}{6}\left(\phi_{ij}^{n+1}-\Delta t\left(\phi_{ij}^{n+1}\right)_t+\frac{\Delta t^2}{2}\left(\phi_{ij}^{n+1}\right)_{tt}+...\right)_{xyy} \\ -(k_2-k_1)(h_1-h_2)\frac{v}{4}\left(\phi_{ij}^{n+1}-\Delta t\left(\phi_{ij}^{n+1}\right)_t+\frac{\Delta t^2}{2}\left(\phi_{ij}^{n+1}\right)_{tt}+...\right)_{xyy} \end{pmatrix}
\end{aligned}
\tag{B.21}
$$

Last part, all the terms of the time derivation part of equation B.13 are expanded about ϕ_{ij}^{n+1} by using spatial and temporal Taylor expansion ($\phi_{ij}^{n+1}-\phi_{ij}^{n}$ is shown by $\Delta\phi_{ij}$).

First spatial expansion:

$$
\begin{aligned}
&Time\ derivative\, part = \\
&\frac{h_1k_2}{36}\left(2\frac{\phi^{n+1}_{i-1j}-\phi^{n}_{i-1j}}{\Delta t}+4\frac{\phi^{n+1}_{ij}-\phi^{n}_{ij}}{\Delta t}+2\frac{\phi^{n+1}_{ij+1}-\phi^{n}_{ij+1}}{\Delta t}+\frac{\phi^{n+1}_{i-1j+1}-\phi^{n}_{i-1j+1}}{\Delta t}\right)\\
&+\frac{h_2k_2}{36}\left(4\frac{\phi^{n+1}_{ij}-\phi^{n}_{ij}}{\Delta t}+2\frac{\phi^{n+1}_{i+1j}-\phi^{n}_{i+1j}}{\Delta t}+\frac{\phi^{n+1}_{i+1j+1}-\phi^{n}_{i+1j+1}}{\Delta t}+2\frac{\phi^{n+1}_{ij+1}-\phi^{n}_{ij+1}}{\Delta t}\right)\\
&+\frac{h_1k_1}{36\Delta t}\left(\frac{\phi^{n+1}_{i-1j-1}-\phi^{n}_{i-1j-1}}{\Delta t}+2\frac{\phi^{n+1}_{ij-1}-\phi^{n}_{ij-1}}{\Delta t}+4\frac{\phi^{n+1}_{ij}-\phi^{n}_{ij}}{\Delta t}+2\frac{\phi^{n+1}_{i-1j}-\phi^{n}_{i-1j}}{\Delta t}\right)\\
&+\frac{h_2k_1}{36\Delta t}\left(2\frac{\phi^{n+1}_{ij-1}-\phi^{n}_{ij-1}}{\Delta t}+\frac{\phi^{n+1}_{i+1j-1}-\phi^{n}_{i+1j-1}}{\Delta t}+2\frac{\phi^{n+1}_{i+1j}-\phi^{n}_{i+1j}}{\Delta t}+4\frac{\phi^{n+1}_{ij}-\phi^{n}_{ij}}{\Delta t}\right)=\\
&+\frac{h_1k_2}{36\Delta t}\left(\begin{array}{l}(9)\,\Delta\phi_{ij}+(-3)\,h_1(\Delta\phi_{ij})_x+\frac{1}{2!}\,(3)\,{h_1}^2(\Delta\phi_{ij})_{xx}+\frac{1}{3!}\,(-3)\,{h_1}^3(\Delta\phi_{ij})_{xxx}\\
+(3)\,k_2(\Delta\phi_{ij})_y+\frac{1}{2!}\,(3)\,{k_2}^2(\Delta\phi_{ij})_{yy}+\frac{1}{3!}\,(3)\,{k_2}^3(\Delta\phi_{ij})_{yyy}\\
+\frac{1}{2!}\,(-2)\,h_1k_2(\Delta\phi_{ij})_{xy}+\frac{1}{3!}\,(3)\,{h_1}^2k_2(\Delta\phi_{ij})_{xxy}+\frac{1}{3!}\,(-3)\,h_1{k_2}^2(\Delta\phi_{ij})_{xyy}\end{array}\right)\\
&+\frac{h_2k_2}{36\Delta t}\left(\begin{array}{l}(9)\,\Delta\phi_{ij}+(3)\,h_2(\Delta\phi_{ij})_x+\frac{1}{2!}\,(3)\,{h_2}^2(\Delta\phi_{ij})_{xx}+\frac{1}{3!}\,(3)\,{h_2}^3(\Delta\phi_{ij})_{xxx}\\
+(3)\,k_2(\Delta\phi_{ij})_y+\frac{1}{2!}\,(3)\,{k_2}^2(\Delta\phi_{ij})_{yy}+\frac{1}{3!}\,(3)\,{k_2}^3(\Delta\phi_{ij})_{yyy}\\
+\frac{1}{2!}\,(2)\,h_2k_2(\Delta\phi_{ij})_{xy}+\frac{1}{3!}\,(3)\,{h_2}^2k_2(\Delta\phi_{ij})_{xxy}+\frac{1}{3!}\,(3)\,h_2{k_2}^2(\Delta\phi_{ij})_{xyy}\end{array}\right)\\
&+\frac{h_1k_1}{36\Delta t}\left(\begin{array}{l}(9)\,\Delta\phi_{ij}+(-3)\,h_1(\Delta\phi_{ij})_x+\frac{1}{2!}\,(3)\,{h_1}^2(\Delta\phi_{ij})_{xx}+\frac{1}{3!}\,(-3)\,{h_1}^3(\Delta\phi_{ij})_{xxx}\\
+(-3)\,k_1(\Delta\phi_{ij})_y+\frac{1}{2!}\,(3)\,{k_1}^2(\Delta\phi_{ij})_{yy}+\frac{1}{3!}\,(-3)\,{k_1}^3(\Delta\phi_{ij})_{yyy}\\
+\frac{1}{2!}\,(2)\,h_1k_1(\Delta\phi_{ij})_{xy}+\frac{1}{3!}\,(-3)\,{h_1}^2k_1(\Delta\phi_{ij})_{xxy}+\frac{1}{3!}\,(-3)\,h_1{k_1}^2(\Delta\phi_{ij})_{xyy}\end{array}\right)\\
&+\frac{h_2k_1}{36\Delta t}\left(\begin{array}{l}(9)\,\Delta\phi_{ij}+(3)\,h_2(\Delta\phi_{ij})_x+\frac{1}{2!}\,(3)\,{h_2}^2(\Delta\phi_{ij})_{xx}+\frac{1}{3!}\,(3)\,{h_2}^3(\Delta\phi_{ij})_{xxx}\\
+(-3)\,k_1(\Delta\phi_{ij})_y+\frac{1}{2!}\,(3)\,{k_1}^2(\Delta\phi_{ij})_{yy}+\frac{1}{3!}\,(-3)\,{k_1}^3(\Delta\phi_{ij})_{yyy}\\
+\frac{1}{2!}\,(-2)\,h_2k_1(\Delta\phi_{ij})_{xy}+\frac{1}{3!}\,(-3)\,{h_2}^2k_1(\Delta\phi_{ij})_{xxy}+\frac{1}{3!}\,(3)\,h_2{k_1}^2(\Delta\phi_{ij})_{xyy}\end{array}\right)=\\
&\frac{1}{4\Delta t}\,(h_1+h_2)\,(k_1+k_2)\,\Delta\phi_{ij}+\frac{1}{12\Delta t}\,(k_1+k_2)\,(h_2-h_1)\,(h_2+h_1)\,(\Delta\phi_{ij})_x\\
&+\frac{1}{12\Delta t}\,(h_2+h_1)\,(k_1+k_2)\,(k_2-k_1)\,(\Delta\phi_{ij})_y\\
&+\frac{1}{24\Delta t}\,(k_1+k_2)\,(h_2+h_1)\left(h_1^2-h_1h_2+h_2^2\right)(\Delta\phi_{ij})_{xx}+\frac{1}{36\Delta t}\left(h_2^2-h_1^2\right)\left(k_2^2-k_1^2\right)(\Delta\phi_{ij})_{xy}\\
&+\frac{1}{24\Delta t}\,(h_2+h_1)\,(k_1+k_2)\left(k_1^2-k_1k_2+k_2^2\right)(\Delta\phi_{ij})_{yy}+\ldots
\end{aligned}
\tag{B.22}
$$

Next, the temporal expansion of equation B.22 could be found by using

$$\frac{\Delta\phi_{ij}}{\Delta t}=\frac{\phi_i^{n+1}-\phi_i^n}{\Delta t}=\left(\phi_{ij}^{n+1}\right)_t-\frac{\Delta t}{2}\left(\phi_{ij}^{n+1}\right)_{tt}+\frac{\Delta t^2}{6}\left(\phi_{ij}^{n+1}\right)_{ttt}+O\left(\Delta t^3\right)$$

Therefore the equation B.22 is rewritten as:

$$\begin{aligned}
&Time\ derivation\, part = \\
&\frac{1}{4}\left(h_1+h_2\right)\left(k_1+k_2\right)\left(\left(\phi_i^{n+1}\right)_t-\frac{\Delta t}{2}\left(\phi_i^{n+1}\right)_{tt}+\frac{\Delta t^2}{6}\left(\phi_i^{n+1}\right)_{ttt}+...\right)\\
&+\frac{1}{12}\left(k_1+k_2\right)\left(h_2-h_1\right)\left(h_2+h_1\right)\left(\left(\phi_i^{n+1}\right)_t-\frac{\Delta t}{2}\left(\phi_i^{n+1}\right)_{tt}+\frac{\Delta t^2}{6}\left(\phi_i^{n+1}\right)_{ttt}+...\right)_x\\
&+\frac{1}{12}\left(h_2+h_1\right)\left(k_1+k_2\right)\left(k_2-k_1\right)\left(\left(\phi_i^{n+1}\right)_t-\frac{\Delta t}{2}\left(\phi_i^{n+1}\right)_{tt}+\frac{\Delta t^2}{6}\left(\phi_i^{n+1}\right)_{ttt}+...\right)_y\\
&+\frac{1}{24}\left(k_1+k_2\right)\left(h_2+h_1\right)\left(h_1^2-h_1h_2+h_2^2\right)\left(\left(\phi_i^{n+1}\right)_t-\frac{\Delta t}{2}\left(\phi_i^{n+1}\right)_{tt}+\frac{\Delta t^2}{6}\left(\phi_i^{n+1}\right)_{ttt}+...\right)_{xx}\\
&+\frac{1}{24}\left(h_2+h_1\right)\left(k_1+k_2\right)\left(k_1^2-k_1k_2+k_2^2\right)\left(\left(\phi_i^{n+1}\right)_t-\frac{\Delta t}{2}\left(\phi_i^{n+1}\right)_{tt}+\frac{\Delta t^2}{6}\left(\phi_i^{n+1}\right)_{ttt}+...\right)_{yy}\\
&+\frac{1}{36}\left(h_2^2-h_1^2\right)\left(k_2^2-k_1^2\right)\left(\left(\phi_i^{n+1}\right)_t-\frac{\Delta t}{2}\left(\phi_i^{n+1}\right)_{tt}+\frac{\Delta t^2}{6}\left(\phi_i^{n+1}\right)_{ttt}+...\right)_{xy}=\\
&\frac{1}{4}\left(h_1+h_2\right)\left(k_1+k_2\right)\times\\
&\left(\begin{aligned}
&\left(\left(\phi_i^{n+1}\right)_t-\frac{\Delta t}{2}\left(\phi_i^{n+1}\right)_{tt}+\frac{\Delta t^2}{6}\left(\phi_i^{n+1}\right)_{ttt}-\frac{\Delta t^3}{24}\left(\phi_i^{n+1}\right)_{tttt}\right)\\
&+\frac{1}{3}\left(h_2-h_1\right)\left(\left(\phi_i^{n+1}\right)_t-\frac{\Delta t}{2}\left(\phi_i^{n+1}\right)_{tt}+\frac{\Delta t^2}{6}\left(\phi_i^{n+1}\right)_{ttt}-\frac{\Delta t^3}{24}\left(\phi_i^{n+1}\right)_{tttt}\right)_x\\
&+\frac{1}{3}\left(k_2-k_1\right)\left(\left(\phi_i^{n+1}\right)_t-\frac{\Delta t}{2}\left(\phi_i^{n+1}\right)_{tt}+\frac{\Delta t^2}{6}\left(\phi_i^{n+1}\right)_{ttt}-\frac{\Delta t^3}{24}\left(\phi_i^{n+1}\right)_{tttt}\right)_y\\
&+\frac{1}{6}\left(h_1^2-h_1h_2+h_2^2\right)\left(\left(\phi_i^{n+1}\right)_t-\frac{\Delta t}{2}\left(\phi_i^{n+1}\right)_{tt}+\frac{\Delta t^2}{6}\left(\phi_i^{n+1}\right)_{ttt}-\frac{\Delta t^3}{24}\left(\phi_i^{n+1}\right)_{tttt}\right)_{xx}\\
&+\frac{1}{9}\left(h_2-h_1\right)\left(k_2-k_1\right)\left(\left(\phi_i^{n+1}\right)_t-\frac{\Delta t}{2}\left(\phi_i^{n+1}\right)_{tt}+\frac{\Delta t^2}{6}\left(\phi_i^{n+1}\right)_{ttt}-\frac{\Delta t^3}{24}\left(\phi_i^{n+1}\right)_{tttt}\right)_{xy}\\
&+\frac{1}{6}\left(k_1^2-k_1k_2+k_2^2\right)\left(\left(\phi_i^{n+1}\right)_t-\frac{\Delta t}{2}\left(\phi_i^{n+1}\right)_{tt}+\frac{\Delta t^2}{6}\left(\phi_i^{n+1}\right)_{ttt}-\frac{\Delta t^3}{24}\left(\phi_i^{n+1}\right)_{tttt}\right)_{yy}+...
\end{aligned}\right)
\end{aligned}\tag{B.23}$$

Now, by assembling diffusion, convection, and time derivative parts, equations

B.17, B.21, and B.23 respectively, the DE about ϕ_{ij}^{n+1} is

$$DE = \frac{(h_1+h_2)(k_1+k_2)}{4}\times \left\{ \begin{array}{l} \frac{\partial \phi}{\partial t} - D\left(\frac{\partial^2\phi}{\partial x^2} + \frac{\partial^2\phi}{\partial x^2}\right) + u\frac{\partial \phi}{\partial x} + v\frac{\partial \phi}{\partial y} \\ +\frac{1}{3}\left((h_2-h_1)\frac{\partial^2\phi}{\partial x\partial t} + (k_2-k_1)\frac{\partial^2\phi}{\partial y\partial t}\right) \\ +\frac{1}{3}\left((k_2-k_1)\left(-\frac{\partial^3\phi}{\partial y^3} - \frac{\partial^3\phi}{\partial x^2\partial y}\right) + (h_2-h_1)\left(-\frac{\partial^3\phi}{\partial x^3} - \frac{\partial^3\phi}{\partial x\partial y^2}\right)\right) \\ +u\left(\frac{1}{2}(h_2-h_1)\frac{\partial^2\phi}{\partial x^2} + \frac{1}{3}(k_2-k_1)\frac{\partial^2\phi}{\partial x\partial y}\right) \\ +v\left(\frac{1}{2}(k_2-k_1)\frac{\partial^2\phi}{\partial y^2} + \frac{1}{3}(h_2-h_1)\frac{\partial^2\phi}{\partial x\partial y}\right) \\ +O(h^2,k^2,hk,h\Delta t,k\Delta t,\Delta t) \end{array} \right\} \quad \text{(B.24)}$$

All terms on the right hand side of equation B.24 are evaluated at (x_i, y_j, t_{n+1}). Re-writing the first order term of the truncation error as

$$\frac{1}{3}\left((k_2-k_1)\frac{\partial}{\partial y}\left(\frac{\partial\phi}{\partial t} - \frac{\partial^2\phi}{\partial x^2} - \frac{\partial^2\phi}{\partial y^2} + u\frac{\partial\phi}{\partial x} + v\frac{\partial\phi}{\partial y}\right)\right) + \frac{u}{6}(h_2-h_1)\frac{\partial^2\phi}{\partial x^2}$$
$$+\frac{1}{3}\left((h_2-h_1)\frac{\partial}{\partial x}\left(\frac{\partial\phi}{\partial t} - \frac{\partial^2\phi}{\partial x^2} - \frac{\partial^2\phi}{\partial y^2} + u\frac{\partial\phi}{\partial x} + v\frac{\partial\phi}{\partial y}\right)\right) + \frac{v}{6}(k_2-k_1)\frac{\partial^2\phi}{\partial y^2}$$

the leading terms on the left must vanish hence the changes in the mesh introduce a spatial first order local error (FOE) equal to

$$FOE = \frac{1}{6}\left(u\,(h_2-h_1)\left(\frac{\partial^2\phi}{\partial x^2}\right)_{ij}^{n+1} + v\,(k_2-k_1)\left(\frac{\partial^2\phi}{\partial y^2}\right)_{ij}^{n+1}\right) \quad \text{(B.25)}$$

This is of the form of an anisotropic artificial diffusion similar to that arising in stabilizing formulations of the upwind type, and is readily eliminated by the addition of an artificial balancing diffusion in the intersected elements [27], which restores the local second order accuracy in the approximation.

