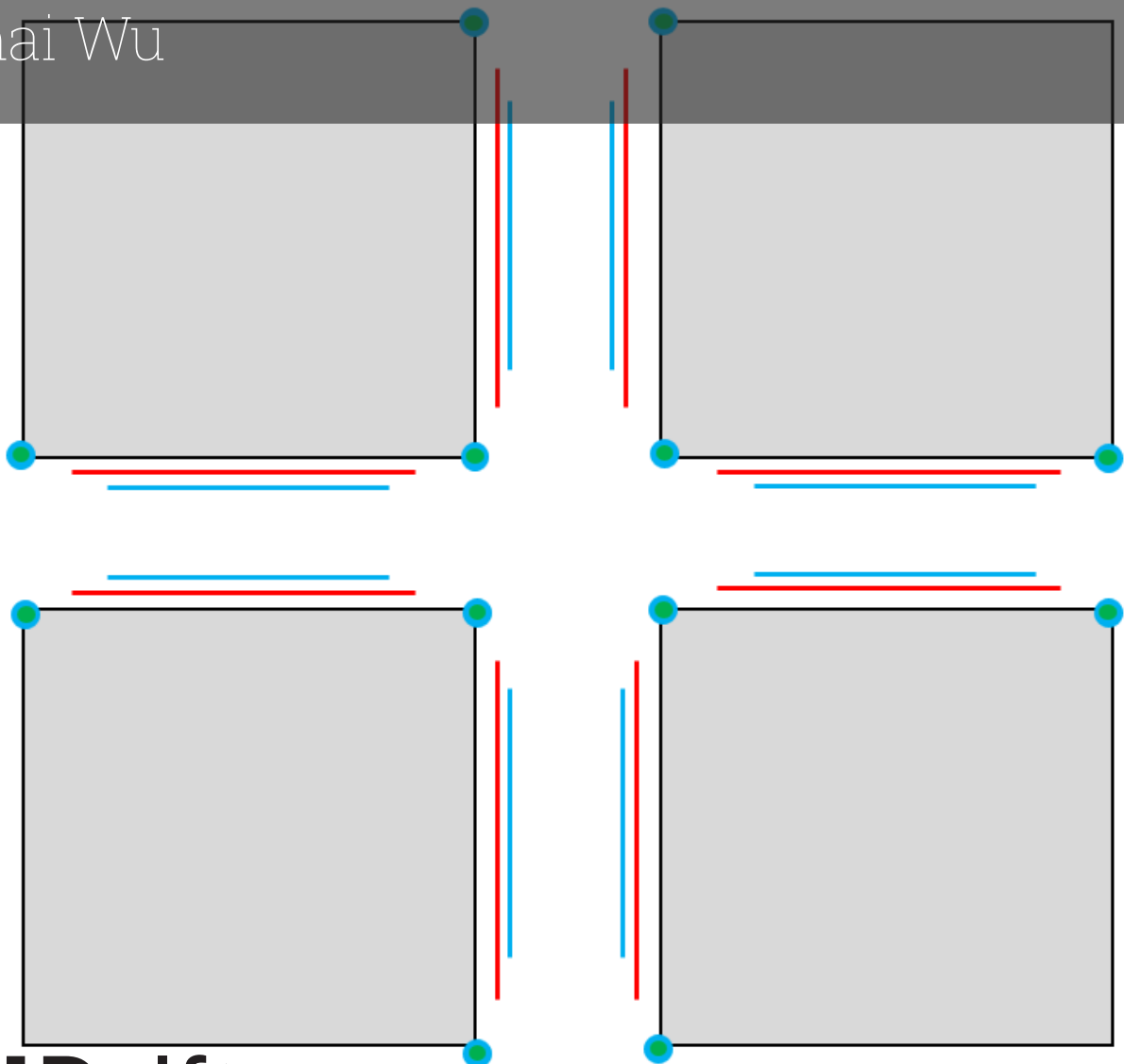


Hybrid Mimetic Finite Element Method with Strong Coupling of Continuity

Applied to Stokes' Equations

MSc. Thesis

Zimai Wu



Hybrid Mimetic Finite Element Method with Strong Coupling of Continuity

Applied to Stokes' Equations

by

Zimai Wu

to obtain the degree of Master of Science
in Aerospace Engineering at Delft University of Technology,
to be defended publicly on 25th August 2026.

Student number: 4649915

Committee:

Dr. ir. M. I. Gerritsma

Dr. S. J. Hulshoff

Dr. ir. F. de Prenter

Dr. A. Palha da Silva Clérigo

TU Delft, supervisor

TU Delft, chair

TU Delft, examiner

TU Delft, examiner

Report template: TU Delft Report Style, with modifications by Daan Zwaneveld

Preface

This paper presents the work of hybrid mimetic spectral element method that applies strong coupling at the interface to maintain continuity, which is the final major effort to obtain the MSc degree.

Firstly, I would like to offer my greatest gratitude to my supervisor, Marc Gerritsma, who guided me patiently along this road, encouraged me when I was in distress and never gives me up of my work, which should have been completed 2 years ago.

I would also like to thank my family, my parents who supported my study abroad and were never disappointed in me; my wife who was by then my girlfriend back in China that stayed up late almost each night to my accompany; and our newborn son, whose birth really encourages me and sweeps away all my distress.

Zimai Wu
August 2026

Abstract

The mimetic spectral element method (MSEM) is a discretization technique that preserves the topological relations and structures presented in PDE's, given certain function spaces and metric-free discrete differential operators that mimic a de Rham or double de Rham complexes. This scheme leads to favorable properties in numerical methods, especially conservation of field variables such as mass or momentum.

To numerically solve PDE's, parallelization of the problem has been well studied to improve efficiency. Domain decomposition is one of the methods, which is self explanatory, and it can be applied to MSEM, called hybrid MSEM. In this paper, hMSEM is proposed in the way that variables at the interfaces between or among subdomains are explicitly coupled with the aid of Lagrange multipliers. A downside in this method is that singularity arises when trying to couple variables assigned to edges. The solution to this issue is discussed in this paper that the number of equations of constraints over edges is reduced by 1, while the discrete system still remains rigorous and can be solved in parallel. Such hMSEM is then implemented and applied to Poisson's equation and Stokes' equations for test, to which the accuracy and convergence rate of this method are verified.

Contents

Preface	i
Abstract	ii
1 Introduction	1
1.1 Research Question	2
1.2 Report Outline	2
2 Mathematical Backbones	3
2.1 Differential Geometry	3
2.1.1 Manifold	3
2.1.2 Tangent and cotangent spaces	3
2.1.3 Differential forms on $\mathbb{R}^3$	5
2.1.4 Exterior derivative	7
2.1.5 Generalized Stokes' theorem	8
2.1.6 Hodge star operator	9
2.2 Algebraic Topology	11
2.2.1 Orientation of the geometric object	11
2.2.2 Cell and chain	11
2.2.3 Boundary operator and incidence matrix	12
2.2.4 Cochains and coboundary	13
3 Mimetic Spectral Element Method	16
3.1 Basic mimetic polynomials in 1-dimension	16
3.1.1 Lagrange polynomials	16
3.1.2 Edge functions	17
3.1.3 Incidence matrix in 1 dimension	18
3.2 Mimetic polynomials in 3-dimension	18
3.2.1 Polynomials on geometry	19
3.2.2 Coordinate transformation	21
3.2.3 Reconstruction	23
3.2.4 Incidence matrices in 3-dimension	24
3.2.5 Double de Rham complex	26
4 Numerical Experiment	27
4.1 Scalar Poisson's equation	27
4.1.1 Discretization of the weak form	27
4.1.2 Numerical results	28
4.2 Vector Poisson's equation	30
4.2.1 Discretization of the weak form	31
4.2.2 Numerical results	32
4.3 Stokes' equations	33
4.3.1 Discretization of the weak form	33
4.3.2 Boundary conditions	34
4.3.3 Numerical results	36
5 Hybrid Mimetic Spectral Element Method	39
5.1 Domain decomposition	39
5.1.1 Reenforcement of continuity	39
5.1.2 Linear system of reenforcement	41
5.2 Numerical experiment	42

6	Conclusion and Recommendation for Future Work	44
6.1	Conclusions	44
6.2	Recommendation for future work	44
	References	46

Introduction

For decades, the Computational Fluids Dynamics (CFD) has been used to numerically solve the fluid-related problems. It can be applied to simple cases, such as incompressible inviscid flows for educational purpose, and also to complex cases that simulate the real-world behaviour of fluids for industrial applications. Therefore, it is widely involved in the designing process of vehicles, aircraft, nozzles, server ventilation, etc [32]. As a numerical method, there are often two concerns with it, i.e. its accuracy that matches the numerical results to the real-world phenomena, and its computational efficiency. In this paper, for the second concern, a novel idea of discretization technique, i.e. domain decomposition, is to be proposed and applied to the Mimetic Spectral Element Method (MSEM).

MSEM is a numerical method that applies the technique of mimetic discretization to the Spectral Element Method. A numerical method solves PDE's, which are described in the continuous domain and illustrate the phenomenon in real physical world, in a discrete algebraic way; and in order to evaluate a certain method, several aspects are considered, such as accuracy, stability, convergence, physical consistency, etc. According to Bochev [4], any numerical scheme that is used to discretize the system may separate the topology from metric. In this case, the stability of the scheme is considered whether the topological structure is well preserved during the discretization; and the physical consistency is whether the metric is well applied, i.e. the approximation of the computed physical solution is properly matched with the actual one. The concept of mimetic method therefore offers great advantages to these properties.