B.2 3-D Domain

Like two dimensional error analysis, assume that the convective velocity field $\mathbf{u} = (u, v, w)^T$ is known and constant.

The weak weighted residuals formulation of equation 4.1 gives

$$\int_{\Omega\ t} \left\{ \mathbf{w} \cdot \left[\frac{\partial \phi}{\partial t} + (\mathbf{u} \cdot \nabla)\phi^n \right] + D \left(\nabla \mathbf{w} . \nabla \phi^{n+1} \right) \right\} d\Omega = 0 \tag{B.26}$$

Where $\mathbf{w}$ denotes the weighting functions.

The ϕ function is discretized over the space as:

$$\phi\left(x, y, z, t\right) \cong \sum_{i=1}^{n} N_i \left(x, y, z, t\right) \phi_i \left(t\right) \tag{B.27}$$

Where N_i are the shape functions over each element, and n is the number of nodes in an element, in this three dimensional case $n = 8$. The weighting functions w_i are set to be equal to shape functions N_i. the final form of the equation 4.2 is

$$\begin{gathered}
\int_0^{\Delta z} \int_0^{\Delta y} \int_0^{\Delta x} N_i \sum_{j=1}^{8} N_j \frac{\partial \phi_j}{\partial t} dxdydz \\
+ \int_0^{\Delta z} \int_0^{\Delta y} \int_0^{\Delta x} \begin{pmatrix} uN_i \sum_{j=1}^{8} \left(\frac{\partial N_j}{\partial x} \phi_j^n \right) \\ +vN_i \sum_{j=1}^{8} \left(\frac{\partial N_j}{\partial y} \phi_j^n \right) \\ +wN_i \sum_{j=1}^{8} \left(\frac{\partial N_j}{\partial z} \phi_j^n \right) \end{pmatrix} dxdydz \\
+ \int_0^{\Delta z} \int_0^{\Delta y} \int_0^{\Delta x} D \begin{pmatrix} \frac{\partial N_i}{\partial x} \sum_{j=1}^{8} \left(\frac{\partial N_j}{\partial x} \phi_j^{n+1} \right) \\ + \frac{\partial N_i}{\partial y} \sum_{j=1}^{8} \left(\frac{\partial N_j}{\partial y} \phi_j^{n+1} \right) \\ + \frac{\partial N_i}{\partial z} \sum_{j=1}^{8} \left(\frac{\partial N_j}{\partial z} \phi_j^{n+1} \right) \end{pmatrix} dxdydz
\end{gathered} \tag{B.28}$$

Another representation of equation B.28 is

$$\begin{aligned}
&\sum_{j=1}^{8}\int_0^{\Delta z}\int_0^{\Delta y}\int_0^{\Delta x} N_i N_j \frac{\partial \phi_j}{\partial t} dxdydz \\
&+u\sum_{j=1}^{8}\int_0^{\Delta z}\int_0^{\Delta y}\int_0^{\Delta x} N_i \frac{\partial N_j}{\partial x} \phi_j^n dxdydz \\
&+v\sum_{j=1}^{8}\int_0^{\Delta z}\int_0^{\Delta y}\int_0^{\Delta x} N_i \frac{\partial N_j}{\partial y} \phi_j^n dxdydz \\
&+w\sum_{j=1}^{8}\int_0^{\Delta z}\int_0^{\Delta y}\int_0^{\Delta x} N_i \frac{\partial N_j}{\partial y} \phi_j^n dxdydz \\
&+D\sum_{j=1}^{8}\int_0^{\Delta z}\int_0^{\Delta y}\int_0^{\Delta x} \frac{\partial N_i}{\partial x}\frac{\partial N_j}{\partial x} \phi_j^{n+1} dxdydz \\
&+D\sum_{j=1}^{8}\int_0^{\Delta z}\int_0^{\Delta y}\int_0^{\Delta x} \frac{\partial N_i}{\partial y}\frac{\partial N_j}{\partial y} \phi_j^{n+1} dxdydz \\
&+D\sum_{j=1}^{8}\int_0^{\Delta z}\int_0^{\Delta y}\int_0^{\Delta x} \frac{\partial N_i}{\partial z}\frac{\partial N_j}{\partial z} \phi_j^{n+1} dxdydz = 0
\end{aligned} \tag{B.29}$$

The shape functions according to figure 4.1(a) are

$$\begin{cases}
N_1 = \left(1-\frac{x}{h}\right)\left(1-\frac{y}{k}\right)\left(1-\frac{z}{l}\right) \\
N_2 = \left(\frac{x}{h}\right)\left(1-\frac{y}{k}\right)\left(1-\frac{z}{l}\right) \\
N_3 = \left(1-\frac{x}{h}\right)\left(\frac{y}{k}\right)\left(1-\frac{z}{l}\right) \\
N_4 = \left(\frac{x}{h}\right)\left(\frac{y}{k}\right)\left(1-\frac{z}{l}\right) \\
N_5 = \left(1-\frac{x}{h}\right)\left(1-\frac{y}{k}\right)\left(\frac{z}{l}\right) \\
N_6 = \left(\frac{x}{h}\right)\left(1-\frac{y}{k}\right)\left(\frac{z}{l}\right) \\
N_7 = \left(1-\frac{x}{h}\right)\left(\frac{y}{k}\right)\left(\frac{z}{l}\right) \\
N_8 = \left(\frac{x}{h}\right)\left(\frac{y}{k}\right)\left(\frac{z}{l}\right)
\end{cases} \tag{B.30}$$

The next task is to calculate the stiffness matrix of an element. By calculating the stiffness matrices the equation B.29 can be written as:

$$S^{11}_{ij}\dot{\phi}_j + S^{22}_{ij}\phi^n_j + S^{33}_{ij}\phi^n_j + S^{44}_{ij}\phi^n_j + S^{55}_{ij}\phi^{n+1}_j + S^{66}_{ij}\phi^{n+1}_j + S^{77}_{ij}\phi^{n+1}_j = 0 \qquad \text{(B.31)}$$

Where the individual S^{mm} are given by

$$S^{11}_{ij} = \frac{\Delta x \Delta y \Delta z}{6^3}\begin{bmatrix} 8 & 4 & 4 & 2 & 4 & 2 & 2 & 1 \\ 4 & 8 & 2 & 4 & 2 & 4 & 1 & 2 \\ 4 & 2 & 8 & 4 & 2 & 1 & 4 & 2 \\ 2 & 4 & 4 & 8 & 1 & 2 & 2 & 4 \\ 4 & 2 & 2 & 1 & 8 & 4 & 4 & 2 \\ 2 & 4 & 1 & 2 & 4 & 8 & 2 & 4 \\ 2 & 1 & 4 & 2 & 4 & 2 & 8 & 4 \\ 1 & 2 & 2 & 4 & 2 & 4 & 4 & 8 \end{bmatrix}$$

$$S^{22}_{ij} = \frac{u \Delta y \Delta z}{72}\begin{bmatrix} -4 & 4 & -2 & 2 & -2 & 2 & -1 & 1 \\ -4 & 4 & -2 & 2 & -2 & 2 & -1 & 1 \\ -2 & 2 & -4 & 4 & -1 & 1 & -2 & 2 \\ -2 & 2 & -4 & 4 & -1 & 1 & -2 & 2 \\ -2 & 2 & -1 & 1 & -4 & 4 & -2 & 2 \\ -2 & 2 & -1 & 1 & -4 & 4 & -2 & 2 \\ -1 & 1 & -2 & 2 & -2 & 2 & -4 & 4 \\ -1 & 1 & -2 & 2 & -2 & 2 & -4 & 4 \end{bmatrix}$$

$$S_{ij}^{33} = \frac{v\Delta x\Delta z}{72}\begin{bmatrix} -4 & -2 & 4 & 2 & -2 & -1 & 2 & 1 \\ -2 & -4 & 2 & 4 & -1 & -2 & 1 & 2 \\ -4 & -2 & 4 & 2 & -2 & -1 & 2 & 1 \\ -2 & -4 & 2 & 4 & -1 & -2 & 1 & 2 \\ -2 & -1 & 2 & 1 & -4 & -2 & 4 & 2 \\ -1 & -2 & 1 & 2 & -2 & -4 & 2 & 4 \\ -2 & -1 & 2 & 1 & -4 & -2 & 4 & 2 \\ -1 & -2 & 1 & 2 & -2 & -4 & 2 & 4 \end{bmatrix}$$

$$S_{ij}^{44} = \frac{w\Delta x\Delta y}{72}\begin{bmatrix} -4 & -2 & -2 & -1 & 4 & 2 & 2 & 1 \\ -2 & -4 & -1 & -2 & 2 & 4 & 1 & 2 \\ -2 & -1 & -4 & -2 & 2 & 1 & 4 & 2 \\ -1 & -2 & -2 & -4 & 1 & 2 & 2 & 4 \\ -4 & -2 & -2 & -1 & 4 & 2 & 2 & 1 \\ -2 & -4 & -1 & -2 & 2 & 4 & 1 & 2 \\ -2 & -1 & -4 & -2 & 2 & 1 & 4 & 2 \\ -1 & -2 & -2 & -4 & 1 & 2 & 2 & 4 \end{bmatrix}$$

$$S_{ij}^{55} = D\frac{\Delta y\Delta z}{36\Delta x}\begin{bmatrix} 4 & -4 & 2 & -2 & 2 & -2 & 1 & -1 \\ -4 & 4 & -2 & 2 & -2 & 2 & -1 & 1 \\ 2 & -2 & 4 & -4 & 1 & -1 & 2 & -2 \\ -2 & 2 & -4 & 4 & -1 & 1 & -2 & 2 \\ 2 & -2 & 1 & -1 & 4 & -4 & 2 & -2 \\ -2 & 2 & -1 & 1 & -4 & 4 & -2 & 2 \\ 1 & -1 & 2 & -2 & 2 & -2 & 4 & -4 \\ -1 & 1 & -2 & 2 & -2 & 2 & -4 & 4 \end{bmatrix}$$

$$S_{ij}^{66} = D\frac{\Delta x \Delta z}{36\Delta y}\begin{bmatrix} 4 & 2 & 2 & 1 & -4 & -2 & -2 & -1 \\ 2 & 4 & 1 & 2 & -2 & -4 & -1 & -2 \\ 2 & 1 & 4 & 2 & -2 & -1 & -4 & -2 \\ 1 & 2 & 2 & 4 & -1 & -2 & -2 & -4 \\ -4 & -2 & -2 & -1 & 4 & 2 & 2 & 1 \\ -2 & -4 & -1 & -2 & 2 & 4 & 1 & 2 \\ -2 & -1 & -4 & -2 & 2 & 1 & 4 & 2 \\ -1 & -2 & -2 & -4 & 1 & 2 & 2 & 4 \end{bmatrix}$$

$$S_{ij}^{77} = D\frac{\Delta x \Delta y}{36\Delta z}\begin{bmatrix} 4 & 2 & -4 & -2 & 2 & 1 & -2 & -1 \\ 2 & 4 & -2 & -4 & 1 & 2 & -1 & -2 \\ -4 & -2 & 4 & 2 & -2 & -1 & 2 & 1 \\ -2 & -4 & 2 & 4 & -1 & -2 & 1 & 2 \\ 2 & 1 & -2 & -1 & 4 & 2 & -4 & -2 \\ 1 & 2 & -1 & -2 & 2 & 4 & -2 & -4 \\ -2 & -1 & 2 & 1 & -4 & -2 & 4 & 2 \\ -1 & -2 & 1 & 2 & -2 & -4 & 2 & 4 \end{bmatrix}$$

The most commonly time integration algorithm normally referring to as the θ method is used. It consists in approximating the time derivative by the backward difference

$$\dot{\phi} \cong \frac{1}{\Delta t}\left(\phi^{n+1} - \phi^{n}\right) \tag{B.32}$$

The transport quantity ϕ is then defined by

$$\phi = \theta\,\phi^{n+1} + (1-\theta)\,\phi^{n} \tag{B.33}$$

in this analysis the relaxation parameter is $\theta = 1$ and, as a result, $\phi = \phi^{n+1}$.

The nodes and dimension for the elements using the notation in figure 4.1 are

first element

nodes

$$\begin{bmatrix} \phi_{i-1j-1k-1} & \phi_{ij-1k-1} & \phi_{i-1jk-1} & \phi_{ijk-1} & \phi_{i-1j-1k} & \phi_{ij-1k} & \phi_{i-1jk} & \phi_{ijk} \end{bmatrix}$$

dimension

$\begin{bmatrix} h_1 & k_1 & l_1 \end{bmatrix}$

second element

nodes

$$\begin{bmatrix} \phi_{ij-1k-1} & \phi_{i+1j-1k-1} & \phi_{ijk-1} & \phi_{i+1jk-1} & \phi_{ij-1k} & \phi_{i+1j-1k} & \phi_{ijk} & \phi_{i+1jk} \end{bmatrix}$$

dimension

$\begin{bmatrix} h_2 & k_1 & l_1 \end{bmatrix}$

third element

nodes

$$\begin{bmatrix} \phi_{i-1jk-1} & \phi_{ijk-1} & \phi_{i-1j+1k-1} & \phi_{ij+1k-1} & \phi_{i-1jk} & \phi_{ijk} & \phi_{i-1j+1k} & \phi_{ij+1k} \end{bmatrix}$$

dimension

$\begin{bmatrix} h_1 & k_2 & l_1 \end{bmatrix}$

fourth element

nodes

$$\begin{bmatrix} \phi_{ijk-1} & \phi_{i+1jk-1} & \phi_{ij+1k-1} & \phi_{i+1j+1k-1} & \phi_{ijk} & \phi_{i+1jk} & \phi_{ij+1k} & \phi_{i+1j+1k} \end{bmatrix}$$

dimension

$\begin{bmatrix} h_2 & k_2 & l_1 \end{bmatrix}$

fifth element

nodes

$$\begin{bmatrix} \phi_{i-1j-1k} & \phi_{ij-1k} & \phi_{i-1jk} & \phi_{ijk} & \phi_{i-1j-1k+1} & \phi_{ij-1k+1} & \phi_{i-1jk+1} & \phi_{ijk+1} \end{bmatrix}$$

dimension

$\begin{bmatrix} h_1 & k_1 & l_2 \end{bmatrix}$

sixth element

nodes

$$\begin{bmatrix} \phi_{ij-1k} & \phi_{i+1j-1k} & \phi_{ijk} & \phi_{i+1jk} & \phi_{ij-1k+1} & \phi_{i+1j-1k+1} & \phi_{ijk+1} & \phi_{i+1jk+1} \end{bmatrix}$$

dimension

$\begin{bmatrix} h_2 & k_1 & l_2 \end{bmatrix}$

seventh element

nodes

$$\begin{bmatrix} \phi_{i-1jk} & \phi_{ijk} & \phi_{i-1j+1k} & \phi_{ij+1k} & \phi_{i-1jk+1} & \phi_{ijk+1} & \phi_{i-1j+1k+1} & \phi_{ij+1k+1} \end{bmatrix}$$

dimension

$\begin{bmatrix} h_1 & k_2 & l_2 \end{bmatrix}$

eighth element

nodes

$$\begin{bmatrix} \phi_{ijk} & \phi_{i+1jk} & \phi_{ij+1k} & \phi_{i+1j+1k} & \phi_{ijk+1} & \phi_{i+1jk+1} & \phi_{ij+1k+1} & \phi_{i+1j+1k+1} \end{bmatrix}$$

dimension

$\begin{bmatrix} h_2 & k_2 & l_2 \end{bmatrix}$

Assembling the element equation contributions to node (x_i, y_i, z_i), using equation B.31, results in the difference equation (DE). Like two dimensional error analysis, differential equation is made up of three different components diffusion, convection, and time derivative.