The major initiation of this work is the idea that the physical quantities in the real world, either spatial or temporal, can be associated and classified to certain groups of geometrical objects according to Tonti [34, 35, 36], who summarized them into the Tonti diagrams. This then implies strong relations between the differential geometry and algebraic topology [37]. This enlightens a hint to separate the topology and metric from the numerical method, and a general framework is proposed by Bochev and Hyman [5], to which the discretization is compatible with the underlying physical laws illustrated by PDE's. For example, inspect the following three fundamental equations in electrostatics [17],

$$\mathbf{E} = -\nabla\varphi \quad (1.1a)$$

$$\nabla \cdot \mathbf{D} = \rho \quad (1.1b)$$

$$\mathbf{D} = \varepsilon \mathbf{E} \quad (1.1c)$$

in which $\mathbf{E}$ and $\mathbf{D}$ are vector fields of electric field strength and electric displacement respectively, φ and ρ are scalar fields of electric potential and electric charge density respectively, and ε is the constant of permittivity. Among these variables of equation (1.1c), the displacement $\mathbf{D}$ and charge density ρ are classified into the source variables, which can be interpreted as the cause of the physical phenomenon and indicate how much quantity there is in the system. The field strength $\mathbf{E}$ and the electric potential φ are, on the other hand, classified into the configuration variable, which can be interpreted as the effects observed in the physical phenomenon and indicate how strong the quantity is in the system [30, 34]. Both equations (1.1a) and (1.1b) illustrate the topological relation beyond the physical phenomenon,

and refer to the conservation law [39], which in this electrostatic case is embedded in the gradient ∇ and divergence $\nabla \cdot$. These vector operators are applied on infinite-dimensional function space according to the common calculus. However, after the mimetic discretization, they would be substituted by mimetic operators that are applied on discrete finite-dimensional function space, which is the subspace of the previous infinite-dimensional space. By this, the crucial mathematical and physical properties observed in the actual physical world can be preserved in the finite-dimensional algebraic counterpart [22], and thus the topological structure of PDE's can consequently be preserved.

So far, there have been quite many implementations on the idea of the mimetic method, see for example the works by Dodziuk that applied the idea to finite difference method [11]; Brezzi Nédélec, et al. that applied to the mixed finite element method [8, 9, 25]; Bossavit that described physical variables by differential forms [7, 6]; Bochev that came up with the idea of two basic operations, the reduction and reconstruction [5]; and Gerritsma [15, 14], Kreeft [18] et al. that proposed the MSEM, and in further works with Zhang, Pal, et al. they demonstrated the conservation properties held by MSEM [40, 41, 26]; and Zhang that extended the MSEM by introducing hybridization (hMSEM) giving a greater efficiency to the method of higher orders [39].

The idea of hybridization proposed by Zhang is actually a common technique in domain decomposition, see Brezzi, Pian et al. [10, 28]. This technique decomposes the computational domain into subdomains for parallel computing, and the discontinuity between borders of neighbor subdomains is solved by applying strong constraints, i.e. the Lagrange multipliers, to the degrees of freedoms at the discontinuity to force them equal. However, the implementation of this idea by Zhang ran into singular matrix when solving incompressible flow problem. Thus in this paper, the aim clearly is to try to solve this.

1.1. Research Question

The major objective of this thesis is to find a method to fix the singularity issue as mentioned above that occurs when applying the hybridization to the MSEM to solve the incompressible flow.

The following sub-questions are listed to support the main objective:

1. Can the singularity issue be eliminated while keeping the idea of hMSEM original, i.e. to find an algebraic way?
2. Is it possible to generalize the proposed method to more common problems, e.g. the Stokes' equations?

1.2. Report Outline

Here concludes the introduction of this thesis. In chapter 2 the related mathematical backbones will be briefly introduced. Then in chapter 3 the numerical method MSEM and its related implementation will be discussed, and tested in chapter 4 by the Poisson's equation and Stokes' equations respectively. The major objective will be proposed and tested in chapter 5, to which the results will finally be presented in chapter 6.

2

Mathematical Backbones

This chapter introduces the mathematical backbones that how MSEM is based on. There are two topics: differential geometry that is discussed in section 2.1, and algebraic topology in section 2.2.

2.1. Differential Geometry

In this section, various concepts of differential geometry are addressed, which eventually lead to the important De Rham complex that provides the solid fundamental to the MSEM.

2.1.1. Manifold

By definition [13, 18], an n -dimensional manifold is a topological space $\mathcal{M}$ with subsets $\mathcal{U}_\alpha \subset \mathcal{M}$, where these subsets $\mathcal{U}_\alpha$ is called the coordinate chart, and each point on $\mathcal{M}$ should be found in at least one of these subsets. Furthermore, there are such one-to-one functions $\varphi_{\mathcal{M}, \alpha}$, called local coordinate maps $\mathcal{U}_\alpha \rightarrow V_\alpha$, where V_α are open subsets of $\mathbb{R}^n$. In general, the manifold can be considered as a generic space, in which the differentiation and integration can be conducted. A generic law of calculus over the manifold can then be specialized into the more familiar vector calculus on Euclidean space, which will be discussed later.

To have a figurative illustration of manifolds, for an improper example, the surface of the earth, which is a sphere, can be considered as a manifold. Any region on earth is one of the subsets of the manifold. The latitude and longitude form a coordinate system but they do not hold the "convenient" properties of the Cartesian system in a 2-dimensional Euclidean space, as the latter one cannot be built over a sphere. However, as the definition states, a local coordinate mapping can rather be used to create the 2-D planar map for the region. After all, the Euclidean space is a case of manifold, and eventually all the numerical calculations will be carried on the Euclidean space.

2.1.2. Tangent and cotangent spaces

While the vector calculus is a friendly language to explain continuum mechanics to most scholars, the calculus on manifolds is, however, rather more suitable and gives fundamental insights in the physical laws that govern the phenomena and interaction between the physical quantities and the geometry that they are assigned to [18]. To perform the integration over a k -dimensional manifold, the concept of differential k -form is introduced, which can be considered as the integrand in such case [12].

Before introducing the differential form, a prior concept of tangent space should be mentioned, to which the differential form can be defined in duality. Consider a 1-dimensional curve $\gamma(x)$ in an n -dimensional manifold $\mathcal{M}$, on which at point $\mathcal{P}$ with $x = 0$, its tangent vector is $\dot{\gamma}(0)$. Such tangent vector can be found at this location over n different curves over $\mathcal{M}$. This may yields n linearly independent vectors, denoted as

$$e_1|_{\mathcal{P}}, \dots, e_n|_{\mathcal{P}} \quad (2.1)$$

If now a Euclidean space with coordinates x^i is introduced locally to the neighborhood at point $\mathcal{P}$,

vector basis equation (2.1) now becomes

$$\frac{\partial}{\partial x^1}, \dots, \frac{\partial}{\partial x^n} \quad (2.2)$$

and they span a tangent vector space at point $\mathcal{P}$ as $T_{\mathcal{P}}\mathcal{M}$, in which the vector is

$$v|_{\mathcal{P}} = \sum_{i=1}^n a^i(\mathcal{P}) \frac{\partial}{\partial x^i}|_{\mathcal{P}} \quad (2.3)$$

equation (2.3) can be considered as the directional derivative $\nabla_v f(x) = v \cdot \frac{\partial f(x)}{\partial x}$ at point $\mathcal{P}$, where the coefficients $a^i(\mathcal{P})$ denote the directional vector v .

With the tangent space $T_{\mathcal{P}}\mathcal{M}$ defined above, the differential forms can now be defined as the elements in the space $T_{\mathcal{P}}^*\mathcal{M}$ that is the dual to $T_{\mathcal{P}}\mathcal{M}$. A dual space V^* to any linear vector space V consists all linear forms that map $V \rightarrow \mathbb{R}$, so for $\alpha \in T_{\mathcal{P}}^*\mathcal{M}$, the linear map is

$$\alpha : T_{\mathcal{P}}\mathcal{M} \rightarrow \mathbb{R} \quad (2.4)$$

and such element α is called the covector at point $\mathcal{P}$. Just like the basis equation (2.1) of the tangent space, one can also define a basis for the covectors as

$$e^1|_{\mathcal{P}}, \dots, e^n|_{\mathcal{P}} \quad (2.5)$$

Furthermore, no matter each element $e_i|_{\mathcal{P}}$ in basis equation (2.1) is orthogonal to each other or not, one can always find the certain covector basis $e^j|_{\mathcal{P}}$ that is orthogonal to each $e_i|_{\mathcal{P}}$ except for the case $i = j$, and this indicates the Kronecker delta property

$$e^i(e_j) = \delta_{ij} \quad (2.6)$$

recalling that $e^i \in T_{\mathcal{M}}^*$ is linear functional that can be applied on e_j . Similar to tangent vectors equation (2.3) that are represented by local coordinates, the covectors can now be represented at point $\mathcal{P}$ by

$$\alpha|_{\mathcal{P}} = \sum_{i=1}^n \alpha_i(\mathcal{P}) dx^i|_{\mathcal{P}} \quad (2.7)$$

where d is the exterior derivative that gives differential 1-form dx^i and α itself. Due to the Kronecker delta property

$$dx^i\left(\frac{\partial}{\partial x^j}\right) = \delta_{ij} \quad (2.8)$$

the functional α applied to the tangent vector v can now be calculated as

$$\alpha(v)|_{\mathcal{P}} = \sum_{i=1}^n \alpha_i(\mathcal{P}) a^i(\mathcal{P}) \quad (2.9)$$

It could be quite confusing at the beginning to understand the result presented in equation (2.8), where dx^i is a differential form, and the exterior derivative d also has its own meaning, and the partial derivative $\partial/\partial x^j$ is rather more familiar as in vector calculus. However, it is by the definition of "what it is supposed to do" that equation (2.8) holds, but not by the mathematical structure underlying, i.e. the duality between two vector spaces $T_{\mathcal{P}}\mathcal{M}$ and $T_{\mathcal{P}}^*\mathcal{M}$ is deliberately designed to satisfy equation (2.8).