Diffusion component of convection-diffusion equation has three parts as the diffusion part of equation B.31 is made up of three matrices S_{ij}^{55},S_{ij}^{66}, and S_{ij}^{77}. Using these matrices, nodes, and dimensions for different neighbor elements of ϕ_{ijk}, defines the diffusion terms.

$$\begin{aligned}
&\phi_{xx}\ component\ of\ diffusion\ terms = \\
&D\tfrac{k_2 l_1}{36h_1}\begin{pmatrix} -2\phi^{n+1}_{i-1jk-1} + 2\phi^{n+1}_{ijk-1} - \phi^{n+1}_{i-1j+1k-1} + \phi^{n+1}_{ij+1k-1} \\ -4\phi^{n+1}_{i-1jk} + 4\phi^{n+1}_{ijk} - 2\phi^{n+1}_{i-1j+1k} + 2\phi^{n+1}_{ij+1k} \end{pmatrix} \\
&+D\tfrac{k_2 l_1}{36h_2}\begin{pmatrix} 2\phi^{n+1}_{ijk-1} - 2\phi^{n+1}_{i+1jk-1} + \phi^{n+1}_{ij+1k-1} - \phi^{n+1}_{i+1j+1k-1} \\ +4\phi^{n+1}_{ijk} - 4\phi^{n+1}_{i+1jk} + 2\phi^{n+1}_{ij+1k} - 2\phi^{n+1}_{i+1j+1k} \end{pmatrix} \\
&+D\tfrac{k_1 l_1}{36h_1}\begin{pmatrix} -\phi^{n+1}_{i-1j-1k-1} + \phi^{n+1}_{ij-1k-1} - 2\phi^{n+1}_{i-1jk-1} + 2\phi^{n+1}_{ijk-1} \\ -2\phi^{n+1}_{i-1j-1k} + 2\phi^{n+1}_{ij-1k} - 4\phi^{n+1}_{i-1jk} + 4\phi^{n+1}_{ijk} \end{pmatrix} \\
&+D\tfrac{k_1 l_1}{36h_2}\begin{pmatrix} \phi^{n+1}_{ij-1k-1} - \phi^{n+1}_{i+1j-1k-1} + 2\phi^{n+1}_{ijk-1} - 2\phi^{n+1}_{i+1jk-1} \\ +2\phi^{n+1}_{ij-1k} - 2\phi^{n+1}_{i+1j-1k} + 4\phi^{n+1}_{ijk} - 4\phi^{n+1}_{i+1jk} \end{pmatrix} \\
&+D\tfrac{k_2 l_2}{36h_1}\begin{pmatrix} -4\phi^{n+1}_{i-1jk} + 4\phi^{n+1}_{ijk} - 2\phi^{n+1}_{i-1j+1k} + 2\phi^{n+1}_{ij+1k} \\ -2\phi^{n+1}_{i-1jk+1} + 2\phi^{n+1}_{ijk+1} - \phi^{n+1}_{i-1j+1k+1} + \phi^{n+1}_{ij+1k+1} \end{pmatrix} \\
&+D\tfrac{k_2 l_2}{36h_2}\begin{pmatrix} 4\phi^{n+1}_{ijk} - 4\phi^{n+1}_{i+1jk} + 2\phi^{n+1}_{ij+1k} - 2\phi^{n+1}_{i+1j+1k} \\ +2\phi^{n+1}_{ijk+1} - 2\phi^{n+1}_{i+1jk+1} + \phi^{n+1}_{ij+1k+1} - \phi^{n+1}_{i+1j+1k+1} \end{pmatrix} \\
&+D\tfrac{k_1 l_2}{36h_1}\begin{pmatrix} -2\phi^{n+1}_{i-1j-1k} + 2\phi^{n+1}_{ij-1k} - 4\phi^{n+1}_{i-1jk} + 4\phi^{n+1}_{ijk} \\ -\phi^{n+1}_{i-1j-1k+1} + \phi^{n+1}_{ij-1k+1} - 2\phi^{n+1}_{i-1jk+1} + 2\phi^{n+1}_{ijk+1} \end{pmatrix} \\
&+D\tfrac{k_1 l_2}{36h_2}\begin{pmatrix} 2\phi^{n+1}_{ij-1k} - 2\phi^{n+1}_{i+1j-1k} + 4\phi^{n+1}_{ijk} - 4\phi^{n+1}_{i+1jk} \\ +\phi^{n+1}_{ij-1k+1} - \phi^{n+1}_{i+1j-1k+1} + 2\phi^{n+1}_{ijk+1} - 2\phi^{n+1}_{i+1jk+1} \end{pmatrix}
\end{aligned} \tag{B.34}$$

The second component of diffusion part of equation B.31 is

$$
\begin{aligned}
&\phi_{yy}\ component\ of\ diffusion\ terms = \\
&D\frac{h_1 l_1}{36k_2}\begin{pmatrix} -2\phi^{n+1}_{i-1jk-1} - 4\phi^{n+1}_{ijk-1} - 1\phi^{n+1}_{i-1j+1k-1} - 2\phi^{n+1}_{ij+1k-1} \\ +2\phi^{n+1}_{i-1jk} + 4\phi^{n+1}_{ijk} + \phi^{n+1}_{i-1j+1k} + 2\phi^{n+1}_{ij+1k} \end{pmatrix} \\
&+D\tfrac{h_2 l_1}{36k_2}\begin{pmatrix} -4\phi^{n+1}_{ijk-1} - 2\phi^{n+1}_{i+1jk-1} - 2\phi^{n+1}_{ij+1k-1} - \phi^{n+1}_{i+1j+1k-1} \\ +4\phi^{n+1}_{ijk} + 2\phi^{n+1}_{i+1jk} + 2\phi^{n+1}_{ij+1k} + \phi^{n+1}_{i+1j+1k} \end{pmatrix} \\
&+D\tfrac{h_1 l_1}{36k_1}\begin{pmatrix} -\phi^{n+1}_{i-1j-1k-1} - 2\phi^{n+1}_{ij-1k-1} - 2\phi^{n+1}_{i-1jk-1} - 4\phi^{n+1}_{ijk-1} \\ +\phi^{n+1}_{i-1j-1k} + 2\phi^{n+1}_{ij-1k} + 2\phi^{n+1}_{i-1jk} + 4\phi^{n+1}_{ijk} \end{pmatrix} \\
&+D\tfrac{h_2 l_1}{36k_1}\begin{pmatrix} -2\phi^{n+1}_{ij-1k-1} - \phi^{n+1}_{i+1j-1k-1} - 4\phi^{n+1}_{ijk-1} - 2\phi^{n+1}_{i+1jk-1} \\ +2\phi^{n+1}_{ij-1k} + \phi^{n+1}_{i+1j-1k} + 4\phi^{n+1}_{ijk} + 2\phi^{n+1}_{i+1jk} \end{pmatrix} \\
&+D\tfrac{h_1 l_2}{36k_2}\begin{pmatrix} 2\phi^{n+1}_{i-1jk} + 4\phi^{n+1}_{ijk} + \phi^{n+1}_{i-1j+1k} + 2\phi^{n+1}_{ij+1k} \\ -2\phi^{n+1}_{i-1jk+1} - 4\phi^{n+1}_{ijk+1} - \phi^{n+1}_{i-1j+1k+1} - 2\phi^{n+1}_{ij+1k+1} \end{pmatrix} \\
&+D\tfrac{h_2 l_2}{36k_2}\begin{pmatrix} 4\phi^{n+1}_{ijk} + 2\phi^{n+1}_{i+1jk} + 2\phi^{n+1}_{ij+1k} + \phi^{n+1}_{i+1j+1k} \\ -4\phi^{n+1}_{ijk+1} - 2\phi^{n+1}_{i+1jk+1} - 2\phi^{n+1}_{ij+1k+1} - \phi^{n+1}_{i+1j+1k+1} \end{pmatrix} \\
&+D\tfrac{h_1 l_2}{36k_1}\begin{pmatrix} \phi^{n+1}_{i-1j-1k} + 2\phi^{n+1}_{ij-1k} + 2\phi^{n+1}_{i-1jk} + 4\phi^{n+1}_{ijk} \\ -\phi^{n+1}_{i-1j-1k+1} - 2\phi^{n+1}_{ij-1k+1} - 2\phi^{n+1}_{i-1jk+1} - 4\phi^{n+1}_{ijk+1} \end{pmatrix} \\
&+D\tfrac{h_2 l_2}{36k_{12}}\begin{pmatrix} 2\phi^{n+1}_{ij-1k} + \phi^{n+1}_{i+1j-1k} + 4\phi^{n+1}_{ijk} + 2\phi^{n+1}_{i+1jk} \\ -2\phi^{n+1}_{ij-1k+1} - \phi^{n+1}_{i+1j-1k+1} - 4\phi^{n+1}_{ijk+1} - 2\phi^{n+1}_{i+1jk+1} \end{pmatrix}
\end{aligned}
\tag{B.35}
$$

The last component of diffusion part is

$$
\begin{aligned}
&\phi_{zz}\ component\ of\ diffusion\ terms = \\
&D\frac{h_1k_2}{36l_1}\begin{pmatrix} \phi^{n+1}_{i-1jk-1} + 2\phi^{n+1}_{ijk-1} - \phi^{n+1}_{i-1j+1k-1} - 2\phi^{n+1}_{ij+1k-1} \\ +2\phi^{n+1}_{i-1jk} + 4\phi^{n+1}_{ijk} - 2\phi^{n+1}_{i-1j+1k} - 4\phi^{n+1}_{ij+1k} \end{pmatrix} \\
&+D\tfrac{h_2k_2}{36l_1}\begin{pmatrix} 2\phi^{n+1}_{ijk-1} + \phi^{n+1}_{i+1jk-1} - 2\phi^{n+1}_{ij+1k-1} - \phi^{n+1}_{i+1j+1k-1} \\ +4\phi^{n+1}_{ijk} + 2\phi^{n+1}_{i+1jk} - 4\phi^{n+1}_{ij+1k} - 2\phi^{n+1}_{i+1j+1k} \end{pmatrix} \\
&+D\tfrac{h_1k_1}{36l_1}\begin{pmatrix} -\phi^{n+1}_{i-1j-1k-1} - 2\phi^{n+1}_{ij-1k-1} + \phi^{n+1}_{i-1jk-1} + 2\phi^{n+1}_{ijk-1} \\ -2\phi^{n+1}_{i-1j-1k} - 4\phi^{n+1}_{ij-1k} + 2\phi^{n+1}_{i-1jk} + 4\phi^{n+1}_{ijk} \end{pmatrix} \\
&+D\tfrac{h_2k_1}{36l_1}\begin{pmatrix} -2\phi^{n+1}_{ij-1k-1} - \phi^{n+1}_{i+1j-1k-1} + 2\phi^{n+1}_{ijk-1} + \phi^{n+1}_{i+1jk-1} \\ -4\phi^{n+1}_{ij-1k} - 2\phi^{n+1}_{i+1j-1k} + 4\phi^{n+1}_{ijk} + 2\phi^{n+1}_{i+1jk} \end{pmatrix} \\
&+D\tfrac{h_1k_2}{36l_2}\begin{pmatrix} 2\phi^{n+1}_{i-1jk} + 4\phi^{n+1}_{ijk} - 2\phi^{n+1}_{i-1j+1k} - 4\phi^{n+1}_{ij+1k} \\ +\phi^{n+1}_{i-1jk+1} + 2\phi^{n+1}_{ijk+1} - \phi^{n+1}_{i-1j+1k+1} - 2\phi^{n+1}_{ij+1k+1} \end{pmatrix} \\
&+D\tfrac{h_2k_2}{36l_2}\begin{pmatrix} 4\phi^{n+1}_{ijk} + 2\phi^{n+1}_{i+1jk} - 4\phi^{n+1}_{ij+1k} - 2\phi^{n+1}_{i+1j+1k} \\ +2\phi^{n+1}_{ijk+1} + \phi^{n+1}_{i+1jk+1} - 2\phi^{n+1}_{ij+1k+1} - \phi^{n+1}_{i+1j+1k+1} \end{pmatrix} \\
&+D\tfrac{h_1k_1}{36l_2}\begin{pmatrix} -2\phi^{n+1}_{i-1j-1k} - 4\phi^{n+1}_{ij-1k} + 2\phi^{n+1}_{i-1jk} + 4\phi^{n+1}_{ijk} \\ -\phi^{n+1}_{i-1j-1k+1} - 2\phi^{n+1}_{ij-1k+1} + \phi^{n+1}_{i-1jk+1} + 2\phi^{n+1}_{ijk+1} \end{pmatrix} \\
&+D\tfrac{h_2k_1}{36l_2}\begin{pmatrix} -4\phi^{n+1}_{ij-1k} - 2\phi^{n+1}_{i+1j-1k} + 4\phi^{n+1}_{ijk} + 2\phi^{n+1}_{i+1jk} \\ -2\phi^{n+1}_{ij-1k+1} - \phi^{n+1}_{i+1j-1k+1} + 2\phi^{n+1}_{ijk+1} + \phi^{n+1}_{i+1jk+1} \end{pmatrix}
\end{aligned}
\tag{B.36}
$$

In the next step, the convection terms are presented. As it is shown in equation B.31, the convection part has three components made up of three matrices S^{22}_{ij},S^{33}_{ij}, and S^{44}_{ij}.

The first component is

$$
\begin{aligned}
&\phi_x \; component \; of \; convection \; part = \\
&u\frac{k_2 l_1}{72}\begin{pmatrix} -2\phi^n_{i-1jk-1} + 2\phi^n_{ijk-1} + \phi^n_{i-1j+1k-1} - \phi^n_{ij+1k-1} \\ -4\phi^n_{i-1jk} + 4\phi^n_{ijk} + 2\phi^n_{i-1j+1k} - 2\phi^n_{ij+1k} \end{pmatrix} \\
&+u\frac{k_2 l_1}{72}\begin{pmatrix} -2\phi^n_{ijk-1} + 2\phi^n_{i+1jk-1} + \phi^n_{ij+1k-1} - \phi^n_{i+1j+1k-1} \\ -4\phi^n_{ijk} + 4\phi^n_{i+1jk} + 2\phi^n_{ij+1k} - 2\phi^n_{i+1j+1k} \end{pmatrix} \\
&+u\tfrac{k_1 l_1}{72}\begin{pmatrix} -\phi^n_{i-1j-1k-1} + \phi^n_{ij-1k-1} + 2\phi^n_{i-1jk-1} - 2\phi^n_{ijk-1} \\ -2\phi^n_{i-1j-1k} + 2\phi^n_{ij-1k} + 4\phi^n_{i-1jk} - 4\phi^n_{ijk} \end{pmatrix} \\
&+u\tfrac{k_1 l_1}{72}\begin{pmatrix} -\phi^n_{ij-1k-1} + \phi^n_{i+1j-1k-1} + 2\phi^n_{ijk-1} - 2\phi^n_{i+1jk-1} \\ -2\phi^n_{ij-1k} + 2\phi^n_{i+1j-1k} + 4\phi^n_{ijk} - 4\phi^n_{i+1jk} \end{pmatrix} \\
&+u\tfrac{k_2 l_2}{72}\begin{pmatrix} -4\phi^n_{i-1jk} + 4\phi^n_{ijk} + 2\phi^n_{i-1j+1k} - 2\phi^n_{ij+1k} \\ -2\phi^n_{i-1jk+1} + 2\phi^n_{ijk+1} + \phi^n_{i-1j+1k+1} - \phi^n_{ij+1k+1} \end{pmatrix} \\
&+u\tfrac{k_2 l_2}{72}\begin{pmatrix} -4\phi^n_{ijk} + 4\phi^n_{i+1jk} + 2\phi^n_{ij+1k} - 2\phi^n_{i+1j+1k} \\ -2\phi^n_{ijk+1} + 2\phi^n_{i+1jk+1} + \phi^n_{ij+1k+1} - \phi^n_{i+1j+1k+1} \end{pmatrix} \\
&+u\tfrac{k_1 l_2}{72}\begin{pmatrix} -2\phi^n_{i-1j-1k} + 2\phi^n_{ij-1k} + 4\phi^n_{i-1jk} - 4\phi^n_{ijk} \\ -\phi^n_{i-1j-1k+1} + \phi^n_{ij-1k+1} + 2\phi^n_{i-1jk+1} - 2\phi^n_{ijk+1} \end{pmatrix} \\
&+u\tfrac{k_1 l_2}{72}\begin{pmatrix} -2\phi^n_{ij-1k} + 2\phi^n_{i+1j-1k} + 4\phi^n_{ijk} - 4\phi^n_{i+1jk} \\ -\phi^n_{ij-1k+1} + \phi^n_{i+1j-1k+1} + 2\phi^n_{ijk+1} - 2\phi^n_{i+1jk+1} \end{pmatrix}
\end{aligned}
\tag{B.37}
$$

The second component of convection part of equation B.31 is

$$
\begin{aligned}
&\phi_y \textit{ component of convection part} = \\
&v\frac{h_1 l_1}{72}\begin{pmatrix} -\phi^n_{i-1jk-1} - 2\phi^n_{ijk-1} + 2\phi^n_{i-1j+1k-1} + \phi^n_{ij+1k-1} \\ -2\phi^n_{i-1jk} - 4\phi^n_{ijk} + 4\phi^n_{i-1j+1k} + 2\phi^n_{ij+1k} \end{pmatrix} \\
&+v\tfrac{h_2 l_1}{72}\begin{pmatrix} -2\phi^n_{ijk-1} - \phi^n_{i+1jk-1} + \phi^n_{ij+1k-1} + 2\phi^n_{i+1j+1k-1} \\ -4\phi^n_{ijk} - 2\phi^n_{i+1jk} + 2\phi^n_{ij+1k} + 4\phi^n_{i+1j+1k} \end{pmatrix} \\
&+v\tfrac{h_1 l_1}{72}\begin{pmatrix} -2\phi^n_{i-1j-1k-1} - \phi^n_{ij-1k-1} + \phi^n_{i-1jk-1} + 2\phi^n_{ijk-1} \\ -4\phi^n_{i-1j-1k} - 2\phi^n_{ij-1k} + 2\phi^n_{i-1jk} + 4\phi^n_{ijk} \end{pmatrix} \\
&+v\tfrac{h_2 l_1}{72}\begin{pmatrix} -\phi^n_{ij-1k-1} - 2\phi^n_{i+1j-1k-1} + 2\phi^n_{ijk-1} + \phi^n_{i+1jk-1} \\ -2\phi^n_{ij-1k} - 4\phi^n_{i+1j-1k} + 4\phi^n_{ijk} + 2\phi^n_{i+1jk} \end{pmatrix} \\
&+v\tfrac{h_1 l_2}{72}\begin{pmatrix} -2\phi^n_{i-1jk} - 4\phi^n_{ijk} + 4\phi^n_{i-1j+1k} + 2\phi^n_{ij+1k} \\ -\phi^n_{i-1jk+1} - 2\phi^n_{ijk+1} + 2\phi^n_{i-1j+1k+1} + \phi^n_{ij+1k+1} \end{pmatrix} \\
&+v\tfrac{h_2 l_2}{72}\begin{pmatrix} -4\phi^n_{ijk} - 2\phi^n_{i+1jk} + 2\phi^n_{ij+1k} + 4\phi^n_{i+1j+1k} \\ -2\phi^n_{ijk+1} - \phi^n_{i+1jk+1} + \phi^n_{ij+1k+1} + 2\phi^n_{i+1j+1k+1} \end{pmatrix} \\
&+v\tfrac{h_1 l_2}{72}\begin{pmatrix} -4\phi^n_{i-1j-1k} - 2\phi^n_{ij-1k} + 2\phi^n_{i-1jk} + 4\phi^n_{ijk} \\ -2\phi^n_{i-1j-1k+1} - \phi^n_{ij-1k+1} + \phi^n_{i-1jk+1} + 2\phi^n_{ijk+1} \end{pmatrix} \\
&+v\tfrac{h_2 l_2}{72}\begin{pmatrix} -2\phi^n_{ij-1k} - 4\phi^n_{i+1j-1k} + 4\phi^n_{ijk} + 2\phi^n_{i+1jk} \\ -\phi^n_{ij-1k+1} - 2\phi^n_{i+1j-1k+1} + 2\phi^n_{ijk+1} + \phi^n_{i+1jk+1} \end{pmatrix}
\end{aligned}
\tag{B.38}
$$