Mathematically, the differential 1-form dx^i can be interpreted as a directional probe that only matches to the information carried by the tangent vector $a^j \partial/\partial x^j$ in the same direction given by $i = j$. For example, consider a scalar function $f(x^1, \dots, x^n)$, which is a 0-form on the manifold $\mathcal{M}$, and applying the exterior derivative to f yields the 1-form, which can be represented by the total derivative as

$$\alpha^{(1)} = df(x^1, \dots, x^n) = \sum_{i=1}^n \frac{\partial f}{\partial x^i} dx^i \quad (2.10)$$

Since the tangent vector v carries the information of arbitrary direction, $\alpha^{(1)}(v)$ gives the directional derivative of f along the direction of v . This is quite opposite to what is conducted in conventional vector calculus, in which the operator of directional derivative (tangent vector) ∇_v is applied to function f ; while in differential geometry the differential form is, however, an operator that is applied to the tangent vector to obtain the same result. This is again simply due to the definition of the duality between the tangent and cotangent spaces.

Physically, the scalar function 0-form f can represent a scalar field such as potential; and the 1-form df can represent a vector field such as force or flow, and the direction is indicated by its basis dx^i . Therefore, integration is also ideally conducted on differential forms as it carries the information of the field, while the integral domain is described by the structure on the manifold. For example, the curve γ with tangent vectors defined on it thus is oriented and functions as the route of line integral.

2.1.3. Differential forms on $\mathbb{R}^3$

In this paper, the physical domain of interest is 3-dimensional as in reality, thus it is embedded in $\mathbb{R}^3$, which is a certain case of 3-dimensional manifold. In the following demonstrate the properties of differential 0- to 3-forms.

The 1-form $\alpha^{(1)}$ at an arbitrary point $\mathcal{P}$ on a k -dimensional manifold $\mathcal{M}$ can be expressed by a linear combination [12] as

$$\alpha^{(1)} = \sum_{i=1}^k \alpha_i dx^i, \text{ with } \alpha_i \in \mathbb{R} \quad (2.11)$$

which spans the space $\Lambda^{(k)}(\mathcal{M})$ of k -forms on manifold $\mathcal{M}$. Following equation (2.11), a 1-form on a 3-dimensional space $\mathbb{R}^3$ can be expressed as

$$\lambda^{(1)} = \lambda_1(x, y, z)dx + \lambda_2(x, y, z)dy + \lambda_3(x, y, z)dz \quad (2.12)$$

where the coefficients $\lambda_1(x, y, z)$, $\lambda_2(x, y, z)$, $\lambda_3(x, y, z)$ are scalar functions defined on $\mathcal{M}$, or in other word the vector proxies of $\lambda^{(1)}$ [14]. The 1-form can be integrated over a 1-dimensional curve C as the line integral. If the curve is parameterized by a single variable $s \in (-\varepsilon, \varepsilon)$ with $\varepsilon > 0$ as $C(s) = (c^1(s), c^2(s), c^3(s))$, its tangent vector can be represented as

$$\dot{C}(s) = \frac{dc^1}{ds} \frac{\partial}{\partial x} + \frac{dc^2}{ds} \frac{\partial}{\partial y} + \frac{dc^3}{ds} \frac{\partial}{\partial z} \quad (2.13)$$

and then the integral turns into

$$\int_C \lambda^{(1)} = \int_{-\varepsilon}^{\varepsilon} \lambda^{(1)}(\dot{C}(s)) = \int_{-\varepsilon}^{\varepsilon} \lambda_1 \frac{dc^1}{ds} + \lambda_2 \frac{dc^2}{ds} + \lambda_3 \frac{dc^3}{ds} \quad (2.14)$$

Integral equation (2.14) demonstrates the dual identities of the differential form, i.e. it functions as an operator that takes a tangent vector, and also as the integrand over a manifold. Such dual identities are united by parameterization, where $\lambda^{(1)}(\dot{C}(s))$ in equation (2.14) clearly shows this process. From the other perspective, for $\lambda^{(1)}$ itself as an integrand, the parameterization is conducted by the pullback operation. Let Φ be a mapping $\mathcal{M} \rightarrow \mathcal{N}$ between two manifolds, and Φ^* be another mapping $\Lambda^k(\mathcal{N}) \rightarrow \Lambda^k(\mathcal{M})$, called pullback, between two spaces of differential forms. Note the direction from $\mathcal{N}$ back to $\mathcal{M}$. This introduces the following dual relation of integral

$$\int_{\Phi(\mathcal{M})} \alpha^{(k)} = \int_{\mathcal{M}} \Phi^* \alpha^{(k)} \quad (2.15)$$

Therefore, the integration equation (2.14) can also be interpreted by equation (2.15), where the differential form $\lambda^{(1)} \in \mathcal{M}$ is now limited over curve C , and the pullback operator Φ now maps $\mathbb{R} \rightarrow C$ and Φ^* maps $\Lambda^1(C) \rightarrow \mathbb{R}$, which is finally expressed as the finite integral of single variable as in equation (2.14).

Specially the 0-form defined on a k -dimensional manifold is just a real-valued scalar function. For example the 0-form $\alpha^{(0)}$ defined on $\mathbb{R}^3$ can be expressed as [14]

$$\alpha^{(0)} = f(x, y, z) \quad (2.16)$$

For consistency, the integration of a 0-form is defined as a sum over a collection of points $\mathcal{P}_1, \dots, \mathcal{P}_k$ as

$$\int_{\mathcal{P}_1, \dots, \mathcal{P}_k} \alpha^{(0)} = \sum_1^k f(\mathcal{P}_i) \quad (2.17)$$

Keep in mind that a k -form can only be integrated over a k -dimensional manifold, and thus the integration of equation (2.17) is the summation of function values over discrete 0-dimensional points.

The k -form with higher degree $k > 1$ can be obtained by taking the sum of the wedge product of 1-forms, and examples of the 2 and 3-forms on $\mathbb{R}^3$ can be expressed as

$$\eta^{(2)} = \eta_1(x, y, z)dx \wedge dy + \eta_2(x, y, z)dy \wedge dz + \eta_3(x, y, z)dz \wedge dx \quad (2.18)$$

$$\omega^{(3)} = \omega(x, y, z)dx \wedge dy \wedge dz \quad (2.19)$$

where $\wedge$ is the exterior or wedge product, and it is skew-symmetric that $dx \wedge dy = -dy \wedge dx$, which indicates that the area denoted by $dx \wedge dy$ is oriented. Specially, $dx \wedge dy \wedge dz$ is called the volume form for it is of the same dimension as the embedded manifold, and for a volume form $\sigma^{(n)}$ its integral of the manifold $\int_{\mathcal{M}} \sigma^{(n)}$ is just the volume of the manifold. Their integrals in $\mathbb{R}^3$ can be found as the surface integral over $\mathcal{S}$ and the volume integral over $\mathcal{V}$ as following,

$$\int_{\mathcal{S}} \eta^{(2)} = \int_{\mathcal{S}} \eta_1(x, y, z)dx \wedge dy + \eta_2(x, y, z)dy \wedge dz + \eta_3(x, y, z)dz \wedge dx \quad (2.20)$$

$$\int_{\mathcal{V}} \omega^{(3)} = \int_{\mathcal{V}} \omega(x, y, z)dx \wedge dy \wedge dz \quad (2.21)$$

Note that the integration of differential forms over manifold is a metric-free operation [13].

These integrals can be expressed as the duality paring between the differential k -form $\alpha^{(k)}$ and the manifold $\mathcal{M}$ as

$$\langle \alpha^{(k)}, \mathcal{M} \rangle = \int_{\mathcal{M}} \alpha^{(k)} \in \mathbb{R} \quad (2.22)$$

in which $\langle \cdot, \cdot \rangle$ is a bilinear map $V^* \times V \rightarrow \mathbb{R}$, recalling that the manifold $\mathcal{M}$ itself is from the chain space generated by the tangent space $T_{\mathcal{P}}\mathcal{M}$ at point $\mathcal{P}$ and the differential form $\alpha^{(k)}$ is from the dual cotangent space $T_{\mathcal{P}}^*\mathcal{M}$ consisting of functionals. Similarly, the application of the differential form to the tangent vector as the integrand in equation (2.14) can also be expressed by the duality paring as

$$\langle \alpha^{(k)}, C \rangle = \int_C \alpha^{(k)} = \int_{-\epsilon}^{\epsilon} \langle \alpha^{(k)}|_{\epsilon}, \dot{C}(s) \rangle \quad (2.23)$$

in which $\dot{C}(s)$ is from the tangent vector space.

The aforementioned wedge product $\wedge$ [12, 33] of two differential forms $\alpha^{(k)} \in \Lambda^{(k)}$ and $\beta^{(l)} \in \Lambda^{(l)}$ on an n -dimensional manifold $\mathcal{M}$, with $k + l \leq n$, is a mapping $\wedge : \Lambda^{(k)}(\mathcal{M}) \times \Lambda^{(l)}(\mathcal{M}) \rightarrow \Lambda^{(k+l)}(\mathcal{M})$. It maps two differential forms of lower degrees to a differential form of higher order, but still living inside the ambient space, i.e. the n -dimensional manifold. The properties that the wedge product satisfy are as follows, given that $\gamma^{(m)} \in \Lambda^{(m)}$ and $f \in \Lambda^{(0)}$

$$\alpha^{(k)} \wedge \beta^{(l)} = (-1)^{kl} \beta^{(l)} \wedge \alpha^{(k)} \quad (2.24a)$$

$$(\alpha^{(k)} + \beta^{(l)}) \wedge \gamma^{(m)} = \alpha^{(k)} \wedge \gamma^{(m)} + \beta^{(l)} \wedge \gamma^{(m)} \quad (2.24b)$$

$$(\alpha^{(k)} \wedge \beta^{(l)}) \wedge \gamma^{(m)} = \alpha^{(k)} \wedge (\beta^{(l)} \wedge \gamma^{(m)}) \quad (2.24c)$$

$$f(\alpha^{(k)} \wedge \beta^{(l)}) = f(\alpha^{(k)}) \wedge \beta^{(l)} = \alpha^{(k)} \wedge f(\beta^{(l)}) \quad (2.24d)$$

equation (2.24a) further implies that

$$\alpha^{(k)} \wedge \alpha^{(k)} = 0 \quad (2.25)$$

which is straightforward, recalling that $\alpha^{(1)} \wedge \beta^{(1)}$ can represent the oriented area of the parallelogram bounded by $\alpha^{(1)}$ and $\beta^{(1)}$, and it becomes zero if $\alpha^{(1)} = \beta^{(1)}$.