The final component of convection part is

$$
\begin{aligned}
&\phi_z \; component \; of \; convection \; part = \\
&w\frac{h_1k_2}{72}\begin{pmatrix} -2\phi^n_{i-1jk-1} - 4\phi^n_{ijk-1} - 2\phi^n_{i-1j+1k-1} - \phi^n_{ij+1k-1} \\ +2\phi^n_{i-1jk} + 4\phi^n_{ijk} + 2\phi^n_{i-1j+1k} + \phi^n_{ij+1k} \end{pmatrix} \\
&+w\frac{h_2k_2}{72}\begin{pmatrix} -4\phi^n_{ijk-1} - 2\phi^n_{i+1jk-1} - \phi^n_{ij+1k-1} - 2\phi^n_{i+1j+1k-1} \\ +4\phi^n_{ijk} + 2\phi^n_{i+1jk} + \phi^n_{ij+1k} + 2\phi^n_{i+1j+1k} \end{pmatrix} \\
&+w\tfrac{h_1k_1}{72}\begin{pmatrix} -2\phi^n_{i-1j-1k-1} - \phi^n_{ij-1k-1} - 2\phi^n_{i-1jk-1} - 4\phi^n_{ijk-1} \\ +2\phi^n_{i-1j-1k} + \phi^n_{ij-1k} + 2\phi^n_{i-1jk} + 4\phi^n_{ijk} \end{pmatrix} \\
&+w\tfrac{h_2k_1}{72}\begin{pmatrix} -\phi^n_{ij-1k-1} - 2\phi^n_{i+1j-1k-1} - 4\phi^n_{ijk-1} - 2\phi^n_{i+1jk-1} \\ +\phi^n_{ij-1k} + 2\phi^n_{i+1j-1k} + 4\phi^n_{ijk} + 2\phi^n_{i+1jk} \end{pmatrix} \\
&+w\tfrac{h_1k_2}{72}\begin{pmatrix} -2\phi^n_{i-1jk} - 4\phi^n_{ijk} - 2\phi^n_{i-1j+1k} - \phi^n_{ij+1k} \\ +2\phi^n_{i-1jk+1} + 4\phi^n_{ijk+1} + 2\phi^n_{i-1j+1k+1} + \phi^n_{ij+1k+1} \end{pmatrix} \\
&+w\tfrac{h_2k_2}{72}\begin{pmatrix} -4\phi^n_{ijk} - 2\phi^n_{i+1jk} - \phi^n_{ij+1k} - 2\phi^n_{i+1j+1k} \\ +4\phi^n_{ijk+1} + 2\phi^n_{i+1jk+1} + \phi^n_{ij+1k+1} + 2\phi^n_{i+1j+1k+1} \end{pmatrix} \\
&+w\tfrac{h_1k_1}{72}\begin{pmatrix} -2\phi^n_{i-1j-1k} - \phi^n_{ij-1k} - 2\phi^n_{i-1jk} - 4\phi^n_{ijk} \\ +2\phi^n_{i-1j-1k+1} + \phi^n_{ij-1k+1} + 2\phi^n_{i-1jk+1} + 4\phi^n_{ijk+1} \end{pmatrix} \\
&+w\tfrac{h_2k_1}{72}\begin{pmatrix} -\phi^n_{ij-1k} - 2\phi^n_{i+1j-1k} - 4\phi^n_{ijk} - 2\phi^n_{i+1jk} \\ +\phi^n_{ij-1k+1} + 2\phi^n_{i+1j-1k+1} + 4\phi^n_{ijk+1} + 2\phi^n_{i+1jk+1} \end{pmatrix}
\end{aligned}
\tag{B.39}
$$

Finally, the time derivative component of differential equation is

$$
\begin{aligned}
&Time\ derivative\ component\ of\ DE = \\
&\frac{h_1k_2l_1}{216}\begin{pmatrix} 2\dot{\phi}_{i-1jk-1} + 4\dot{\phi}_{ijk-1} + \dot{\phi}_{i-1j+1k-1} + 2\dot{\phi}_{ij+1k-1} \\ +4\dot{\phi}_{i-1jk} + 8\dot{\phi}_{ijk} + 2\dot{\phi}_{i-1j+1k} + 4\dot{\phi}_{ij+1k} \end{pmatrix} \\
&+\frac{h_2k_2l_1}{216}\begin{pmatrix} 4\dot{\phi}_{ijk-1} + 2\dot{\phi}_{i+1jk-1} + 2\dot{\phi}_{ij+1k-1} + \dot{\phi}_{i+1j+1k-1} \\ +8\dot{\phi}_{ijk} + 4\dot{\phi}_{i+1jk} + 4\dot{\phi}_{ij+1k} + 2\dot{\phi}_{i+1j+1k} \end{pmatrix} \\
&+\frac{h_1k_1l_1}{216}\begin{pmatrix} \dot{\phi}_{i-1j-1k-1} + 2\dot{\phi}_{ij-1k-1} + 2\dot{\phi}_{i-1jk-1} + 4\dot{\phi}_{ijk-1} \\ +2\dot{\phi}_{i-1j-1k} + 4\dot{\phi}_{ij-1k} + 4\dot{\phi}_{i-1jk} + 8\dot{\phi}_{ijk} \end{pmatrix} \\
&+\frac{h_2k_1l_1}{216}\begin{pmatrix} 2\dot{\phi}_{ij-1k-1} + \dot{\phi}_{i+1j-1k-1} + 4\dot{\phi}_{ijk-1} + 2\dot{\phi}_{i+1jk-1} \\ +4\dot{\phi}_{ij-1k} + 2\dot{\phi}_{i+1j-1k} + 8\dot{\phi}_{ijk} + 4\dot{\phi}_{i+1jk} \end{pmatrix} \\
&+\frac{h_1k_2l_2}{216}\begin{pmatrix} 4\dot{\phi}_{i-1jk} + 8\dot{\phi}_{ijk} + 2\dot{\phi}_{i-1j+1k} + 4\dot{\phi}_{ij+1k} \\ +2\dot{\phi}_{i-1jk+1} + 4\dot{\phi}_{ijk+1} + \dot{\phi}_{i-1j+1k+1} + 2\dot{\phi}_{ij+1k+1} \end{pmatrix} \\
&+\frac{h_2k_2l_2}{216}\begin{pmatrix} 8\dot{\phi}_{ijk} + 4\dot{\phi}_{i+1jk} + 4\dot{\phi}_{ij+1k} + 2\dot{\phi}_{i+1j+1k} \\ +4\dot{\phi}_{ijk+1} + 2\dot{\phi}_{i+1jk+1} + 2\dot{\phi}_{ij+1k+1} + \dot{\phi}_{i+1j+1k+1} \end{pmatrix} \\
&+\frac{h_1k_1l_2}{216}\begin{pmatrix} 2\dot{\phi}_{i-1j-1k} + 4\dot{\phi}_{ij-1k} + 4\dot{\phi}_{i-1jk} + 8\dot{\phi}_{ijk} \\ +\dot{\phi}_{i-1j-1k+1} + 2\dot{\phi}_{ij-1k+1} + 2\dot{\phi}_{i-1jk+1} + 4\dot{\phi}_{ijk+1} \end{pmatrix} \\
&+\frac{h_2k_1l_2}{216}\begin{pmatrix} 4\dot{\phi}_{ij-1k} + 2\dot{\phi}_{i+1j-1k} + 8\dot{\phi}_{ijk} + 4\dot{\phi}_{i+1jk} \\ +2\dot{\phi}_{ij-1k+1} + \dot{\phi}_{i+1j-1k+1} + 4\dot{\phi}_{ijk+1} + 2\dot{\phi}_{i+1jk+1} \end{pmatrix}
\end{aligned}
\tag{B.40}
$$

where $\dot{\phi} \cong \frac{1}{\Delta t}\left(\phi^{n+1} - \phi^{n}\right)$

All the terms in DE are expanded in Taylor series about $\phi_{i\,j\,k}^{n+1}$. For example:

$$\phi_{i-1j-1k-1} = \phi_{ijk} - \Big(h_1(\phi_{ijk})_x + k_1(\phi_{ijk})_y + l_1(\phi_{ijk})_z\Big)$$
$$+\frac{1}{2!}\begin{pmatrix} {h_1}^2(\phi_{ijk})_{xx} + 2h_1k_1(\phi_{ijk})_{xy} + 2h_1l_1(\phi_{ijk})_{xz} \\ +{k_1}^2(\phi_{ijk})_{yy} + 2k_1l_1(\phi_{ijk})_{yz} + {l_1}^2(\phi_{ijk})_{zz} \end{pmatrix}$$
$$-\frac{1}{3!}\begin{pmatrix} {h_1}^3(\phi_{ijk})_{xxx} + 3{h_1}^2k_1(\phi_{ijk})_{xxy} + 3{h_1}^2l_1(\phi_{ijk})_{xxz} \\ +3h_1{k_1}^2(\phi_{ijk})_{xyy} + 6h_1k_1l_1(\phi_{ijk})_{xyz} + 3h_1{l_1}^2(\phi_{ijk})_{xzz} \\ +{k_1}^3(\phi_{ijk})_{yyy} + 3{k_1}^2l_1(\phi_{ijk})_{yyz} + 3k_1{l_1}^2(\phi_{ijk})_{yzz} + {l_1}^3(\phi_{ijk})_{zzz} \end{pmatrix}$$

and

$$\phi_{i+1j+1k+1} = \phi_{ijk} + \Big(h_2(\phi_{ijk})_x + k_2(\phi_{ijk})_y + l_2(\phi_{ijk})_z\Big)$$
$$+\frac{1}{2!}\begin{pmatrix} {h_2}^2(\phi_{ijk})_{xx} + 2h_2k_2(\phi_{ijk})_{xy} + 2h_2l_2(\phi_{ijk})_{xz} \\ +{k_2}^2(\phi_{ijk})_{yy} + 2k_2l_2(\phi_{ijk})_{yz} + {l_2}^2(\phi_{ijk})_{zz} \end{pmatrix}$$
$$+\frac{1}{3!}\begin{pmatrix} {h_2}^3(\phi_{ijk})_{xxx} + 3{h_2}^2k_2(\phi_{ijk})_{xxy} + 3{h_2}^2l_2(\phi_{ijk})_{xxz} \\ +3h_2{k_2}^2(\phi_{ijk})_{xyy} + 6h_2k_2l_2(\phi_{ijk})_{xyz} + 3h_2{l_2}^2(\phi_{ijk})_{xzz} \\ +{k_2}^3(\phi_{ijk})_{yyy} + 3{k_2}^2l_2(\phi_{ijk})_{yyz} + 3k_2{l_2}^2(\phi_{ijk})_{yzz} + {l_2}^3(\phi_{ijk})_{zzz} \end{pmatrix}$$

The diffusion terms, convection terms, and time derivation terms in equation B.31 are shown respectively on the following pages. First, the diffusion parts shown in three parts about $\phi_{i\,j\,k}^{n+1}$ are

$$\phi_{xx} \ \ component\ of\ diffusion\ terms =$$
$$\frac{D}{36}\left(\begin{array}{l} -\frac{1}{2!}9\left(\begin{array}{l} h_1k_1l_1+h_2k_1l_1+h_1k_2l_1+h_2k_2l_1 \\ +h_1k_1l_2+h_2k_1l_2+h_1k_2l_2+h_2k_2l_2 \end{array}\right)\left(\phi^{n+1}_{ijk}\right)_{xx} \\ +\frac{1}{3!}9\left(\begin{array}{l} h_1^2k_1l_1-h_2^2k_1l_1+h_1^2k_2l_1-h_2^2k_2l_1 \\ +h_1^2k_1l_2-h_2^2k_1l_2+h_1^2k_2l_2-h_2^2k_2l_2 \end{array}\right)\left(\phi^{n+1}_{ijk}\right)_{xxx} \\ +\frac{1}{3!}9\left(\begin{array}{l} -h_1k_1^2l_1-h_2k_1^2l_1+h_1k_2^2l_1+h_2k_2^2l_1 \\ -h_1k_1^2l_2-h_2k_1^2l_2+h_1k_2^2l_2+h_2k_2^2l_2 \end{array}\right)\left(\phi^{n+1}_{ijk}\right)_{xxy} \\ +\frac{1}{3!}9\left(\begin{array}{l} h_1k_1l_1^2+h_2k_1l_1^2+h_1k_2l_1^2+h_2k_2l_1^2 \\ -h_1k_1l_2^2-h_2k_1l_2^2-h_1k_2l_2^2-h_2k_2l_2^2 \end{array}\right)\left(\phi^{n+1}_{ijk}\right)_{xxz} \end{array}\right) \tag{B.41}$$

the second component of diffusion part is

$$\phi_{yy}\ component\ of\ diffusion\ terms =$$
$$\frac{D}{36}\left(\begin{array}{l} -\frac{1}{2!}9\left(\begin{array}{l} h_1k_1l_1+h_2k_1l_1+h_1k_2l_1+h_2k_2l_1 \\ +h_1k_1l_2+h_2k_1l_2+h_1k_2l_2+h_2k_2l_2 \end{array}\right)\left(\phi^{n+1}_{ijk}\right)_{yy} \\ +\frac{1}{3!}9\left(\begin{array}{l} h_1^2k_1l_1-h_2^2k_1l_1+h_1^2k_2l_1-h_2^2k_2l_1 \\ +h_1^2k_1l_2-h_2^2k_1l_2+h_1^2k_2l_2-h_2^2k_2l_2 \end{array}\right)\left(\phi^{n+1}_{ijk}\right)_{xyy} \\ +\frac{1}{3!}9\left(\begin{array}{l} -h_1k_1^2l_1-h_2k_1^2l_1+h_1k_2^2l_1+h_2k_2^2l_1 \\ -h_1k_1^2l_2-h_2k_1^2l_2+h_1k_2^2l_2+h_2k_2^2l_2 \end{array}\right)\left(\phi^{n+1}_{ijk}\right)_{yyy} \\ +\frac{1}{3!}9\left(\begin{array}{l} h_1k_1l_1^2+h_2k_1l_1^2+h_1k_2l_1^2+h_2k_2l_1^2 \\ -h_1k_1l_2^2-h_2k_1l_2^2-h_1k_2l_2^2-h_2k_2l_2^2 \end{array}\right)\left(\phi^{n+1}_{ijk}\right)_{yyz} \end{array}\right) \tag{B.42}$$

Final component of diffusion part is

$$\phi_{zz}\ component\ of\ diffusion\ terms =$$

$$\frac{D}{36}\left(\begin{array}{l} -\frac{1}{2!}9\begin{pmatrix} h_1k_1l_1 + h_2k_1l_1 + h_1k_2l_1 + h_2k_2l_1 \\ +h_1k_1l_2 + h_2k_1l_2 + h_1k_2l_2 + h_2k_2l_2 \end{pmatrix}\left(\phi_{ijk}^{n+1}\right)_{zz} \\ +\frac{1}{3!}9\begin{pmatrix} h_1^2k_1l_1 - h_2^2k_1l_1 + h_1^2k_2l_1 - h_2^2k_2l_1 \\ +h_1^2k_1l_2 - h_2^2k_1l_2 + h_1^2k_2l_2 - h_2^2k_2l_2 \end{pmatrix}\left(\phi_{ijk}^{n+1}\right)_{xzz} \\ +\frac{1}{3!}9\begin{pmatrix} -h_1k_1^2l_1 - h_2k_1^2l_1 + h_1k_2^2l_1 + h_2k_2^2l_1 \\ -h_1k_1^2l_2 - h_2k_1^2l_2 + h_1k_2^2l_2 + h_2k_2^2l_2 \end{pmatrix}\left(\phi_{ijk}^{n+1}\right)_{yzz} \\ +\frac{1}{3!}9\begin{pmatrix} h_1k_1l_1^2 + h_2k_1l_1^2 + h_1k_2l_1^2 + h_2k_2l_1^2 \\ -h_1k_1l_2^2 - h_2k_1l_2^2 - h_1k_2l_2^2 - h_2k_2l_2^2 \end{pmatrix}\left(\phi_{ijk}^{n+1}\right)_{zzz} \end{array}\right) \tag{B.43}$$