2.1.4. Exterior derivative

In the previous section, the underlying mathematics of the exterior derivative d is ignored, and the duality between the differential forms and the tangent vectors works simply "by definition". In this section, the basics of the exterior derivative will be introduced and its powerful essence to the conventional vector calculus will also be illustrated. In the scope of vector calculus, operators of gradient, curl and divergence are quite useful and neat, which are fundamental to PDE's that dominate the physical phenomena. However, in the scope of differential geometry, all these three operators are generalized into a single metric-free one, the exterior derivative.

The exterior derivative [13, 12] applied to the differential form on an n -dimensional manifold $\mathcal{M}$ is a mapping $d : \Lambda^{(k)}(\mathcal{M}) \rightarrow \Lambda^{(k+1)}(\mathcal{M})$. The properties that are satisfied by the exterior derivative are as following, given that α and β are differential forms and f is a 0-form,

$$d(d\alpha^{(k)}) = 0 \quad (2.26a)$$

$$d(\alpha^{(k)} + \beta^{(k)}) = d\alpha^{(k)} + d\beta^{(k)} \quad (2.26b)$$

$$d(\alpha^{(k)} \wedge \beta^{(l)}) = d\alpha^{(k)} \wedge \beta^{(l)} + (-1)^k \alpha^{(k)} \wedge d\beta^{(l)} \quad (2.26c)$$

$$df = \sum_i \frac{\partial f}{\partial x_i} dx_i \quad (2.26d)$$

equation (2.26d) simply illustrates the gradient operator ∇ in 3-dimensional Euclidean space by applying the exterior derivative to a 0-form $\alpha^{(0)} = f(x, y, z)$ as

$$d\alpha^{(0)} = \frac{\partial f}{\partial x} dx + \frac{\partial f}{\partial y} dy + \frac{\partial f}{\partial z} dz \quad (2.27)$$

in which on the right-hand side is a linear combination of 1-forms similar to equation (2.12).

Now consider a 1-form $\lambda^{(1)}$ defined on $\mathbb{R}^3$, as

$$\lambda^{(1)} = \lambda_1 dx + \lambda_2 dy + \lambda_3 dz \quad (2.28)$$

Its exterior derivative $d\lambda^{(1)}$ can be calculated by the nilpotent property equation (2.26a) and graded product rule equation (2.26c) as

$$d\lambda^{(1)} = d\lambda_1 \wedge dx + d\lambda_2 \wedge dy + d\lambda_3 \wedge dz \quad (2.29)$$

in which the newly derived 1-form λ_1 can be found by the total derivative of the scalar function λ_1 as

$$d\lambda_1 = \frac{\partial \lambda_1}{\partial x} dx + \frac{\partial \lambda_1}{\partial y} dy + \frac{\partial \lambda_1}{\partial z} dz \quad (2.30)$$

and so are λ_2 and λ_3 . This finally gives the exterior derivative $d\lambda^{(1)}$ as

$$\begin{aligned} d\lambda^{(1)} = & \left(\frac{\partial \lambda_3}{\partial y} - \frac{\partial \lambda_2}{\partial z} \right) dy \wedge dz + \left(\frac{\partial \lambda_1}{\partial z} - \frac{\partial \lambda_3}{\partial x} \right) dz \wedge dx \\ & + \left(\frac{\partial \lambda_2}{\partial x} - \frac{\partial \lambda_1}{\partial y} \right) dx \wedge dy \end{aligned} \quad (2.31)$$

equation (2.31) is found to be the sum of the vector components of the curl operator $\nabla \times$ applied to a vector (1-form) on $\mathbb{R}^3$, in which, the wedge product, for example $dy \wedge dz$, can be interpreted as the oriented infinitesimal surface element along the x direction. A benefit here of using wedge product is that the direction is automatically handled and can be reversed naturally by switching the order of the product as $dz \wedge dy$.

Similarly, applying the exterior derivative to a 2-form $\eta^{(2)}$ on $\mathbb{R}^3$ yields

$$d\eta^{(2)} = d\eta_1 dy \wedge dz + d\eta_2 dz \wedge dx + d\eta_3 dx \wedge dy \quad (2.32)$$

in which the first term for example, can be found as

$$\begin{aligned} d\eta_1 dy \wedge dz &= \left(\frac{\partial \eta_1}{\partial x} dx + \frac{\partial \eta_1}{\partial y} dy + \frac{\partial \eta_1}{\partial z} dz \right) dy \wedge dz \\ &= \frac{\partial \eta_1}{\partial x} dx \wedge dy \wedge dz + \frac{\partial \eta_1}{\partial y} dy \wedge dy \wedge dz + \frac{\partial \eta_1}{\partial z} dz \wedge dy \wedge dz \end{aligned} \quad (2.33)$$

$$= \frac{\partial \eta_1}{\partial x} dx \wedge dy \wedge dz \quad (2.34)$$

and so are the rest two terms in equation (2.32). This finally leads to the result of the exterior derivative of the 2-form as

$$\begin{aligned} d\eta^{(2)} &= \frac{\partial \eta_1}{\partial x} dx \wedge dy \wedge dz + \frac{\partial \eta_2}{\partial y} dy \wedge dz \wedge dx + \frac{\partial \eta_3}{\partial z} dz \wedge dx \wedge dy \\ &= \left(\frac{\partial \eta_1}{\partial x} + \frac{\partial \eta_2}{\partial y} + \frac{\partial \eta_3}{\partial z} \right) dx \wedge dy \wedge dz \end{aligned} \quad (2.35)$$

which clearly shows the divergence operator $\nabla \cdot$ in $\mathbb{R}^3$.

Lastly, one can also apply the exterior derivative to a 3-form in $\mathbb{R}^3$, giving

$$d\omega^{(3)} = d\omega dx \wedge dy \wedge dz \quad (2.36)$$

in which $d\omega$ includes terms of dx , dy and dz that will all vanish when applying the wedge product to $dx \wedge dy \wedge dz$. Therefore, the exterior derivative applied to a 3-form in $\mathbb{R}^3$ is 0.

Apart from the interpretation of the exterior derivative on differential forms on $\mathbb{R}^3$ that they represent the conventional vector operators, the nilpotent property equation (2.26a) of the exterior product further implies the two well-known vector calculus identities

$$\nabla \times (\nabla) = 0 \quad (2.37a)$$

$$\nabla \cdot (\nabla \times) = 0 \quad (2.37b)$$

The examples above of applying the exterior derivative to differential forms show the fact that the spaces $\Lambda^{(k)}(\mathcal{M})$ of differential forms are connected sequentially by the exterior derivative. Such sequence is clearly represented by the De Rham complex [38, 3, 2, 5], for example over a 3-dimensional manifold as

$$0 \rightarrow \Lambda^{(0)}(\mathcal{M}) \xrightarrow{\nabla} \Lambda^{(1)}(\mathcal{M}) \xrightarrow{\nabla \times} \Lambda^{(2)}(\mathcal{M}) \xrightarrow{\nabla \cdot} \Lambda^{(3)}(\mathcal{M}) \rightarrow 0 \quad (2.38)$$

2.1.5. Generalized Stokes' theorem

Recall the Stokes' theorem and the Gauss divergence theorem on $\mathbb{R}^3$ defined by the vector calculus,

$$\iint_S (\nabla \times \mathbf{F}) \cdot d\mathbf{S} = \oint_{\partial S} \mathbf{F} \cdot d\mathbf{\Gamma} \quad (2.39)$$

$$\iiint_V (\nabla \cdot \mathbf{F}) dV = \oint_{\partial V} \mathbf{F} \cdot d\mathbf{S} \quad (2.40)$$

where $\mathbf{F}$ is a vector field on $\mathbb{R}^3$, and $\mathbf{\Gamma}$, $\mathbf{S}$ and V are the closed oriented curve, closed oriented surface and volume respectively. Another integration that shares similar structure includes the gradient, as

$$\int_C \nabla \varphi \cdot d\mathbf{C} = \varphi|_{\partial C} = \varphi(\mathcal{P}_2) - \varphi(\mathcal{P}_1) \quad (2.41)$$

where φ is a scalar function defined on $\mathbb{R}^3$, C is an orientated curve and $\mathcal{P}_1$ and $\mathcal{P}_2$ are the two end points on C . In $\mathbb{R}$, equation (2.41) can be reduced to the well-known Newton-Leibniz theorem that

calculate the integral of a single-variable function over a closed interval by the difference of its primitive function at the end points.