The summation of diffusion terms is

$$\frac{D}{36}\left(\begin{array}{l}
-\frac{1}{2!}9\left(\begin{array}{l}h_1k_1l_1+h_2k_1l_1+h_1k_2l_1+h_2k_2l_1\\+h_1k_1l_2+h_2k_1l_2+h_1k_2l_2+h_2k_2l_2\end{array}\right)\left(\phi_{ijk}^{n+1}\right)_{xx}\\
-\frac{1}{2!}9\left(\begin{array}{l}h_1k_1l_1+h_2k_1l_1+h_1k_2l_1+h_2k_2l_1\\+h_1k_1l_2+h_2k_1l_2+h_1k_2l_2+h_2k_2l_2\end{array}\right)\left(\phi_{ijk}^{n+1}\right)_{yy}\\
-\frac{1}{2!}9\left(\begin{array}{l}h_1k_1l_1+h_2k_1l_1+h_1k_2l_1+h_2k_2l_1\\+h_1k_1l_2+h_2k_1l_2+h_1k_2l_2+h_2k_2l_2\end{array}\right)\left(\phi_{ijk}^{n+1}\right)_{zz}\\
+\frac{1}{3!}9\left(\begin{array}{l}h_1^2k_1l_1-h_2^2k_1l_1+h_1^2k_2l_1-h_2^2k_2l_1\\+h_1^2k_1l_2-h_2^2k_1l_2+h_1^2k_2l_2-h_2^2k_2l_2\end{array}\right)\left(\phi_{ijk}^{n+1}\right)_{xxx}\\
+\frac{1}{3!}9\left(\begin{array}{l}-h_1k_1^2l_1-h_2k_1^2l_1+h_1k_2^2l_1+h_2k_2^2l_1\\-h_1k_1^2l_2-h_2k_1^2l_2+h_1k_2^2l_2+h_2k_2^2l_2\end{array}\right)\left(\phi_{ijk}^{n+1}\right)_{yyy}\\
+\frac{1}{3!}9\left(\begin{array}{l}h_1k_1l_1^2+h_2k_1l_1^2+h_1k_2l_1^2+h_2k_2l_1^2\\-h_1k_1l_2^2-h_2k_1l_2^2-h_1k_2l_2^2-h_2k_2l_2^2\end{array}\right)\left(\phi_{ijk}^{n+1}\right)_{zzz}\\
+\frac{1}{3!}9\left(\begin{array}{l}-h_1k_1^2l_1-h_2k_1^2l_1+h_1k_2^2l_1+h_2k_2^2l_1\\-h_1k_1^2l_2-h_2k_1^2l_2+h_1k_2^2l_2+h_2k_2^2l_2\end{array}\right)\left(\phi_{ijk}^{n+1}\right)_{xxy}\\
+\frac{1}{3!}9\left(\begin{array}{l}h_1k_1l_1^2+h_2k_1l_1^2+h_1k_2l_1^2+h_2k_2l_1^2\\-h_1k_1l_2^2-h_2k_1l_2^2-h_1k_2l_2^2-h_2k_2l_2^2\end{array}\right)\left(\phi_{ijk}^{n+1}\right)_{xxz}\\
+\frac{1}{3!}9\left(\begin{array}{l}h_1^2k_1l_1-h_2^2k_1l_1+h_1^2k_2l_1-h_2^2k_2l_1\\+h_1^2k_1l_2-h_2^2k_1l_2+h_1^2k_2l_2-h_2^2k_2l_2\end{array}\right)\left(\phi_{ijk}^{n+1}\right)_{xyy}\\
+\frac{1}{3!}9\left(\begin{array}{l}h_1^2k_1l_1-h_2^2k_1l_1+h_1^2k_2l_1-h_2^2k_2l_1\\+h_1^2k_1l_2-h_2^2k_1l_2+h_1^2k_2l_2-h_2^2k_2l_2\end{array}\right)\left(\phi_{ijk}^{n+1}\right)_{xzz}\\
+\frac{1}{3!}9\left(\begin{array}{l}h_1k_1l_1^2+h_2k_1l_1^2+h_1k_2l_1^2+h_2k_2l_1^2\\-h_1k_1l_2^2-h_2k_1l_2^2-h_1k_2l_2^2-h_2k_2l_2^2\end{array}\right)\left(\phi_{ijk}^{n+1}\right)_{yyz}\\
+\frac{1}{3!}9\left(\begin{array}{l}-h_1k_1^2l_1-h_2k_1^2l_1+h_1k_2^2l_1+h_2k_2^2l_1\\-h_1k_1^2l_2-h_2k_1^2l_2+h_1k_2^2l_2+h_2k_2^2l_2\end{array}\right)\left(\phi_{ijk}^{n+1}\right)_{yzz}
\end{array}\right) \tag{B.44}$$

After some mathematical manipulations the diffusion terms are

$$Diffusion\ term = \frac{1}{8}\left(h_1 + h_2\right)\left(k_1 + k_2\right)\left(l_1 + l_2\right) \times$$

$$D\left(\begin{array}{l} -\left(\phi_{ijk}^{n+1}\right)_{xx} - \left(\phi_{ijk}^{n+1}\right)_{yy} - \left(\phi_{ijk}^{n+1}\right)_{zz} \\ +\frac{1}{3}\left(h_1 - h_2\right)\left(\left(\phi_{ijk}^{n+1}\right)_{xxx} + \left(\phi_{ijk}^{n+1}\right)_{xyy} + \left(\phi_{ijk}^{n+1}\right)_{xzz}\right) \\ +\frac{1}{3}\left(k_1 - k_2\right)\left(\left(\phi_{ijk}^{n+1}\right)_{xxy} + \left(\phi_{ijk}^{n+1}\right)_{yyy} + \left(\phi_{ijk}^{n+1}\right)_{zzy}\right) \\ +\frac{1}{3}\left(l_1 - l_2\right)\left(\left(\phi_{ijk}^{n+1}\right)_{xxz} + \left(\phi_{ijk}^{n+1}\right)_{yyz} + \left(\phi_{ijk}^{n+1}\right)_{zzz}\right) \end{array}\right) \tag{B.45}$$

In the next step, all the terms in convection part of equation B.31 are expanded in Taylor series about $\phi_{i\,j\,k}^{n+1}$

First part is

$$\frac{u}{72}\left(\begin{array}{l}
+9\begin{pmatrix} h_1k_1l_1+h_2k_1l_1+h_1k_2l_1+h_2k_2l_1 \\ +h_1k_1l_2+h_2k_1l_2+h_1k_2l_2+h_2k_2l_2 \end{pmatrix}\left(\phi_{ijk}^{n}\right)_x \\
+\frac{1}{2!}9\begin{pmatrix} -h_1^2k_1l_1+h_2^2k_1l_1-h_1^2k_2l_1+h_2^2k_2l_1 \\ -h_1^2k_1l_2+h_2^2k_1l_2-h_1^2k_2l_2+h_2^2k_2l_2 \end{pmatrix}\left(\phi_{ijk}^{n}\right)_{xx} \\
+\frac{1}{2!}6\begin{pmatrix} h_1k_1^2l_1+h_2k_1^2l_1-h_1k_2^2l_1-h_2k_2^2l_1 \\ +h_1k_1^2l_2+h_2k_1^2l_2-h_1k_2^2l_2-h_2k_2^2l_2 \end{pmatrix}\left(\phi_{ijk}^{n}\right)_{xy} \\
+\frac{1}{2!}6\begin{pmatrix} -h_1k_1l_1^2-h_2k_1l_1^2-h_1k_2l_1^2-h_2k_2l_1^2 \\ +h_1k_1l_2^2+h_2k_1l_2^2+h_1k_2l_2^2+h_2k_2l_2^2 \end{pmatrix}\left(\phi_{ijk}^{n}\right)_{xz} \\
+\frac{1}{3!}9\begin{pmatrix} h_1^3k_1l_1+h_2^3k_1l_1+h_1^3k_2l_1+h_2^3k_2l_1 \\ +h_1^3k_1l_2+h_2^3k_1l_2+h_1^3k_2l_2+h_2^3k_2l_2 \end{pmatrix}\left(\phi_{ijk}^{n}\right)_{xxx} \\
+\frac{1}{3!}9\begin{pmatrix} -h_1^2k_1^2l_1+h_2^2k_1^2l_1+h_1^2k_2^2l_1-h_2^2k_2^2l_1 \\ -h_1^2k_1^2l_2+h_2^2k_1^2l_2+h_1^2k_2^2l_2-h_2^2k_2^2l_2 \end{pmatrix}\left(\phi_{ijk}^{n}\right)_{xxy} \\
+\frac{1}{3!}9\begin{pmatrix} h_1^2k_1l_1^2-h_2^2k_1l_1^2+h_1^2k_2l_1^2-h_2^2k_2l_1^2 \\ -h_1^2k_1l_2^2+h_2^2k_1l_2^2-h_1^2k_2l_2^2+h_2^2k_2l_2^2 \end{pmatrix}\left(\phi_{ijk}^{n}\right)_{xxz} \\
+\frac{1}{3!}9\begin{pmatrix} h_1k_1^3l_1+h_2k_1^3l_1+h_1k_2^3l_1+h_2k_2^3l_1 \\ +h_1k_1^3l_2+h_2k_1^3l_2+h_1k_2^3l_2+h_2k_2^3l_2 \end{pmatrix}\left(\phi_{ijk}^{n}\right)_{xyy} \\
+\frac{1}{3!}6\begin{pmatrix} -h_1k_1^2l_1^2-h_2k_1^2l_1^2+h_1k_2^2l_1^2+h_2k_2^2l_1^2 \\ +h_1k_1^2l_2^2+h_2k_1^2l_2^2-h_1k_2^2l_2^2-h_2k_2^2l_2^2 \end{pmatrix}\left(\phi_{ijk}^{n}\right)_{xyz} \\
+\frac{1}{3!}9\begin{pmatrix} h_1k_1l_1^3+h_2k_1l_1^3+h_1k_2l_1^3+h_2k_2l_1^3 \\ +h_1k_1l_2^3+h_2k_1l_2^3+h_1k_2l_2^3+h_2k_2l_2^3 \end{pmatrix}\left(\phi_{ijk}^{n+1}\right)_{xzz}
\end{array}\right) \tag{B.46}$$

After some mathematical calculations the first part can be rewritten as

$$Convection\,part\,one = \frac{1}{8}\left(h_1+h_2\right)\left(k_1+k_2\right)\left(l_1+l_2\right)\times$$
$$u\begin{pmatrix} \left(\phi^n_{ijk}\right)_x \\ +\frac{1}{2}\left(h_2-h_1\right)\left(\phi^n_{ijk}\right)_{xx} \\ +\frac{1}{3}\left(k_2-k_1\right)\left(\phi^n_{ijk}\right)_{xy} \\ +\frac{1}{3}\left(l_2-l_1\right)\left(\phi^n_{ijk}\right)_{xz} \\ +\frac{1}{6}\left(h_1^2-h_1h_2+h_2^2\right)\left(\phi^n_{ijk}\right)_{xxx} \\ +\frac{1}{6}\left(h_2-h_1\right)\left(k_2-k_1\right)\left(\phi^n_{ijk}\right)_{xxy} \\ +\frac{1}{6}\left(h_1-h_2\right)\left(l_1-l_2\right)\left(\phi^n_{ijk}\right)_{xxz} \\ +\frac{1}{6}\left(k_1^2-k_1k_2+k_2^2\right)\left(\phi^n_{ijk}\right)_{xyy} \\ +\frac{1}{9}\left(k_1-k_2\right)\left(l_1-l_2\right)\left(\phi^n_{ijk}\right)_{xyz} \\ +\frac{1}{6}\left(l_1^2-l_1l_2+l_2^2\right)\left(\phi^{n+1}_{ijk}\right)_{xzz} \end{pmatrix} \tag{B.47}$$

the second component of convection part is

$$
\begin{aligned}
&\mathit{Convection\ part\,two} = \frac{1}{8}\left(h_1+h_2\right)\left(k_1+k_2\right)\left(l_1+l_2\right)\times \\
&v\left(\begin{array}{l}
\left(\phi_{ijk}^{n+1}\right)_y \\
+\frac{1}{3}\left(h_2-h_1\right)\left(\phi_{ijk}^{n+1}\right)_{xy} \\
+\frac{1}{2}\left(k_2-k_1\right)\left(\phi_{ijk}^{n+1}\right)_{yy} \\
+\frac{1}{3}\left(l_2-l_1\right)\left(\phi_{ijk}^{n+1}\right)_{yz} \\
+\frac{1}{6}\left(h_1^2-h_1h_2+h_2^2\right)\left(\phi_{ijk}^{n+1}\right)_{xxy} \\
+\frac{1}{6}\left(h_2-h_1\right)\left(k_2-k_1\right)\left(\phi_{ijk}^{n+1}\right)_{xyy} \\
+\frac{1}{9}\left(h_1-h_2\right)\left(l_1-l_2\right)\left(\phi_{ijk}^{n+1}\right)_{xyz} \\
+\frac{1}{6}\left(k_1^2-k_1k_2+k_2^2\right)\left(\phi_{ijk}^{n+1}\right)_{yyy} \\
+\frac{1}{6}\left(k_1-k_2\right)\left(l_1-l_2\right)\left(\phi_{ijk}^{n+1}\right)_{yyz} \\
+\frac{1}{6}\left(l_1^2-l_1l_2+l_2^2\right)\left(\phi_{ijk}^{n+1}\right)_{yzz}
\end{array}\right)
\end{aligned}
\tag{B.48}
$$

the last component of convection part is

$$Convection\ part\, three = \frac{1}{8}\left(h_1+h_2\right)\left(k_1+k_2\right)\left(l_1+l_2\right)\times$$
$$w\begin{pmatrix} \left(\phi^n_{ijk}\right)_z \\ +\frac{1}{3}\left(h_2-h_1\right)\left(\phi^n_{ijk}\right)_{xz} \\ +\frac{1}{3}\left(k_2-k_1\right)\left(\phi^n_{ijk}\right)_{yz} \\ +\frac{1}{2}\left(l_2-l_1\right)\left(\phi^n_{ijk}\right)_{zz} \\ +\frac{1}{6}\left(h_1^2-h_1h_2+h_2^2\right)\left(\phi^n_{ijk}\right)_{xxz} \\ +\frac{1}{9}\left(h_2-h_1\right)\left(k_2-k_1\right)\left(\phi^n_{ijk}\right)_{xyz} \\ +\frac{1}{6}\left(h_1-h_2\right)\left(l_1-l_2\right)\left(\phi^n_{ijk}\right)_{xzz} \\ +\frac{1}{6}\left(k_1^2-k_1k_2+k_2^2\right)\left(\phi^n_{ijk}\right)_{yyz} \\ +\frac{1}{6}\left(k_1-k_2\right)\left(l_1-l_2\right)\left(\phi^n_{ijk}\right)_{yzz} \\ +\frac{1}{6}\left(l_1^2-l_1l_2+l_2^2\right)\left(\phi^n_{ijk}\right)_{zzz} \end{pmatrix} \tag{B.49}$$

the summation of all three components of convection part is

$$Convection\ part\ = \frac{1}{8}\left(h_1+h_2\right)\left(k_1+k_2\right)\left(l_1+l_2\right)\times$$
$$\begin{pmatrix} u\left(\phi^n_{ijk}\right)_x+v\left(\phi^n_{ijk}\right)_y+w\left(\phi^n_{ijk}\right)_z \\ +\frac{1}{3}\left(h_2-h_1\right)\left(u\left(\phi^n_{ijk}\right)_{xx}+v\left(\phi^n_{ijk}\right)_{xy}+w\left(\phi^n_{ijk}\right)_{xz}\right)+\frac{u}{6}\left(h_2-h_1\right)\left(\phi^n_{ijk}\right)_{xx} \\ +\frac{1}{3}\left(k_2-k_1\right)\left(u\left(\phi^n_{ijk}\right)_{xy}+v\left(\phi^n_{ijk}\right)_{yy}+w\left(\phi^n_{ijk}\right)_{yz}\right)+\frac{v}{6}\left(k_2-k_1\right)\left(\phi^n_{ijk}\right)_{yy} \\ +\frac{1}{3}\left(l_2-l_1\right)\left(u\left(\phi^n_{ijk}\right)_{xz}+v\left(\phi^n_{ijk}\right)_{yz}+w\left(\phi^n_{ijk}\right)_{zz}\right)+\frac{w}{6}\left(l_2-l_1\right)\left(\phi^n_{ijk}\right)_{zz} \\ +O\left(h^2,\, hl,\, l^2\right) \end{pmatrix} \tag{B.50}$$

In this step, all the terms are expanded about $\phi^{n+1}_{i\,j\,k}$ by using temporal Taylor expansion

$$\phi^{n}_{ijk} = \phi^{n+1}_{ijk} - \Delta t\left(\phi^{n+1}_{ijk}\right)_t + \frac{\Delta t^2}{2}\left(\phi^{n+1}_{ijk}\right)_{tt} + O\left(\Delta t^3\right)$$