All these three equations (2.39) to (2.41) demonstrate that the integration over a certain geometry, curve, surface or volume, can be transferred to finding the integral over the corresponding boundary of this geometry. This can then be condensed to the generalized Stokes' theorem [33] as

$$\int_{\mathcal{M}} d\alpha^{(k)} = \int_{\partial\mathcal{M}} \alpha^{(k)} \quad (2.42)$$

where ∂ here is the boundary operator that finds the boundary of the manifold $\mathcal{M}$. Note its nilpotent property $\partial\partial = 0$ that the boundary of a boundary is null, just similar to $dd = 0$. equation (2.42) can also be expressed in the form of duality pairing as

$$\langle d\alpha^{(k)}, \mathcal{M} \rangle = \langle \alpha^{(k)}, \partial\mathcal{M} \rangle \quad (2.43)$$

which shows that the exterior derivative d is the formal adjoint of the boundary operator ∂ [27]. Note that the boundary operator ∂ uses the same symbol as the partial derivative $\partial/\partial x^i$ or ∂_i , but they are two different operations. However, they are still relevant due to the adjoint relation to the exterior derivative. Recall that in the previous section, the exterior derivative can be considered as the analogy to conventional gradient, curl and divergence operators in $\mathbb{R}^3$, and all these operators includes the partial derivatives.

2.1.6. Hodge star operator

The Hodge star $\star$ operator is a mapping [13, 18] $\Lambda^k(\mathcal{M}) \rightarrow \Lambda^{(n-k)}(\mathcal{M})$, defined on an n -dimensional manifold $\mathcal{M}$. An important property that can be derived from the definition is

$$\alpha^{(k)} \wedge \star\beta^{(k)} = \langle \alpha^{(k)}, \beta^{(k)} \rangle \sigma^{(n)} \quad (2.44)$$

where $\sigma^{(n)}$ is the volume form. Recall that the wedge product of two differential forms of the same k -dimension yields a new one of $2k$ -dimension, which is not necessarily equal to the dimension of the manifold n . This raises a problem that the integral of such product cannot be evaluated over the manifold for $2k \neq n$. equation (2.44), however, gives the solution that it always yields a result of n -form, by which the L^2 inner product of two k -forms is defined as

$$\langle \alpha^{(k)}, \beta^{(k)} \rangle_{L^2} = \int_{\mathcal{M}} \langle \alpha^{(k)}, \beta^{(k)} \rangle \sigma^{(n)} = \int_{\mathcal{M}} \alpha^{(k)} \wedge \star\beta^{(k)} \quad (2.45)$$

Since the paring here is conducted between the same two spaces (not dual ones, and thus unlike the duality paring, which is metric-free), extra structure is required, i.e. the Hodge star operator, and it introduces metrics into the process [18].

An example of the application of the Hodge star operator is illustrated by [14]. Consider the Poisson equation $\nabla \cdot (\nabla\varphi) = f$ decomposed into a first-order system

$$\nabla \cdot \mathbf{q} = f \quad (2.46a)$$

$$\nabla\varphi = \mathbf{u} \quad (2.46b)$$

$$\mathbf{u} = \mathbf{q} \quad (2.46c)$$

in which $\mathbf{q}$ and $\mathbf{u}$ are vector fields and φ and f are scalar fields. Now recall the exterior derivatives discussed in section 2.1.4, in $\mathbb{R}^3$ the divergence operator $\nabla \cdot$ acts on a 2-form, and the gradient operator ∇ acts on the 1-form. Therefore, the vector field $\mathbf{q}$ can be interpreted as a 2-form $q^{(2)}$, and as a result f must be a 3-form $f^{(3)}$, which turns equation (2.46a) into the form

$$dq^{(2)} = f^{(3)} \quad (2.47)$$

Similarly, since the gradient operator ∇ acts on a 0-form, equation (2.46b) can be interpreted as

$$d\varphi^{(0)} = u^{(1)} \quad (2.48)$$

However, such interpretation results in a dilemma to the last equation (2.46c) as

$$u^{(1)} = q^{(2)} \quad (2.49)$$

which makes no sense, while equation (2.46c) still holds meaningful to the conventional differential calculus.

Such dilemma is solved by introducing a the Hodge $\star$ operator, which conducts the transform to equation (2.49) in $\mathbb{R}^3$ as

$$\star u^{(1)} = q^{(2)} \text{ or } \star q^{(2)} = u^{(1)} \quad (2.50)$$

in either way, and a deeper insight to this is expressed as

$$\star dx_1 = dx_2 \wedge dx_3 \text{ or } \star (dx_2 \wedge dx_3) = dx_1 \quad (2.51)$$

If the Hodge star is applied twice, the resulted differential form returns to the original k -form but the sign could be flipped depending on the dimension of the differential form itself and that of the ambient manifold as

$$\star \star \alpha^{(k)} = (-1)^{k(n-k)} \alpha^{(k)} \quad (2.52)$$

It is worth noting that the Hodge operator introduces the metric tensor to explain the curvature of the manifold, while the other operators introduced before, such as the exterior derivative and the wedge product, are purely topological. This property plays an important role in discretization that will be introduced in chapter 5.

One of the functions of the Hodge star operator as illustrated by equation (2.50) is that it connects two de Rham complices in opposite direction. Such dual de Rham complex in $\mathbb{R}^3$ is illustrated as

$$\begin{array}{ccccccc} 0 & \rightarrow & \Lambda^{(0)}(\mathcal{M}) & \xrightarrow{d} & \Lambda^{(1)}(\mathcal{M}) & \xrightarrow{d} & \Lambda^{(2)}(\mathcal{M}) & \xrightarrow{d} & \Lambda^{(3)}(\mathcal{M}) & \rightarrow & 0 \\ & & \updownarrow \star & & \updownarrow \star & & \updownarrow \star & & \updownarrow \star & & \\ 0 & \leftarrow & \tilde{\Lambda}^{(3)}(\mathcal{M}) & \xleftarrow{d} & \tilde{\Lambda}^{(2)}(\mathcal{M}) & \xleftarrow{d} & \tilde{\Lambda}^{(1)}(\mathcal{M}) & \xleftarrow{d} & \tilde{\Lambda}^{(0)}(\mathcal{M}) & \leftarrow & 0 \end{array} \quad (2.53)$$

in which the tilde on the second row indicates that $\tilde{\Lambda}^{(n-k)}(\mathcal{M})$ is a dual space of differential form $\Lambda^{(k)}(\mathcal{M})$, connected by the Hodge star operator.

Another important function of the Hodge star operator is that it defines the codifferential operator δ as

$$\delta = (-1)^{n(k+1)+1} \star d \star \quad (2.54)$$

which is a mapping $\Lambda^k(\mathcal{M}) \rightarrow \Lambda^{(k-1)}(\mathcal{M})$ as opposite to the exterior derivative d , and it also has the nilpotent property $\delta^2 = 0$. In addition, it is the formal adjoint of d as

$$\int_{\partial \mathcal{M}} \alpha^{(k-1)} \wedge \star \beta^{(k)} = \langle d\alpha^{(k-1)}, \beta^{(k)} \rangle - \langle \alpha^{(k-1)}, \delta \beta^{(k)} \rangle \quad (2.55)$$

which can be interpreted as the integration by parts of the differential form over manifold. Note that in the integral of the boundary term both $\partial \mathcal{M}$ and $\alpha^{(k-1)} \wedge \star \beta^{(k)}$ are $(n-1)$ -dimensional, and that since the definition of the codifferential δ includes the Hodge star operator, it thus introduces metrics, too.

The exterior derivative and the codifferential now can be used to build another dual de Rham complex as

$$\begin{array}{ccccccc} 0 & \rightarrow & \Lambda^{(0)}(\mathcal{M}) & \xrightarrow{d} & \Lambda^{(1)}(\mathcal{M}) & \xrightarrow{d} & \Lambda^{(2)}(\mathcal{M}) & \xrightarrow{d} & \Lambda^{(3)}(\mathcal{M}) & \rightarrow & 0 \\ & & \updownarrow & & \updownarrow & & \updownarrow & & \updownarrow & & \\ 0 & \leftarrow & \tilde{\Lambda}^{(0)}(\mathcal{M}) & \xleftarrow{\delta} & \tilde{\Lambda}^{(1)}(\mathcal{M}) & \xleftarrow{\delta} & \tilde{\Lambda}^{(2)}(\mathcal{M}) & \xleftarrow{\delta} & \tilde{\Lambda}^{(3)}(\mathcal{M}) & \leftarrow & 0 \end{array} \quad (2.56)$$

In the dual de Rham complex as shown in equation (2.53) constructed by only the exterior derivative, the spaces $\Lambda^{(k)}(\mathcal{M})$ and $\tilde{\Lambda}^{(n-k)}(\mathcal{M})$ are placed at opposite locations and connected by the Hodge star operator. The dual complex as shown in equation (2.56) constructed by both the exterior derivative and the codifferential, however, reverses the sequence of the dual spaces so that $\Lambda^{(k)}(\mathcal{M})$ and $\tilde{\Lambda}^{(k)}(\mathcal{M})$ are now placed at the opposite locations. Thus they are no longer connected by the Hodge star operator since they are of the same dimension, but are connected by the duality identity of equation (2.55).

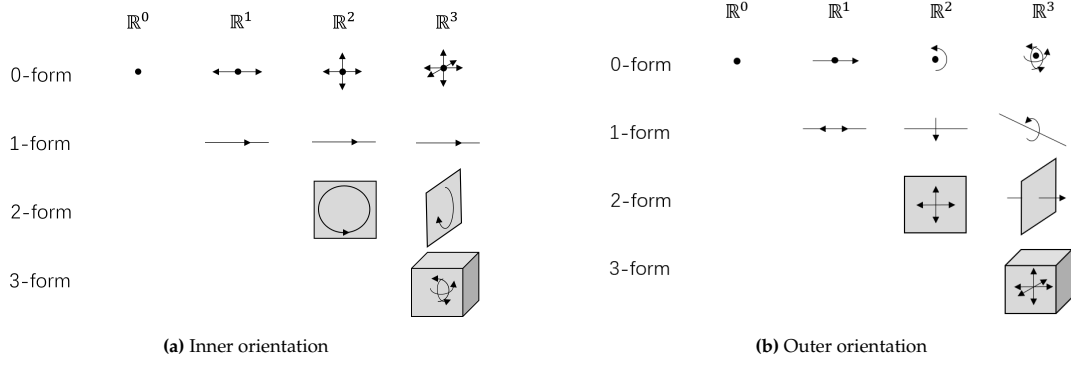


Figure 2.1: Demonstration of the inner and outer orientations of objects in 0, 1, 2 and 3-dimensional spaces [18, 31].

2.2. Algebraic Topology

When numerically solving a physical problem, such as the potential field caused by an electric charge that is governed by the Poisson's equation, it is important to discretize the physical space into non-overlapping subspaces, on which the solution is built by the chosen numerical method. Such physical space can be mathematically expressed by the aforementioned manifold, and the algebraic topology is then a discrete analogue or counterpart [18, 14] to the manifold.

By topology, one is focusing on the geometric parts instead of the metric parts. The geometry includes, for example, nodes, edges, faces and volumes, which by the language of algebraic topology are called cells. These geometric elements are connected topologically, in which the information of length, angles, curvatures, etc. do not matter at all, since it is captured by the metric parts.

This topological property is found to be applicable to the discretization of certain mathematical concepts [21], such as operators of gradient, curl and divergence that play an important role in PDE's [30]. The nature of these operators is well captured and preserved during the process of discretization, while the approximation happens at the metric part, for example depending on the quality and density of the mesh grid; and these two individual parts can then be well separated.

2.2.1. Orientation of the geometric object

When solving for a physical problem, such as the thermal conduction, the definition of the orientation of geometric objects, to which the physical quantity of interest is assigned matters [22]. For example, the heat source of a volume radiates energy through the volume's boundary to its surroundings; the Fourier's law describes the energy flow from one side of the surface to the other, i.e. the heat flux. These two examples illustrate the so called outer orientation in an $\mathbb{R}^3$ space as shown in figure 2.1b, and the qualifier "outer" indicates that the arrow that represents the direction does not lie on the object, but points outward. This then implies that the outer orientation of a geometric object of certain dimension depends on the dimension of the embedded ambient space, which is illustrated by the line object in figure 2.1b that the orientation in the 2-D space is perpendicular to the line object while in the 3-D space is circulating around the line object.

On the contrary to the outer orientation, the inner orientation assigns the direction arrow within the geometric object as shown in figure 2.1a and therefore it is independent of the the dimension of its ambient space. The 1-D line object is assigned with the orientation along itself in all 1, 2 and 3-dimensional spaces.

2.2.2. Cell and chain

In simple words, a k -cell $c_{(k)}$ on an n -dimensional manifold $\mathcal{M}$ with $n \geq k$ is a set of points on $\mathcal{M}$ [16, 23], and the collection of all these k -cells and their connections forms a topological space, called cell complex. It can be considered as a discrete tool built over the manifold, on which scalars and vectors can be defined and assigned. Note that it is not an instance of the manifold, such as the Euclidean $\mathbb{R}^3$, but on the other hand it is an algebraic counterpart to the manifold. For physical applications in reality, the dimension of the manifold of interest in this section is still limited to 3-dimension.

In $\mathbb{R}^3$, the most fundamental cell is the 0-cell, which is a 0-dimensional object, node, denoted as $c_{(0)}$. 0-cells spread in the space and their locations are irrelevant, but each of them is numbered uniquely as $c_{(0),i}$. Each of these 0-cell is embedded with an orientation previously discussed as in figure 2.1, and a positive orientation is defined arbitrarily but in consistence and applied to all the cells.

For cells of higher dimensions in $\mathbb{R}^3$, they can be easily described as edges $c_{(1)}$, faces $c_{(2)}$ and volumes $c_{(3)}$, and their respective orientations are also illustrated in figure 2.1. Such cell of higher dimension is constructed and bounded by those of lower dimension, so for example, a 1-cell is obviously bounded by 2 0-cells. However, its shape, whether straight or curved, is again irrelevant, while its orientation and relations to its boundary cells are important in topological space, and this will be illustrated in the next section.

A series of N k -cells of the same dimension can be grouped together by a formal sum as

$$c_{(k)} = \sum_{i=1}^N c^i c_{(k),i} \quad (2.57)$$

resulting a k -chain [20, 14, 27]. In this sum, a weight c^i is assigned to each k -cell with value of -1 , 0 or 1 , in which a positive one means that this cell is included in the space with a defined positive orientation, while a negative one means the opposite orientation, and a zero means that this certain cell is excluded from the chain. Finally, all cells of arbitrary dimensions defined in a certain topological space can then be further grouped together by the formal sum into a cell complex. For example, in figure 2.2 is a

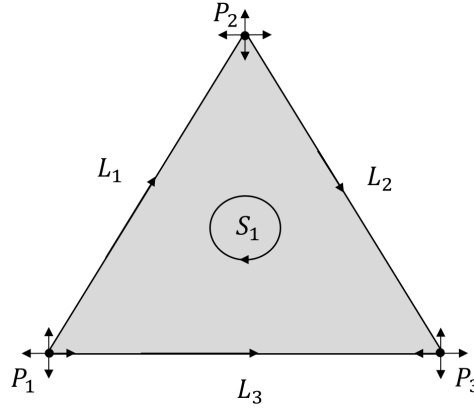


Figure 2.2: A 2-dimensional cell complex.

two-dimensional cell complex that partitions a 2-dimensional space. It consists of a 2-cell (denoted by S_i) bounded by 3 edges (denoted by L_i) of 1-cells, each of which is then bounded by 2 nodes (denoted by P_i) of 0-cells. Inner orientation is assigned to each cell in the complex as indicated by arrows, thus the 1-chain for example can be expressed by the formal sum as

$$c_{(1)} = (+1) \cdot L_1 + (+1) \cdot L_2 + (-1) \cdot L_3 \quad (2.58)$$

2.2.3. Boundary operator and incidence matrix

Recall that the cell complex is a discrete algebraic counterpart of the manifold, thus a similar boundary operator ∂ as in $\partial\mathcal{M}$ can be defined over a k -chain [23, 16, 27] as

$$\partial c_{(k)} = \partial \sum_i c^i c_{(k),i} = \sum_i c^i \partial c_{(k),i} \quad (2.59)$$

in which the boundary of a k -cell is obtained by $(k-1)$ -cells at its boundary as

$$\partial c_{(k),i} = \sum_j e_{ij} c_{(k-1),j} \quad (2.60)$$

in which e_{ij} is the weight that again takes a value of -1, 0 or 1, such that if the orientation of $c_{(k-1),i}$ is equal to that of $c_{(k)}$, c^i takes 1, otherwise if opposite, c^i takes -1, and if $c_{(k-1),i}$ is not included in the boundary of $c_{(k)}$, c^i takes 0.

For example, again examine the 2-dimensional cell complex in figure 2.2. All the 0-cells in the cell complex are assigned with outward positive, i.e. each node is a source. The boundary of a 1-cell can then be expressed algebraically by a 0-chain, e.g. for the edge labeled with L_1 , its boundary is

$$\partial L_1 = (-1) \cdot P_1 + (+1) \cdot P_2 \quad (2.61)$$

When applied to a 1-chain, the boundary of all oriented edges in figure 2.2 can be expressed as

$$\partial \begin{bmatrix} L_1 \\ L_2 \\ L_3 \end{bmatrix} = \begin{bmatrix} \partial L_1 \\ \partial L_2 \\ \partial L_3 \end{bmatrix} = \begin{bmatrix} P_1 - P_2 \\ P_2 - P_3 \\ P_1 - P_3 \end{bmatrix} = \begin{bmatrix} 1 & -1 & 0 \\ 0 & 1 & -1 \\ 1 & 0 & -1 \end{bmatrix} \begin{bmatrix} P_1 \\ P_2 \\ P_3 \end{bmatrix} \quad (2.62)$$

Similarly, the boundary of the 2-chain can be found as

$$\partial S_1 = L_1 + L_2 - L_3 = \begin{bmatrix} 1 & 1 & -1 \end{bmatrix} \begin{bmatrix} L_1 \\ L_2 \\ L_3 \end{bmatrix} \quad (2.63)$$

The matrices that contain only -1, 0 and 1 in equations (2.62) and (2.63) are the incidence matrix, denoted by $\mathbb{E}^{(k,k-1)}$ with k being the dimension of the k -chain whose boundary is built by a $(k-1)$ -chain. It is now easily observed that the boundary of a k -chain in the topological space is well resolved into the incidence matrix without any approximation, which is a quite important and favorable feature in any numerical method where the partial derivative is encountered. It is worth noting the influence of the numbering and defined positive orientation of cells on the structure of the incidence matrix: the numbering of the k -cells in the k -chain on the left-hand side corresponds to rows of the incidence matrix, while that of the $(k-1)$ -cells on the right-hand side constituting the boundary corresponds to the columns of the matrix, so any swapping of numbering would result in the same swapping in either corresponding rows or columns; the defined positive orientation of each k - and $(k-1)$ -cells together determines the sign of each element in the incidence matrix.

The simple cell complex depicted in figure 2.2 can be readily expanded to a furthermore complicated network-shape one that consists of more nodes, edges, faces and even volumes when a third dimension is added to the example space in figure 2.2. However, no matter how ugly or messy the assembled cell complex could be, one should always keep in mind that it is the connectivity among the cells that matters but not the complex's shape. Therefore, in order to build the incidence matrices of any cell complex, one should focus on tracking the assigned number and positive orientation of each cell. As mentioned before, the numbering can be assigned in any order as long as each cell gets its own unique number, and the default positive orientation can also be given arbitrarily. However, for convenience, it is recommended to keep the numbering in a natural order and keep the default positive orientation of each k -cell consistent.

2.2.4. Cochains and coboundary

In section 2.1.2, the concept of duality is introduced, such that the cotangent space is the dual space of the tangent space, and duality pairing between the differential forms and the manifold. Such duality can also be defined to the chain, which introduces the cochain as a counterpart of the differential forms.