The convection part about $\phi^{n+1}_{i\,j}$ is

$$\begin{aligned}
&Convection\ part = \frac{1}{8}\left(h_1+h_2\right)\left(k_1+k_2\right)\left(l_1+l_2\right)\times\\
&\left(\begin{array}{l}
\left(\begin{array}{l}
u\left(\phi^{n+1}_{ijk}\right)_x + v\left(\phi^{n+1}_{ijk}\right)_y + w\left(\phi^{n+1}_{ijk}\right)_z\\
+\frac{1}{3}\left(h_2-h_1\right)\left(u\left(\phi^{n+1}_{ijk}\right)_{xx} + v\left(\phi^{n+1}_{ijk}\right)_{xy} + w\left(\phi^{n+1}_{ijk}\right)_{xz}\right) + \frac{u}{6}\left(h_2-h_1\right)\left(\phi^{n+1}_{ijk}\right)_{xx}\\
+\frac{1}{3}\left(k_2-k_1\right)\left(u\left(\phi^{n+1}_{ijk}\right)_{xy} + v\left(\phi^{n+1}_{ijk}\right)_{yy} + w\left(\phi^{n+1}_{ijk}\right)_{yz}\right) + \frac{v}{6}\left(k_2-k_1\right)\left(\phi^{n+1}_{ijk}\right)_{yy}\\
+\frac{1}{3}\left(l_2-l_1\right)\left(u\left(\phi^{n+1}_{ijk}\right)_{xz} + v\left(\phi^{n+1}_{ijk}\right)_{yz} + w\left(\phi^{n+1}_{ijk}\right)_{zz}\right) + \frac{w}{6}\left(l_2-l_1\right)\left(\phi^{n+1}_{ijk}\right)_{zz}
\end{array}\right)\\
-\Delta t\left(\begin{array}{l}
u\left(\phi^{n+1}_{ijk}\right)_{tx} + v\left(\phi^{n+1}_{ijk}\right)_{ty} + w\left(\phi^{n+1}_{ijk}\right)_{tz}\\
+\frac{1}{3}\left(h_2-h_1\right)\left(u\left(\phi^{n+1}_{ijk}\right)_{txx} + v\left(\phi^{n+1}_{ijk}\right)_{txy} + w\left(\phi^{n+1}_{ijk}\right)_{txz}\right) + \frac{u}{6}\left(h_2-h_1\right)\left(\phi^{n+1}_{ijk}\right)_{txx}\\
+\frac{1}{3}\left(k_2-k_1\right)\left(u\left(\phi^{n+1}_{ijk}\right)_{txy} + v\left(\phi^{n+1}_{ijk}\right)_{tyy} + w\left(\phi^{n+1}_{ijk}\right)_{tyz}\right) + \frac{v}{6}\left(k_2-k_1\right)\left(\phi^{n+1}_{ijk}\right)_{tyy}\\
+\frac{1}{3}\left(l_2-l_1\right)\left(u\left(\phi^{n+1}_{ijk}\right)_{txz} + v\left(\phi^{n+1}_{ijk}\right)_{tyz} + w\left(\phi^{n+1}_{ijk}\right)_{tzz}\right) + \frac{w}{6}\left(l_2-l_1\right)\left(\phi^{n+1}_{ijk}\right)_{tzz}
\end{array}\right)\\
+O\left(h^2,\, hl,\, l^2,\, \Delta t^2 ...\right)
\end{array}\right)
\end{aligned} \tag{B.51}$$

Last part, all the components of the time derivation part of equation B.31 are expanded about $\phi^{n+1}_{i\,j\,k}$ by using spatial and temporal Taylor expansion ($\phi^{n+1}_{ij} - \phi^{n}_{ij}$ is shown by $\Delta\phi_{ij}$). First spatial expansion:

$$\begin{aligned}
&\mathit{Time\ derivative\ part} = \\
&\quad \frac{h_1k_2l_1}{216}\left(27\dot{\phi}_{ijk} - 9h_1\left(\dot{\phi}_{ijk}\right)_x + 9k_2\left(\dot{\phi}_{ijk}\right)_y - 9l_1\left(\dot{\phi}_{ijk}\right)_z\right) \\
&+\frac{h_2k_2l_1}{216}\left(27\dot{\phi}_{ijk} + 9h_2\left(\dot{\phi}_{ijk}\right)_x + 9k_2\left(\dot{\phi}_{ijk}\right)_y - 9l_1\left(\dot{\phi}_{ijk}\right)_z\right) \\
&+\frac{h_1k_1l_1}{216}\left(27\dot{\phi}_{ijk} - 9h_1\left(\dot{\phi}_{ijk}\right)_x - 9k_1\left(\dot{\phi}_{ijk}\right)_y - 9l_1\left(\dot{\phi}_{ijk}\right)_z\right) \\
&+\frac{h_2k_1l_1}{216}\left(27\dot{\phi}_{ijk} + 9h_2\left(\dot{\phi}_{ijk}\right)_x - 9k_1\left(\dot{\phi}_{ijk}\right)_y - 9l_1\left(\dot{\phi}_{ijk}\right)_z\right) \\
&+\frac{h_1k_2l_2}{216}\left(27\dot{\phi}_{ijk} - 9h_1\left(\dot{\phi}_{ijk}\right)_x + 9k_2\left(\dot{\phi}_{ijk}\right)_y + 9l_2\left(\dot{\phi}_{ijk}\right)_z\right) \\
&+\frac{h_2k_2l_2}{216}\left(27\dot{\phi}_{ijk} + 9h_2\left(\dot{\phi}_{ijk}\right)_x + 9k_2\left(\dot{\phi}_{ijk}\right)_y + 9l_2\left(\dot{\phi}_{ijk}\right)_z\right) \\
&+\frac{h_1k_1l_2}{216}\left(27\dot{\phi}_{ijk} - 9h_1\left(\dot{\phi}_{ijk}\right)_x - 9k_1\left(\dot{\phi}_{ijk}\right)_y + 9l_2\left(\dot{\phi}_{ijk}\right)_z\right) \\
&+\frac{h_2k_1l_2}{216}\left(27\dot{\phi}_{ijk} + 9h_2\left(\dot{\phi}_{ijk}\right)_x - 9k_1\left(\dot{\phi}_{ijk}\right)_y + 9l_2\left(\dot{\phi}_{ijk}\right)_z\right) \\
&+\cdots
\end{aligned} \tag{B.52}$$

after rearranging the equation B.52 becomes

$$\begin{aligned}
&\mathit{Time\ derivative\ part} = \frac{1}{8}\left(h_1+h_2\right)\left(k_1+k_2\right)\left(l_1+l_2\right)\times \\
&\left(\dot{\phi}_{ijk} + \frac{1}{3}\left(h_2-h_1\right)\left(\dot{\phi}_{ijk}\right)_x + \frac{1}{3}\left(k_2-k_1\right)\left(\dot{\phi}_{ijk}\right)_y + \frac{1}{3}\left(l_2-l_1\right)\left(\dot{\phi}_{ijk}\right)_z\right) \\
&+\cdots
\end{aligned} \tag{B.53}$$

where $\dot{\phi} \cong \frac{1}{\Delta t}\left(\phi^{n+1}-\phi^{n}\right) = \frac{\Delta\phi}{\Delta t}$ and

$$\dot{\phi}_{ijk} = \frac{\Delta\phi_{ijk}}{\Delta t} = \frac{\phi^{n+1}_{ijk}-\phi^{n}_{ijk}}{\Delta t} = \left(\phi^{n+1}_{ijk}\right)_t - \frac{\Delta t}{2}\left(\phi^{n+1}_{ijk}\right)_{tt} + \frac{\Delta t^2}{6}\left(\phi^{n+1}_{ijk}\right)_{ttt} + O\left(\Delta t^3\right)$$

The final form of equation B.53 is

$$\begin{aligned}
&Time\ derivative\ part = \frac{1}{8}\left(h_1+h_2\right)\left(k_1+k_2\right)\left(l_1+l_2\right)\times \\
&\left(\begin{array}{l}
\left(\left(\phi_{ijk}^{n+1}\right)_t - \frac{\Delta t}{2}\left(\phi_{ijk}^{n+1}\right)_{tt} + O\left(\Delta t^2\right)\right) \\
+\frac{1}{3}\left(h_2-h_1\right)\left(\left(\phi_{ijk}^{n+1}\right)_t - \frac{\Delta t}{2}\left(\phi_{ijk}^{n+1}\right)_{tt} + O\left(\Delta t^2\right)\right)_x \\
+\frac{1}{3}\left(k_2-k_1\right)\left(\left(\phi_{ijk}^{n+1}\right)_t - \frac{\Delta t}{2}\left(\phi_{ijk}^{n+1}\right)_{tt} + O\left(\Delta t^2\right)\right)_y \\
+\frac{1}{3}\left(l_2-l_1\right)\left(\left(\phi_{ijk}^{n+1}\right)_t - \frac{\Delta t}{2}\left(\phi_{ijk}^{n+1}\right)_{tt} + O\left(\Delta t^2\right)\right)_z
\end{array}\right) \\
&+\cdots
\end{aligned} \tag{B.54}$$

Now, by assembling diffusion, convection, and time derivative parts, equations B.45, B.51, and B.54 respectively, the three dimensional truncation error terms in the Taylor expansion about $\phi_{i\,j}^{n+1}$ are

$$\begin{aligned}
DE &= \frac{\partial\phi}{\partial t} - D\left(\frac{\partial^2\phi}{\partial x^2}+\frac{\partial^2\phi}{\partial y^2}+\frac{\partial^2\phi}{\partial z^2}\right) + u\frac{\partial\phi}{\partial x} + v\frac{\partial\phi}{\partial y} + w\frac{\partial\phi}{\partial z} \\
&+\frac{1}{3}\left((h_2-h_1)\frac{\partial}{\partial x}\left(\frac{\partial\phi}{\partial t} - D\left(\frac{\partial^2\phi}{\partial x^2}+\frac{\partial^2\phi}{\partial y^2}+\frac{\partial^2\phi}{\partial z^2}\right) + u\frac{\partial\phi}{\partial x} + v\frac{\partial\phi}{\partial y} + w\frac{\partial\phi}{\partial z}\right)\right) \\
&+\frac{1}{3}\left((k_2-k_1)\frac{\partial}{\partial y}\left(\frac{\partial\phi}{\partial t} - D\left(\frac{\partial^2\phi}{\partial x^2}+\frac{\partial^2\phi}{\partial y^2}+\frac{\partial^2\phi}{\partial z^2}\right) + u\frac{\partial\phi}{\partial x} + v\frac{\partial\phi}{\partial y} + w\frac{\partial\phi}{\partial z}\right)\right) \\
&+\frac{1}{3}\left((l_2-l_1)\frac{\partial}{\partial z}\left(\frac{\partial\phi}{\partial t} - D\left(\frac{\partial^2\phi}{\partial x^2}+\frac{\partial^2\phi}{\partial y^2}+\frac{\partial^2\phi}{\partial z^2}\right) + u\frac{\partial\phi}{\partial x} + v\frac{\partial\phi}{\partial y} + w\frac{\partial\phi}{\partial z}\right)\right) \\
&+\frac{u}{6}(h_2-h_1)\frac{\partial^2\phi}{\partial x^2} + \frac{v}{6}(k_2-k_1)\frac{\partial^2\phi}{\partial y^2} + \frac{w}{6}(l_2-l_1)\frac{\partial^2\phi}{\partial z^2} + HOT
\end{aligned} \tag{B.55}$$

where l_1 and l_2 are the different mesh sizes in the z-direction. The same manipulations as in two dimensions show that the local first order error introduced by the mesh changes is

$$FOE = \frac{1}{6}\begin{bmatrix} u\left(h_2 - h_1\right)\left(\dfrac{\partial^2\phi}{\partial x^2}\right)_{i\,j}^{n+1} \\ +v\left(k_2 - k_1\right)\left(\dfrac{\partial^2\phi}{\partial y^2}\right)_{i\,j}^{n+1} \\ +w\left(l_2 - l_1\right)\left(\dfrac{\partial^2\phi}{\partial z^2}\right)_{i\,j}^{n+1} \end{bmatrix} \tag{B.56}$$

Therefore the approximation to the convection diffusion equation requires a correction to eliminate the artificial diffusion introduced by the changes in the mesh. This is readily accomplished by means of any of the procedures already known to eliminate artificial numerical diffusion, and can be implemented in a variety of ways. In particular this correction is similar to the stabilization of SUPG type required for highly convective flows. However, in the present case the additional error is strictly localized next to the interfaces and does not have the global effect of a stabilized Petrov-Galerkin formulation. Moreover, so far numerical experiments have shown that this error is small in the sense that it only increases the relative error at nodes adjacent to the boundary by two or three percent, but this conclusion is based on a limited number of measurements.

Appendix C

Poisson Equation Truncation Error Analysis

C.1 2-D Domain

The Poisson's Equation is

$$-\nabla^2 p = f \tag{C.1}$$

where

$$f = -\frac{1}{\Delta t}\nabla \cdot \mathbf{u}^* \tag{C.2}$$

The weak weighted residuals formulation of equation 4.1 gives

$$\int_\Omega \left(\nabla \mathbf{w}.\nabla p - \mathbf{w} f\right) d\Omega = 0 \tag{C.3}$$

Where $\mathbf{w}$ denotes the weighting functions.

The p and f functions are discretized over the space as:

$$p\left(x, y\right) \cong \sum_{i=1}^{n} N_i\left(x, y\right) p_i \qquad f\left(x, y\right) \cong \sum_{i=1}^{n} N_i\left(x, y\right) f_i \tag{C.4}$$

Where N_i are the shape functions over each element, and n is the number of nodes in an element, in this two dimensional case $n = 4$. The weighting functions w_i are set to be equal to shape functions N_i. the final form of the equation C.3 is

$$\int_0^{\Delta y}\int_0^{\Delta x}\left(\frac{\partial N_i}{\partial x}\sum_{j=1}^{4}\left(\frac{\partial N_j}{\partial x}p_j\right)+\frac{\partial N_i}{\partial y}\sum_{j=1}^{4}\left(\frac{\partial N_j}{\partial y}p_j\right)\right)dxdy$$
$$-\int_0^{\Delta y}\int_0^{\Delta x}N_i\sum_{j=1}^{4}N_jf_jdxdy = 0 \tag{C.5}$$

Another representation of equation C.5 is

$$\sum_{j=1}^{4}\int_0^{\Delta y}\int_0^{\Delta x}\frac{\partial N_i}{\partial x}\frac{\partial N_j}{\partial x}p_jdxdy+\sum_{j=1}^{4}\int_0^{\Delta y}\int_0^{\Delta x}\frac{\partial N_i}{\partial y}\frac{\partial N_j}{\partial y}p_jdxdy$$
$$-\sum_{j=1}^{4}\int_0^{\Delta y}\int_0^{\Delta x}N_iN_jf_jdxdy = 0 \tag{C.6}$$

The shape functions according to figure 4.1(a) are

$$\begin{cases} N_1 = \left(1-\frac{x}{h}\right)\left(1-\frac{y}{k}\right) \\ N_2 = \left(\frac{x}{h}\right)\left(1-\frac{y}{k}\right) \\ N_3 = \left(1-\frac{x}{h}\right)\left(\frac{y}{k}\right) \\ N_4 = \left(\frac{x}{h}\right)\left(\frac{y}{k}\right) \end{cases} \tag{C.7}$$

The next task is to calculate the stiffness matrix of an element. By calculating the stiffness matrices the equation C.6 can be written as:

$$M_{ij}^{11}p_j + M_{ij}^{22}p_j + M_{ij}^{33}f_j = 0 \tag{C.8}$$

Where M^{mm} are stiffness matrices calculated as

$M_{ij}^{11} = \frac{\Delta y}{6\Delta x}\begin{bmatrix} 2 & -2 & -1 & 1 \\ -2 & 2 & 1 & -1 \\ -1 & 1 & 2 & -2 \\ 1 & -1 & -2 & 2 \end{bmatrix}$, $M_{ij}^{22} = \frac{\Delta x}{6\Delta y}\begin{bmatrix} 2 & 1 & -1 & -2 \\ 1 & 2 & -2 & -1 \\ -1 & -2 & 2 & 1 \\ -2 & -1 & 1 & 2 \end{bmatrix}$, and

$M_{ij}^{33} = -\frac{\Delta x \Delta y}{36}\begin{bmatrix} 4 & 2 & 1 & 2 \\ 2 & 4 & 2 & 1 \\ 1 & 2 & 4 & 2 \\ 2 & 1 & 2 & 4 \end{bmatrix}$