Let $C_{(k)}$ be the chain space of k -chains, and its dual space is defined as the cochain space $C^{(k)}$ constituted by k -cochains $c^{(k)}$ [16]. The k -cochain can also be written as a formal sum as

$$c^{(k)} = \sum_{i=1}^N c_i c^{(k),i} \quad (2.64)$$

where $c_i \in \mathbb{R}$ are coefficients that are associated with corresponding k -cells, and $c^{(k),i}$ are dual bases to k -cells $c_{(k),i}$ that satisfy the Kronecker delta property as defined by equation (2.6), which gives the

duality pairing

$$\langle c^{(k)}, c_{(k)} \rangle = \sum_i c_i c^{(k),i} (\sum_j c^j c_{(k),j}) = \sum_i c_i c^i \quad (2.65)$$

equation (2.65) resembles the discrete representation of the duality pairing between the differential form and the embedded manifold $\langle \alpha^{(n)}, \mathcal{M} \rangle$. This can be seen as a discrete counterpart of the integral of a field function over a weighted domain [21], in which the k -cochain is the analogue to the differential form with coefficients c_i representing integrated values assigned over certain k -cells, while the k -chain is the analogue to the manifold [14].

The coboundary operator δ (do not confuse with the codifferential δ in equation (2.54) that is applied on a differential form), by definition [16], is a mapping from the space of k -cochains to the space of $(k+1)$ -cochains $C^{(k)} \mapsto C^{(k+1)}$, similar to the 'exterior derivative defined in section 2.1.4 that is a mapping from a k -form to a $(k+1)$ -form. The coboundary operator is thus the formal adjoint of the boundary operator ∂ [27] as

$$\langle \delta c^{(k)}, c_{(k+1)} \rangle = \langle c^{(k)}, \partial c_{(k+1)} \rangle \quad (2.66)$$

which recalls equation (2.43) that over the manifold the exterior derivative d is the formal adjoint of the boundary operator ∂ . The coboundary operator is nilpotent, too, just like the exterior derivative

$$\delta(\delta c^{(k)}) = 0 \quad (2.67)$$

This property is illustrated in figure 2.3 [5], in which a 0-cell in $\mathbb{R}^2$ with an outer orientation is depicted;

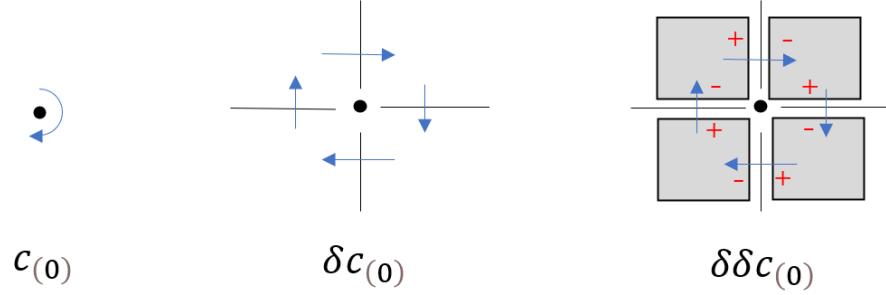


Figure 2.3: Illustration of applying the coboundary operator twice.

when the coboundary operator is applied twice, each of the four surrounding 2-cells has zero net flux (supposing outflow being positive) as indicated by the + and - signs as a result of the positive and negative contributions from the two adjacent 1-cells. Furthermore, by the duality pairing equation (2.66) and the nilpotent equation (2.67),

$$\begin{aligned} \langle c_{(k+2)}, \delta \delta c^{(k)} \rangle &= \langle \partial c_{(k+2)}, \delta c^{(k)} \rangle \\ &= \langle \partial \partial c_{(k+2)}, c^{(k)} \rangle \\ &= 0 \end{aligned} \quad (2.68)$$

the boundary operator ∂ can be proven nilpotent as well

$$\partial(\partial c_{(k)}) = 0 \quad (2.69)$$

Now a cochain complex in $\mathbb{R}^3$ can be built in a similar way to the de Rham sequence of the exterior derivative depicted in equation (2.38) as

$$0 \rightarrow c^{(0)} \xrightarrow{\delta} c^{(1)} \xrightarrow{\delta} c^{(2)} \xrightarrow{\delta} c^{(3)} \rightarrow 0 \quad (2.70)$$

Here, the coboundary operators applied to the 0-, 1- and 2-cochains are the metric-free discrete counterparts of the gradient, curl and divergence operators respectively; and the nilpotent property equation (2.67) can be interpreted as the discrete version of the vector calculus identities equation (2.37b).

A summary of concepts introduced in this chapter about continuous manifold and discrete chains are presented in table 2.1.

Table 2.1: Counterparts between the manifold and the k -chain.

Continuous	Discrete
Manifold $\mathcal{M}$	k -chain $c_{(k)}$
Differential form $\alpha^{(k)}$	k -cochain $c^{(k)}$
Duality pairing $\langle \alpha^{(k)}, \mathcal{M} \rangle$	$\langle c^{(k)}, c_{(k)} \rangle$
Tangent vector basis ∂_i	Chain basis k -cell $c_{(k),i}$
Cotangent vector basis dx^i	Cochain basis $c^{(k),i}$
Kronecker delta $dx^i(\partial_j) = \delta_{ij}$	$c^{(k),i}(c_{(k),j}) = \delta_{ij}$
Boundary operator $\partial\mathcal{M}$	$\partial c_{(k)}$
Exterior derivative d	Coboundary operator δ
Formal adjoint $\langle d\alpha^{(k)}, \mathcal{M} \rangle = \langle \alpha^{(k)}, \partial\mathcal{M} \rangle$	$\langle \delta c^{(k)}, c_{(k+1)} \rangle = \langle c^{(k)}, \partial c_{(k+1)} \rangle$

Mimetic Spectral Element Method

In this chapter, the implementation of the MSEM is presented. Firstly in section 3.1, the two fundamental polynomials on 1-dimensional domain are introduced, which are the building blocks of polynomials of higher dimensions. Then in section 3.2, the polynomials in $\mathbb{R}^3$ are constructed and their relevant algebraic application is introduced.

3.1. Basic mimetic polynomials in 1-dimension

The PDE problem to be solved by the MSEM is usually 3-dimensional in space, which is the case as in the real life. Therefore, a proper selection of the basis functions that discretize the problem in 3-dimension with preserved de Rham sequence is necessary. In this paper, the so-called mimetic polynomials [39] are used and each of them is assigned to a certain geometry, i.e. the nodes, edges, faces and volumes. These functions are constructed by 2 types of 1-dimensional polynomials, i.e. Lagrange polynomials in section 3.1.1 and the edge functions [15] in section 3.1.2. These two polynomials by nature hold a topological derivative relation, which can be represented by the a metric-free incidence matrix presented in section 3.1.3.

3.1.1. Lagrange polynomials

The Lagrange polynomials of degree N can be described as

$$\ell_i(\xi) = \prod_{j=0, j \neq i}^N \frac{\xi - \xi_j}{\xi_i - \xi_j}, \text{ for } i \in \{0, 1, \dots, N\} \quad (3.1)$$

for $N + 1$ nodes

$$-1 = \xi_0 < \xi_1 < \dots < \xi_{N-1} < \xi_N = 1 \quad (3.2)$$

on the reference domain $\Omega_{\text{ref}} = [-1, 1]$. This domain is useful that any arbitrary actual domain can be reduced to or reconstructed from it. equation (3.1) gives the following Kronecker delta property for each node x_j

$$\ell_i(\xi_j) = \delta_{ij} = \begin{cases} 0 & \text{if } i \neq j \\ 1 & \text{if } i = j \end{cases} \quad (3.3)$$

An example of 4-degree Lagrange polynomials is shown in figure 3.1, where the spacing and placing of these $N + 1$ nodes ξ_j are distributed according to the Gauss-Lobatto nodes.

The Kronecker delta property equation (3.3) of the Lagrange polynomials allows the construction of an N -degree polynomial in 1-D

$$p^h(\xi) = \sum_{i=0}^N p_i \ell_i(\xi) \quad (3.4)$$

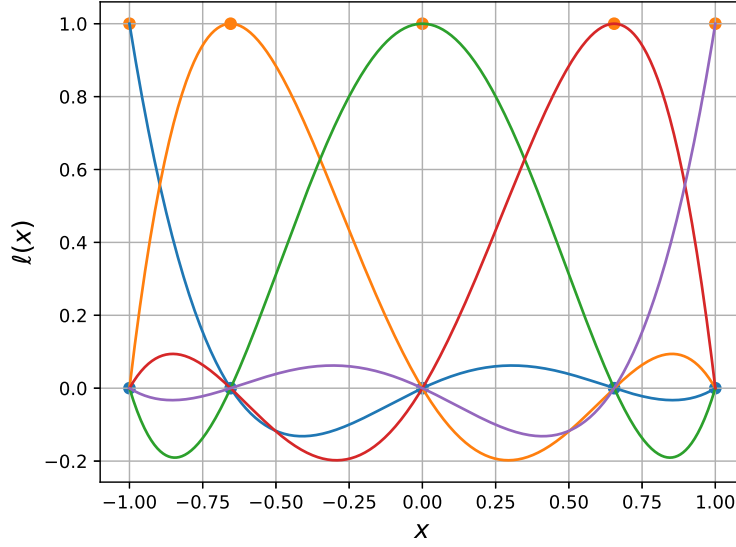


Figure 3.1: Lagrange polynomials of degree 4.

in which the superscript h denotes that this polynomial p^h is constructed by polynomials that span in a discrete space. The coefficient p_i is called the degree of freedom (DoF), and its value is just that of the polynomial $p(\xi_i)$ at node ξ_i

$$p^h(\xi_i) = p_i \quad (3.5)$$

3.1.2. Edge functions

The edge functions are polynomials defined based on the sum of derivatives of the Lagrange polynomials equation (3.1) as

$$e_i(\xi) = \sum_{j=i}^N \frac{d}{d\xi} \ell_j(\xi) = - \sum_{j=0}^{i-1} \frac{d}{d\xi} \ell_j(\xi), \text{ for } i \in \{1, \dots, N\} \quad (3.6)$$

which also gives a similar Kronecker delta property but in the sense of integration on each interval enclosed by the Lobatto nodes ξ_j , as

$$\int_{\xi_{j-1}}^{\xi_j} e_i(\xi) d\xi = \delta_{ij} = \begin{cases} 0 & \text{if } i \neq j \\ 1 & \text{if } i = j \end{cases} \quad (3.7)$$

An example of 4-degree edge functions plotted over the reference domain is shown in figure 3.2, in which the integral of each edge functions in its corresponding interval is colored and the values are all equal to 1.