The element equations are

first element

$$\left(\frac{k_1}{6h_1}\begin{bmatrix} 2 & -2 & -1 & 1 \\ -2 & 2 & 1 & -1 \\ -1 & 1 & 2 & -2 \\ 1 & -1 & -2 & 2 \end{bmatrix} + \frac{h_1}{6k_1}\begin{bmatrix} 2 & 1 & -1 & -2 \\ 1 & 2 & -2 & -1 \\ -1 & -2 & 2 & 1 \\ -2 & -1 & 1 & 2 \end{bmatrix}\right)\begin{bmatrix} p_{i-1j-1} \\ p_{ij-1} \\ p_{ij} \\ p_{i-1j} \end{bmatrix} = \frac{h_1 k_1}{36}\begin{bmatrix} 4 & 2 & 1 & 2 \\ 2 & 4 & 2 & 1 \\ 1 & 2 & 4 & 2 \\ 2 & 1 & 2 & 4 \end{bmatrix}\begin{bmatrix} f_{i-1j-1} \\ f_{ij-1} \\ f_{ij} \\ f_{i-1j} \end{bmatrix} \tag{C.9}$$

second element

$$\left(\frac{k_1}{6h_2}\begin{bmatrix} 2 & -2 & -1 & 1 \\ -2 & 2 & 1 & -1 \\ -1 & 1 & 2 & -2 \\ 1 & -1 & -2 & 2 \end{bmatrix} + \frac{h_2}{6k_1}\begin{bmatrix} 2 & 1 & -1 & -2 \\ 1 & 2 & -2 & -1 \\ -1 & -2 & 2 & 1 \\ -2 & -1 & 1 & 2 \end{bmatrix}\right)\begin{bmatrix} p_{ij-1} \\ p_{i+1j-1} \\ p_{i+1j} \\ p_{ij} \end{bmatrix} = \frac{h_2k_1}{36}\begin{bmatrix} 4 & 2 & 1 & 2 \\ 2 & 4 & 2 & 1 \\ 1 & 2 & 4 & 2 \\ 2 & 1 & 2 & 4 \end{bmatrix}\begin{bmatrix} f_{ij-1} \\ f_{i+1j-1} \\ f_{i+1j} \\ f_{ij} \end{bmatrix} \tag{C.10}$$

third element

$$\left(\frac{k_2}{6h_1}\begin{bmatrix} 2 & -2 & -1 & 1 \\ -2 & 2 & 1 & -1 \\ -1 & 1 & 2 & -2 \\ 1 & -1 & -2 & 2 \end{bmatrix} + \frac{h_1}{6k_2}\begin{bmatrix} 2 & 1 & -1 & -2 \\ 1 & 2 & -2 & -1 \\ -1 & -2 & 2 & 1 \\ -2 & -1 & 1 & 2 \end{bmatrix}\right)\begin{bmatrix} p_{i-1j} \\ p_{ij} \\ p_{ij+1} \\ p_{i-1j+1} \end{bmatrix} = \frac{h_1k_2}{36}\begin{bmatrix} 4 & 2 & 1 & 2 \\ 2 & 4 & 2 & 1 \\ 1 & 2 & 4 & 2 \\ 2 & 1 & 2 & 4 \end{bmatrix}\begin{bmatrix} f_{i-1j} \\ f_{ij} \\ f_{ij+1} \\ f_{i-1j+1} \end{bmatrix} \tag{C.11}$$

fourth element

$$\left(\frac{k_2}{6h_2}\begin{bmatrix} 2 & -2 & -1 & 1 \\ -2 & 2 & 1 & -1 \\ -1 & 1 & 2 & -2 \\ 1 & -1 & -2 & 2 \end{bmatrix} + \frac{h_2}{6k_2}\begin{bmatrix} 2 & 1 & -1 & -2 \\ 1 & 2 & -2 & -1 \\ -1 & -2 & 2 & 1 \\ -2 & -1 & 1 & 2 \end{bmatrix}\right)\begin{bmatrix} p_{ij} \\ p_{i+1j} \\ p_{i+1j+1} \\ p_{ij+1} \end{bmatrix} = \frac{h_2k_2}{36}\begin{bmatrix} 4 & 2 & 1 & 2 \\ 2 & 4 & 2 & 1 \\ 1 & 2 & 4 & 2 \\ 2 & 1 & 2 & 4 \end{bmatrix}\begin{bmatrix} f_{ij} \\ f_{i+1j} \\ f_{i+1j+1} \\ f_{ij+1} \end{bmatrix} \tag{C.12}$$

and assembling the difference equation for node (x_i, y_i) yields

$$\begin{aligned} DE \equiv\ & \frac{k_2}{6h_1}\left(-2p_{i-1j} + 2p_{ij} + p_{ij+1} - p_{i-1j+1}\right) + \frac{h_1}{6k_2}\left(p_{i-1j} + 2p_{ij} - 2p_{ij+1} - p_{i-1j+1}\right) \\ & + \frac{k_2}{6h_2}\left(2p_{ij} - 2p_{i+1j} - p_{i+1j+1} + p_{ij+1}\right) + \frac{h_2}{6k_2}\left(2p_{ij} + p_{i+1j} - p_{i+1j+1} - 2p_{ij+1}\right) \\ & + \frac{k_1}{6h_1}\left(-p_{i-1j-1} + p_{ij-1} + 2p_{ij} - 2p_{i-1j}\right) + \frac{h_1}{6k_1}\left(-p_{i-1j-1} - 2p_{ij-1} + 2p_{ij} + p_{i-1j}\right) \\ & + \frac{k_1}{6h_2}\left(p_{ij-1} - p_{i+1j-1} - 2p_{i+1j} + 2p_{ij}\right) + \frac{h_2}{6k_1}\left(-2p_{ij-1} - p_{i+1j-1} + p_{i+1j} + 2p_{ij}\right) \\ & - \frac{h_1k_2}{36}\left(2f_{i-1j} + 4f_{ij} + 2f_{ij+1} + f_{i-1j+1}\right) - \frac{h_2k_2}{36}\left(4f_{ij} + 2f_{i+1j} + f_{i+1j+1} + 2f_{ij+1}\right) \\ & - \frac{h_1k_1}{36}\left(f_{i-1j-1} + 2f_{ij-1} + 4f_{ij} + 2f_{i-1j}\right) - \frac{h_2k_1}{36}\left(2f_{ij-1} + f_{i+1j-1} + 2f_{i+1j} + 4f_{ij}\right) = 0 \end{aligned} \tag{C.13}$$

All the terms in DE are expanded in Taylor series about ϕ_{ij}^{n+1}. For example:

$$\begin{aligned} p_{i+1j+1} = p_{ij} & + \left(\Delta x (p_{ij})_x + \Delta y (p_{ij})_y\right) + \frac{1}{2!}\left(\Delta x^2 (p_{ij})_{xx} + 2\Delta x\Delta y (p_{ij})_{xy} + \Delta y^2 (p_{ij})_{yy}\right) \\ & + \frac{1}{3!}\left(\Delta x^3 (p_{ij})_{xxx} + 3\Delta x^2\Delta y (p_{ij})_{xxy} + 3\Delta x\Delta y^2 (p_{ij})_{xyy} + \Delta y^3 (p_{ij})_{yyy}\right) \\ & + O\left(\Delta x^4,\ \Delta x^3\Delta y,\ \Delta x^2\Delta y^2,\ \Delta x\Delta y^3,\ \Delta y^4\right) \end{aligned}$$

and

$$p_{i-1j-1} = p_{ij} - \left(\Delta x(p_{ij})_x + \Delta y(p_{ij})_y\right) + \frac{1}{2!}\left(\Delta x^2(p_{ij})_{xx} + 2\Delta x\Delta y(p_{ij})_{xy} + \Delta y^2(p_{ij})_{yy}\right)$$
$$- \frac{1}{3!}\left(\Delta x^3(p_{ij})_{xxx} + 3\Delta x^2\Delta y(p_{ij})_{xxy} + 3\Delta x\Delta y^2(p_{ij})_{xyy} + \Delta y^3(p_{ij})_{yyy}\right)$$
$$+O\left(\Delta x^4,\ \Delta x^3\Delta y,\ \Delta x^2\Delta y^2,\ \Delta x\Delta y^3,\ \Delta y^4\right)$$

The Taylor series expansion about $p_{i\,j}$ gives

$$DE = \frac{(h_1+h_2)(k_1+k_2)}{4}\times \left(\begin{array}{l} \left(-\frac{\partial^2 p}{\partial x^2} - \frac{\partial^2 p}{\partial x^2} - f\right) + \frac{1}{3}\left(\begin{array}{c} (k_2-k_1)\left(-\frac{\partial^3 p}{\partial y^3} - \frac{\partial^3 p}{\partial x^2 \partial y}\right) \\ +(h_2-h_1)\left(-\frac{\partial^3 p}{\partial y^3} - \frac{\partial^3 p}{\partial x \partial y^2}\right)\end{array}\right) \\ -\frac{1}{3}\left[(k_2-k_1)f_y + (h_2-h_1)f_x\right] + O(h^2,k^2,hk) \end{array}\right) \tag{C.14}$$

Note that the leading first order term in the truncation error is equal to

$$FOE = \frac{1}{3}\left(\begin{array}{c} (k_2-k_1)\frac{\partial}{\partial y}\left(-\frac{\partial^2 p_{ij}}{\partial x^2} - \frac{\partial^2 p_{ij}}{\partial y^2} - f_{ij}\right) \\ +(h_2-h_1)\frac{\partial}{\partial x}\left(-\frac{\partial^2 p_{ij}}{\partial x^2} - \frac{\partial^2 p_{ij}}{\partial y^2} - f_{ij}\right)\end{array}\right) \equiv 0 \tag{C.15}$$

Provided that the finite element discretization of the right hand side is fully consistent; Therefore, this error vanishes and the method is locally second order accurate regardless of abrupt changes in the mesh. However, if the formulation is not fully consistent, such as the case reduced integration is used to evaluate the pressure gradients in , then a first order error is introduced.

C.2 3-D Domain

The three dimensional Poisson's Equation is

$$-\nabla^2 p = f \tag{C.16}$$

where

$$f = -\frac{1}{\Delta t}\nabla \cdot \mathbf{u}^* \tag{C.17}$$

The weak weighted residuals formulation of equation 4.1 gives

$$\int_\Omega (\nabla \mathbf{w}.\nabla p - \mathbf{w} f)\, d\Omega = 0 \tag{C.18}$$

Where $\mathbf{w}$ denotes the weighting functions.
The p and f functions are discretized over the space as:

$$p(x, y, z) \cong \sum_{i=1}^{n} N_i(x, y, z)\, p_i \tag{C.19}$$

$$f(x, y, z) \cong \sum_{i=1}^{n} N_i(x, y, z)\, f_i \tag{C.20}$$

Where N_i are the shape functions over each element, and n is the number of nodes in an element, in this two dimensional case $n = 8$. The weighting functions w_i are set to be equal to shape functions N_i. the final form of the equation C.18 is

$$\int_0^{\Delta z}\int_0^{\Delta y}\int_0^{\Delta x}\left(\frac{\partial N_i}{\partial x}\sum_{j=1}^{8}\left(\frac{\partial N_j}{\partial x}p_j\right) + \frac{\partial N_i}{\partial y}\sum_{j=1}^{8}\left(\frac{\partial N_j}{\partial y}p_j\right) + \frac{\partial N_i}{\partial z}\sum_{j=1}^{8}\left(\frac{\partial N_j}{\partial z}p_j\right)\right) dxdydz$$
$$-\int_0^{\Delta z}\int_0^{\Delta y}\int_0^{\Delta x} N_i \sum_{j=1}^{8} N_j f_j dxdydz = 0 \tag{C.21}$$

Another representation of equation C.21 is

$$\begin{aligned}
&\sum_{j=1}^{8}\int_0^{\Delta z}\int_0^{\Delta y}\int_0^{\Delta x}\frac{\partial N_i}{\partial x}\frac{\partial N_j}{\partial x}p_j dxdydz \\
&+\sum_{j=1}^{8}\int_0^{\Delta z}\int_0^{\Delta y}\int_0^{\Delta x}\frac{\partial N_i}{\partial y}\frac{\partial N_j}{\partial y}p_j dxdydz \\
&+\sum_{j=1}^{8}\int_0^{\Delta z}\int_0^{\Delta y}\int_0^{\Delta x}\frac{\partial N_i}{\partial z}\frac{\partial N_j}{\partial z}p_j dxdydz \\
&-\sum_{j=1}^{8}\int_0^{\Delta z}\int_0^{\Delta y}\int_0^{\Delta x} N_i N_j f_j dxdy = 0
\end{aligned} \tag{C.22}$$

The shape functions according to figure 4.1(a) are

$$\begin{cases}
N_1 = \left(1-\frac{x}{h}\right)\left(1-\frac{y}{k}\right)\left(1-\frac{z}{l}\right) \\
N_2 = \left(\frac{x}{h}\right)\left(1-\frac{y}{k}\right)\left(1-\frac{z}{l}\right) \\
N_3 = \left(1-\frac{x}{h}\right)\left(\frac{y}{k}\right)\left(1-\frac{z}{l}\right) \\
N_4 = \left(\frac{x}{h}\right)\left(\frac{y}{k}\right)\left(1-\frac{z}{l}\right) \\
N_5 = \left(1-\frac{x}{h}\right)\left(1-\frac{y}{k}\right)\left(\frac{z}{l}\right) \\
N_6 = \left(\frac{x}{h}\right)\left(1-\frac{y}{k}\right)\left(\frac{z}{l}\right) \\
N_7 = \left(1-\frac{x}{h}\right)\left(\frac{y}{k}\right)\left(\frac{z}{l}\right) \\
N_8 = \left(\frac{x}{h}\right)\left(\frac{y}{k}\right)\left(\frac{z}{l}\right)
\end{cases} \tag{C.23}$$

The next task is to calculate the stiffness matrix of an element. By calculating the stiffness matrices the equation C.22 can be written as:

$$M_{ij}^{11}p_j + M_{ij}^{22}p_j + M_{ij}^{33}p_j + M_{ij}^{44}f_j = 0 \tag{C.24}$$

In this formula, M^{mm} are stiffness matrices given as

$$M_{ij}^{11} = \frac{kl}{36h}\begin{bmatrix} 4 & -4 & 2 & -2 & 2 & -2 & 1 & -1 \\ -4 & 4 & -2 & 2 & -2 & 2 & -1 & 1 \\ 2 & -2 & 4 & -4 & 1 & -1 & 2 & -2 \\ -2 & 2 & -4 & 4 & -1 & 1 & -2 & 2 \\ 2 & -2 & 1 & -1 & 4 & -4 & 2 & -2 \\ -2 & 2 & -1 & 1 & -4 & 4 & -2 & 2 \\ 1 & -1 & 2 & -2 & 2 & -2 & 4 & -4 \\ -1 & 1 & -2 & 2 & -2 & 2 & -4 & 4 \end{bmatrix},$$

$$M_{ij}^{22} = \frac{hl}{36k}\begin{bmatrix} 4 & 2 & -4 & -2 & 2 & 1 & -2 & -1 \\ 2 & 4 & -2 & -4 & 1 & 2 & -1 & -2 \\ -4 & -2 & 4 & 2 & -2 & -1 & 2 & 1 \\ -2 & -4 & 2 & 4 & -1 & -2 & 1 & 2 \\ 2 & 1 & -2 & -1 & 4 & 2 & -4 & -2 \\ 1 & 2 & -1 & -2 & 2 & 4 & -2 & -4 \\ -2 & -1 & 2 & 1 & -4 & -2 & 4 & 2 \\ -1 & -2 & 1 & 2 & -2 & -4 & 2 & 4 \end{bmatrix},$$

$$M_{ij}^{33} = \frac{hk}{36l}\begin{bmatrix} 4 & 2 & 2 & 1 & -4 & -2 & -2 & -1 \\ 2 & 4 & 1 & 2 & -2 & -4 & -1 & -2 \\ 2 & 1 & 4 & 2 & -2 & -1 & -4 & -2 \\ 1 & 2 & 2 & 4 & -1 & -2 & -2 & -4 \\ -4 & -2 & -2 & -1 & 4 & 2 & 2 & 1 \\ -2 & -4 & -1 & -2 & 2 & 4 & 1 & 2 \\ -2 & -1 & -4 & -2 & 2 & 1 & 4 & 2 \\ -1 & -2 & -2 & -4 & 1 & 2 & 2 & 4 \end{bmatrix}, \text{ and}$$

$$M_{ij}^{44} = -\frac{hkl}{216}\begin{bmatrix} 8 & 4 & 4 & 2 & 4 & 2 & 2 & 1 \\ 4 & 8 & 2 & 4 & 2 & 4 & 1 & 2 \\ 4 & 2 & 8 & 4 & 2 & 1 & 4 & 2 \\ 2 & 4 & 4 & 8 & 1 & 2 & 2 & 4 \\ 4 & 2 & 2 & 1 & 8 & 4 & 4 & 2 \\ 2 & 4 & 1 & 2 & 4 & 8 & 2 & 4 \\ 2 & 1 & 4 & 2 & 4 & 2 & 8 & 4 \\ 1 & 2 & 2 & 4 & 2 & 4 & 4 & 8 \end{bmatrix}$$

The nodes and dimension for the elements using the notation in figure 4.1 are **first** element

nodes

$$\begin{bmatrix} \phi_{i-1j-1k-1} & \phi_{ij-1k-1} & \phi_{i-1jk-1} & \phi_{ijk-1} & \phi_{i-1j-1k} & \phi_{ij-1k} & \phi_{i-1jk} & \phi_{ijk} \end{bmatrix}$$

dimension

$\begin{bmatrix} h_1 & k_1 & l_1 \end{bmatrix}$

second element

nodes

$$\begin{bmatrix} \phi_{ij-1k-1} & \phi_{i+1j-1k-1} & \phi_{ijk-1} & \phi_{i+1jk-1} & \phi_{ij-1k} & \phi_{i+1j-1k} & \phi_{ijk} & \phi_{i+1jk} \end{bmatrix}$$

dimension

$\begin{bmatrix} h_2 & k_1 & l_1 \end{bmatrix}$

third element

nodes

$$\begin{bmatrix} \phi_{i-1jk-1} & \phi_{ijk-1} & \phi_{i-1j+1k-1} & \phi_{ij+1k-1} & \phi_{i-1jk} & \phi_{ijk} & \phi_{i-1j+1k} & \phi_{ij+1k} \end{bmatrix}$$

dimension

$\begin{bmatrix} h_1 & k_2 & l_1 \end{bmatrix}$

fourth element

nodes

$$\left[\begin{array}{cccccccc} \phi_{ijk-1} & \phi_{i+1jk-1} & \phi_{ij+1k-1} & \phi_{i+1j+1k-1} & \phi_{ijk} & \phi_{i+1jk} & \phi_{ij+1k} & \phi_{i+1j+1k} \end{array}\right]$$

dimension

$\left[\begin{array}{ccc} h_2 & k_2 & l_1 \end{array}\right]$

fifth element

nodes

$$\left[\begin{array}{cccccccc} \phi_{i-1j-1k} & \phi_{ij-1k} & \phi_{i-1jk} & \phi_{ijk} & \phi_{i-1j-1k+1} & \phi_{ij-1k+1} & \phi_{i-1jk+1} & \phi_{ijk+1} \end{array}\right]$$

dimension

$\left[\begin{array}{ccc} h_1 & k_1 & l_2 \end{array}\right]$

sixth element

nodes

$$\left[\begin{array}{cccccccc} \phi_{ij-1k} & \phi_{i+1j-1k} & \phi_{ijk} & \phi_{i+1jk} & \phi_{ij-1k+1} & \phi_{i+1j-1k+1} & \phi_{ijk+1} & \phi_{i+1jk+1} \end{array}\right]$$

dimension

$\left[\begin{array}{ccc} h_2 & k_1 & l_2 \end{array}\right]$

seventh element

nodes

$$\left[\begin{array}{cccccccc} \phi_{i-1jk} & \phi_{ijk} & \phi_{i-1j+1k} & \phi_{ij+1k} & \phi_{i-1jk+1} & \phi_{ijk+1} & \phi_{i-1j+1k+1} & \phi_{ij+1k+1} \end{array}\right]$$

dimension

$\left[\begin{array}{ccc} h_1 & k_2 & l_2 \end{array}\right]$

eighth element

nodes

$$\left[\begin{array}{cccccccc} \phi_{ijk} & \phi_{i+1jk} & \phi_{ij+1k} & \phi_{i+1j+1k} & \phi_{ijk+1} & \phi_{i+1jk+1} & \phi_{ij+1k+1} & \phi_{i+1j+1k+1} \end{array}\right]$$

dimension

$$\begin{bmatrix} h_2 & k_2 & l_2 \end{bmatrix}$$

assembling the difference equation for node (x_i, y_i) yields

$$DE \equiv DE_1 + DE_2 + DE_3 + DE_4 \tag{C.25}$$

where

$$\begin{aligned}
&DE_1 \equiv \\
&\frac{k_2 l_1}{36 h_1}\left(-2p_{i-1jk-1} + 2p_{ijk-1} - p_{i-1j+1k-1} + p_{ij+1k-1} - 4p_{i-1jk} + 4p_{ijk} - 2p_{i-1j+1k} + 2p_{ij+1k}\right) \\
&+\frac{k_2 l_1}{36 h_2}\left(+2p_{ijk-1} - 2p_{i+1jk-1} + p_{ij+1k-1} - p_{i+1j+1k-1} + 4p_{ijk} - 4p_{i+1jk} + 2p_{ij+1k} - 2p_{i+1j+1k}\right) \\
&+\frac{k_1 l_1}{36 h_1}\left(-p_{i-1j-1k-1} + p_{ij-1k-1} - 2p_{i-1jk-1} + 2p_{ijk-1} - 2p_{i-1j-1k} + 2p_{ij-1k} - 4p_{i-1jk} + 4p_{ijk}\right) \\
&+\frac{k_1 l_1}{36 h_2}\left(+p_{ij-1k-1} - p_{i+1j-1k-1} + 2p_{ijk-1} - 2p_{i+1jk-1} + 2p_{ij-1k} - 2p_{i+1j-1k} + 4p_{ijk} - 4p_{i+1jk}\right) \\
&+\frac{k_2 l_2}{36 h_1}\left(-4p_{i-1jk} + 4p_{ijk} - 2p_{i-1j+1k} + 2p_{ij+1k} - 2p_{i-1jk+1} + 2p_{ijk+1} - p_{i-1j+1k+1} + p_{ij+1k+1}\right) \\
&+\frac{k_2 l_2}{36 h_2}\left(+4p_{ijk} - 4p_{i+1jk} + 2p_{ij+1k} - 2p_{i+1j+1k} + 2p_{ijk+1} - 2p_{i+1jk+1} + p_{ij+1k+1} - p_{i+1j+1k+1}\right) \\
&+\frac{k_1 l_2}{36 h_1}\left(-2p_{i-1j-1k} + 2p_{ij-1k} - 4p_{i-1jk} + 4p_{ijk} - p_{i-1j-1k+1} + p_{ij-1k+1} - 2p_{i-1jk+1} + 2p_{ijk+1}\right) \\
&+\frac{k_1 l_2}{36 h_2}\left(+2p_{ij-1k} - 2p_{i+1j-1k} + 4p_{ijk} - 4p_{i+1jk} + p_{ij-1k+1} - p_{i+1j-1k+1} + 2p_{ijk+1} - 2p_{i+1jk+1}\right)
\end{aligned} \tag{C.26}$$

and

$$
\begin{aligned}
DE_2 \equiv & \qquad\qquad (C.27)\\
&+\frac{h_1 l_1}{36k_2}\left(p_{i-1jk-1}+2p_{ijk-1}-p_{i-1j+1k-1}-2p_{ij+1k-1}+2p_{i-1jk}+4p_{ijk}-2p_{i-1j+1k}-4p_{ij+1k}\right)\\
&+\frac{h_2 l_1}{36k_2}\left(+2p_{ijk-1}+p_{i+1jk-1}-2p_{ij+1k-1}-p_{i+1j+1k-1}+4p_{ijk}+2p_{i+1jk}-4p_{ij+1k}-2p_{i+1j+1k}\right)\\
&+\frac{h_1 l_1}{36k_1}\left(-p_{i-1j-1k-1}-2p_{ij-1k-1}+p_{i-1jk-1}+2p_{ijk-1}-2p_{i-1j-1k}-4p_{ij-1k}+2p_{i-1jk}+4p_{ijk}\right)\\
&+\frac{h_2 l_1}{36k_1}\left(-2p_{ij-1k-1}-p_{i+1j-1k-1}+2p_{ijk-1}+p_{i+1jk-1}-4p_{ij-1k}-2p_{i+1j-1k}+4p_{ijk}+2p_{i+1jk}\right)\\
&+\frac{h_1 l_2}{36k_2}\left(+2p_{i-1jk}+4p_{ijk}-2p_{i-1j+1k}-4p_{ij+1k}+p_{i-1jk+1}+2p_{ijk+1}-p_{i-1j+1k+1}-2p_{ij+1k+1}\right)\\
&+\frac{h_2 l_2}{36k_2}\left(+4p_{ijk}+2p_{i+1jk}-4p_{ij+1k}-2p_{i+1j+1k}+2p_{ijk+1}+p_{i+1jk+1}-2p_{ij+1k+1}-p_{i+1j+1k+1}\right)\\
&+\frac{h_1 l_2}{36k_1}\left(-2p_{i-1j-1k}-4p_{ij-1k}+2p_{i-1jk}+4p_{ijk}-p_{i-1j-1k+1}-2p_{ij-1k+1}+p_{i-1jk+1}+2p_{ijk+1}\right)\\
&+\frac{h_2 l_2}{36k_1}\left(-4p_{ij-1k}-2p_{i+1j-1k}+4p_{ijk}+2p_{i+1jk}-2p_{ij-1k+1}-p_{i+1j-1k+1}+2p_{ijk+1}+p_{i+1jk+1}\right)
\end{aligned}
$$

and

$$
\begin{aligned}
DE_3 \equiv & \qquad\qquad (C.28)\\
&+\frac{h_1 k_2}{36l_1}\left(-2p_{i-1jk-1}-4p_{ijk-1}-p_{i-1j+1k-1}-2p_{ij+1k-1}+2p_{i-1jk}+4p_{ijk}+p_{i-1j+1k}+2p_{ij+1k}\right)\\
&+\frac{h_2 k_2}{36{l_1}^2}\left(-4p_{ijk-1}-2p_{i+1jk-1}-2p_{ij+1k-1}-p_{i+1j+1k-1}+4p_{ijk}+2p_{i+1jk}+2p_{ij+1k}+p_{i+1j+1k}\right)\\
&+\frac{h_1 k_1}{36l_1}\left(-p_{i-1j-1k-1}-2p_{ij-1k-1}-2p_{i-1jk-1}-4p_{ijk-1}+p_{i-1j-1k}+2p_{ij-1k}+2p_{i-1jk}+4p_{ijk}\right)\\
&+\frac{h_2 k_1}{36l_1}\left(-2p_{ij-1k-1}-p_{i+1j-1k-1}-4p_{ijk-1}-2p_{i+1jk-1}+2p_{ij-1k}+p_{i+1j-1k}+4p_{ijk}+2p_{i+1jk}\right)\\
&+\frac{h_1 k_2}{36l_2}\left(+2p_{i-1jk}+4p_{ijk}+p_{i-1j+1k}+2p_{ij+1k}-2p_{i-1jk+1}-4p_{ijk+1}-p_{i-1j+1k+1}-2p_{ij+1k+1}\right)\\
&+\frac{h_2 k_2}{36l_2}\left(+4p_{ijk}+2p_{i+1jk}+2p_{ij+1k}+p_{i+1j+1k}-4p_{ijk+1}-2p_{i+1jk+1}-2p_{ij+1k+1}-p_{i+1j+1k+1}\right)\\
&+\frac{h_1 k_1}{36l_2}\left(+p_{i-1j-1k}+2p_{ij-1k}+2p_{i-1jk}+4p_{ijk}-p_{i-1j-1k+1}-2p_{ij-1k+1}-2p_{i-1jk+1}-4p_{ijk+1}\right)\\
&+\frac{h_2 k_1}{36l_2}\left(+2p_{ij-1k}+p_{i+1j-1k}+4p_{ijk}+2p_{i+1jk}-2p_{ij-1k+1}-p_{i+1j-1k+1}-4p_{ijk+1}-2p_{i+1jk+1}\right)
\end{aligned}
$$

finally

$$
\begin{aligned}
&DE_4 \equiv \\
&-\frac{h_1k_2l_1}{216}\left(+2f_{i-1jk-1}+4f_{ijk-1}+f_{i-1j+1k-1}+2f_{ij+1k-1}+4f_{i-1jk}+8f_{ijk}+2f_{i-1j+1k}+4f_{ij+1k}\right)\\
&-\frac{h_2k_2l_1}{216}\left(+4f_{ijk-1}+2f_{i+1jk-1}+2f_{ij+1k-1}+f_{i+1j+1k-1}+8f_{ijk}+4f_{i+1jk}+4f_{ij+1k}+2f_{i+1j+1k}\right)\\
&-\frac{h_1k_1l_1}{216}\left(+f_{i-1j-1k-1}+2f_{ij-1k-1}+2f_{i-1jk-1}+4f_{ijk-1}+2f_{i-1j-1k}+4f_{ij-1k}+4f_{i-1jk}+8f_{ijk}\right)\\
&-\frac{h_2k_1l_1}{216}\left(+2f_{ij-1k-1}+f_{i+1j-1k-1}+4f_{ijk-1}+2f_{i+1jk-1}+4f_{ij-1k}+2f_{i+1j-1k}+8f_{ijk}+4f_{i+1jk}\right)\\
&-\frac{h_1k_2l_2}{216}\left(+4f_{i-1jk}+8f_{ijk}+2f_{i-1j+1k}+4f_{ij+1k}+2f_{i-1jk+1}+4f_{ijk+1}+f_{i-1j+1k+1}+2f_{ij+1k+1}\right)\\
&-\frac{h_2k_2l_2}{216}\left(+8f_{ijk}+4f_{i+1jk}+4f_{ij+1k}+2f_{i+1j+1k}+4f_{ijk+1}+2f_{i+1jk+1}+2f_{ij+1k+1}+f_{i+1j+1k+1}\right)\\
&-\frac{h_1k_1l_2}{216}\left(+2f_{i-1j-1k}+4f_{ij-1k}+4f_{i-1jk}+8f_{ijk}+f_{i-1j-1k+1}+2f_{ij-1k+1}+2f_{i-1jk+1}+4f_{ijk+1}\right)\\
&-\frac{h_2k_1l_2}{216}\left(+4f_{ij-1k}+2f_{i+1j-1k}+8f_{ijk}+4f_{i+1jk}+2f_{ij-1k+1}+f_{i+1j-1k+1}+4f_{ijk+1}+2f_{i+1jk+1}\right)
\end{aligned}
\tag{C.29}
$$

All the terms in DE are expanded in Taylor series about ϕ_{ij}^{n+1}. For example:

$$
\begin{aligned}
p_{i+1j+1} = p_{ij} &+ \Big(\Delta x(p_{ij})_x + \Delta y(p_{ij})_y\Big) + \frac{1}{2!}\Big(\Delta x^2(p_{ij})_{xx} + 2\Delta x\Delta y(p_{ij})_{xy} + \Delta y^2(p_{ij})_{yy}\Big)\\
&+ \frac{1}{3!}\Big(\Delta x^3(p_{ij})_{xxx} + 3\Delta x^2\Delta y(p_{ij})_{xxy} + 3\Delta x\Delta y^2(p_{ij})_{xyy} + \Delta y^3(p_{ij})_{yyy}\Big)\\
&+O\left(\Delta x^4,\ \Delta x^3\Delta y,\ \Delta x^2\Delta y^2,\ \Delta x\Delta y^3,\ \Delta y^4\right)
\end{aligned}
$$

and

$$
\begin{aligned}
p_{i-1j-1} = p_{ij} &- \Big(\Delta x(p_{ij})_x + \Delta y(p_{ij})_y\Big) + \frac{1}{2!}\Big(\Delta x^2(p_{ij})_{xx} + 2\Delta x\Delta y(p_{ij})_{xy} + \Delta y^2(p_{ij})_{yy}\Big)\\
&- \frac{1}{3!}\Big(\Delta x^3(p_{ij})_{xxx} + 3\Delta x^2\Delta y(p_{ij})_{xxy} + 3\Delta x\Delta y^2(p_{ij})_{xyy} + \Delta y^3(p_{ij})_{yyy}\Big)\\
&+O\left(\Delta x^4,\ \Delta x^3\Delta y,\ \Delta x^2\Delta y^2,\ \Delta x\Delta y^3,\ \Delta y^4\right)
\end{aligned}
$$

The Taylor series expansion about p_{ij} gives

$$DE = \frac{1}{8}(k_1 + k_2)(l_1 + l_2)(h_1 + h_2) \times \left(\begin{array}{l} \left(-(p_{ijk})_{xx} - (p_{ijk})_{yy} - (p_{ijk})_{zz} - (f_{ijk})\right) \\ +\frac{1}{3}(h_2 - h_1)\frac{\partial}{\partial x}\left(-(p_{ijk})_{xx} - (p_{ijk})_{yy} - (p_{ijk})_{zz} - (f_{ijk})\right) \\ +\frac{1}{3}(k_2 - k_1)\frac{\partial}{\partial y}\left(-(p_{ijk})_{xx} - (p_{ijk})_{yy} - (p_{ijk})_{zz} - (f_{ijk})\right) \\ +\frac{1}{3}(l_2 - l_1)\frac{\partial}{\partial z}\left(-(p_{ijk})_{xx} - (p_{ijk})_{yy} - (p_{ijk})_{zz} - (f_{ijk})\right) \end{array} \right) \tag{C.30}$$

Note that the leading first order term in the truncation error is equal to

$$FOE = \frac{1}{3}\left(\begin{array}{c} (h_2 - h_1)\frac{\partial}{\partial x}\left(-\frac{\partial^2 p_{ijk}}{\partial x^2} - \frac{\partial^2 p_{ijk}}{\partial y^2} - \frac{\partial^2 p_{ijk}}{\partial z^2} - f_{ijk}\right) \\ +(k_2 - k_1)\frac{\partial}{\partial y}\left(-\frac{\partial^2 p_{ijk}}{\partial x^2} - \frac{\partial^2 p_{ijk}}{\partial y^2} - \frac{\partial^2 p_{ijk}}{\partial z^2} - f_{ijk}\right) \\ +(l_2 - l_1)\frac{\partial}{\partial z}\left(-\frac{\partial^2 p_{ijk}}{\partial x^2} - \frac{\partial^2 p_{ijk}}{\partial y^2} - \frac{\partial^2 p_{ijk}}{\partial z^2} - f_{ijk}\right) \end{array} \right) \equiv 0 \tag{C.31}$$

Provided that the finite element discretization of the right hand side is fully consistent; Therefore, this error vanishes and the method is locally second order accurate regardless of abrupt changes in the mesh. However, if the formulation is not fully consistent, such as the case reduced integration is used to evaluate the pressure gradients in , then a first order error is introduced.