By the nature of the edge functions, i.e. its definition, the derivative of polynomial $p^h(\xi)$ as defined by equation (3.4) can be built by the edge functions as

$$q^h(\xi) = \frac{d}{d\xi} p^h(\xi) = \sum_i^N q_i e_i(\xi) \quad (3.8)$$

in which q_i here is the DoF and its value also satisfies a similar Kronecker delta property similar to equation (3.5) but again in the sense of integration, as

$$\int_{\xi_{i-1}}^{\xi_i} q^h(\xi) d\xi = q_i \quad (3.9)$$

which offers a good property of reconstructing the derivatives of functions built by the Lagrange polynomials in a metric-free way. This is the key of the MSEM and will be illustrated later.

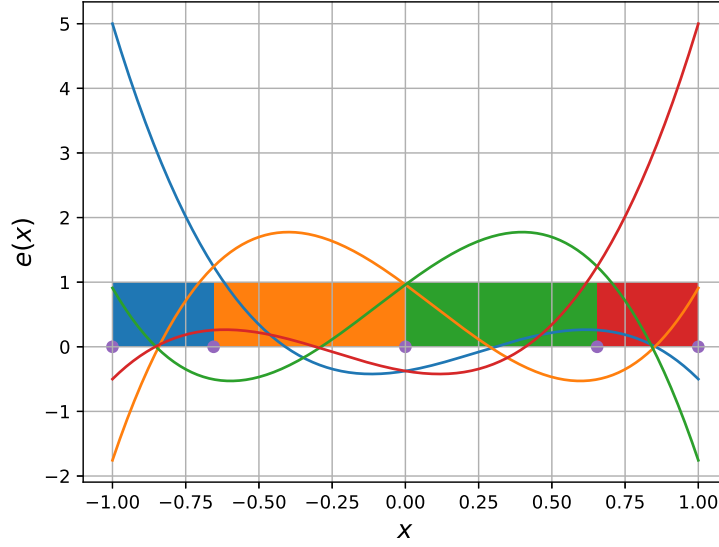


Figure 3.2: Edge polynomials of degree 4.

3.1.3. Incidence matrix in 1 dimension

With the Kronecker delta properties of both $p^h(\xi)$ and $q^h(\xi)$ as given by equations (3.5) and (3.9), the integral relation between DoF's p_i and q_i can be found as

$$q_i = p_i - p_{i-1}, \text{ for } i \in \{1, \dots, N\} \quad (3.10)$$

by which a linear algebraic system can be built.

Consider two vectors $\mathbf{p}$ and $\mathbf{q}$ that are composed of DoF p_i and DoF q_i respectively. A matrix $\mathbb{E}$ of size $N \times (N + 1)$ can be found to satisfy

$$\mathbf{q} = \mathbb{E}\mathbf{p} \quad (3.11)$$

where the only non-zero elements in $\mathbb{E}$ are -1 and 1. An example of size 4×5 is shown as following,

$$\mathbb{E} = \begin{bmatrix} -1 & 1 & 0 & 0 & 0 \\ 0 & -1 & 1 & 0 & 0 \\ 0 & 0 & -1 & 1 & 0 \\ 0 & 0 & 0 & -1 & 1 \end{bmatrix} \quad (3.12)$$

assuming that elements of both vectors $\mathbf{p}$ and $\mathbf{q}$ are in a natural order, i.e. $\mathbf{p} = [p_0 \ p_1 \ p_2 \ p_3 \ p_4]$ and $\mathbf{q} = [q_1 \ q_2 \ q_3 \ q_4]$. If any other arbitrary order is applied, the corresponding places of non-zero elements in $\mathbb{E}$ should be adjusted accordingly. However, in order to build a robust algorithm of MSEM, it is always recommended to adhere to a simple, consistent and developer friendly sequence. Such sequence used in this paper is based on the work by Zhang [39].

It is worth noting that the incidence matrix $\mathbb{E}$ is purely topological, and only depends on the topological nature of the grid, i.e. the ordering of $\mathbf{p}$ and $\mathbf{q}$ as discussed above. The derivative is handled by the edge polynomials and thus this system is structure-preserving.

3.2. Mimetic polynomials in 3-dimension

For basis polynomials in $\mathbb{R}^3$, it is recommended to consult [39] by Zhang for more detailed motivations and derivations. In this paper, terms and notations will be kept consistent with his work.

Consider in $\mathbb{R}^3$ a reference domain $\Omega_{\text{ref}} = [-1, 1]^3$, where the superscript 3 denotes that the interval of the domain in all 3 dimensions are all $[-1, 1]$, and a set of nodes distributed along each dimensions,

$$\{\xi_0, \xi_1, \dots, \xi_{N_\xi}\}, \{\eta_0, \eta_1, \dots, \eta_{N_\eta}\}, \{\sigma_0, \sigma_1, \dots, \sigma_{N_\sigma}\} \quad (3.13)$$

In this paper, the distribution of these nodes will follow the Gauss-Lobatto nodes. Over these nodes, the previously defined Lagrange and edge polynomials can also be constructed. Such reference domain is the basis of any domains of arbitrary sizes for later computation.

3.2.1. Polynomials on geometry

For simplicity, in this section the reference domain Ω_{ref} is evenly distributed along all 3 dimensions with $N_\xi = N_\eta = N_\sigma = N$ degrees. The super- or subscripts i and l correspond to the first dimension, j and m to the second, and k and n to the third.

Node polynomials

The node polynomials $\text{lll}(\xi, \eta, \sigma)$ are a set of product of Lagrange polynomials defined as following,

$$\{\text{lll}^{i,j,k}(\xi, \eta, \sigma) | i, j, k \in \{0, 1, \dots, N\}\} \quad (3.14)$$

in which

$$\text{lll}^{i,j,k}(\xi, \eta, \sigma) = \ell^i(\xi)\ell^j(\eta)\ell^k(\sigma) \quad (3.15)$$

Similar to the Lagrange and edge polynomials, the node polynomials also show a Kronecker delta property in $\mathbb{R}^3$ as

$$\text{lll}^{i,j,k}(\xi_l, \eta_m, \sigma_n) = \ell^i(\xi_l)\ell^j(\eta_m)\ell^k(\sigma_n) = \begin{cases} 1 & \text{if } i = l, j = m \text{ and } k = n \\ 0 & \text{else} \end{cases} \quad (3.16)$$

where $(\xi_l, \eta_m, \sigma_n)$ is one of the nodes in the grid with $l, m, n \in \{0, 1, \dots, N\}$.

These node polynomials span a discrete function space $\text{NP}_N(\Omega_{\text{ref}})$ that can be defined as

$$\text{NP}_N(\Omega_{\text{ref}}) = \text{span} \left(\{\text{lll}^{i,j,k}(\xi, \eta, \sigma) | i, j, k \in \{0, 1, \dots, N\}\} \right) \quad (3.17)$$

Edge polynomials

The edge polynomials $\text{ell}(\xi, \eta, \sigma)$, $\text{lel}(\xi, \eta, \sigma)$ and $\text{lle}(\xi, \eta, \sigma)$ are a set of product of Lagrange polynomials and edge functions, defined as following,

$$\{\text{ell}^{i,j,k}(\xi, \eta, \sigma) | i \in \{1, 2, \dots, N\}, j, k \in \{0, 1, \dots, N\}\} \quad (3.18a)$$

$$\{\text{lel}^{i,j,k}(\xi, \eta, \sigma) | j \in \{1, 2, \dots, N\}, i, k \in \{0, 1, \dots, N\}\} \quad (3.18b)$$

$$\{\text{lle}^{i,j,k}(\xi, \eta, \sigma) | k \in \{1, 2, \dots, N\}, i, j \in \{0, 1, \dots, N\}\} \quad (3.18c)$$

in which

$$\text{ell}^{i,j,k}(\xi, \eta, \sigma) = e^i(\xi)\ell^j(\eta)\ell^k(\sigma) \quad (3.19a)$$

$$\text{lel}^{i,j,k}(\xi, \eta, \sigma) = \ell^i(\xi)e^j(\eta)\ell^k(\sigma) \quad (3.19b)$$

$$\text{lle}^{i,j,k}(\xi, \eta, \sigma) = \ell^i(\xi)\ell^j(\eta)e^k(\sigma) \quad (3.19c)$$

Since the edge polynomials include the edge functions, its Kronecker delta property thus as expected would include integration over certain interval. Let $[\xi_l - 1, \xi_l]$ denote an interval and $([\xi_{l-1}, \xi_l], \eta_m, \sigma_n)$ an edge, the Kronecker delta property can thus be expressed as line integrals,

$$\int_{([\xi_{l-1}, \xi_l], \eta_m, \sigma_n)} \text{ell}^{i,j,k}(\xi, \eta, \sigma) d\mathbf{r} = \left(\int_{\xi_{l-1}}^{\xi_l} e^i(\xi) d\xi \right) \ell^j(\eta_m) \ell^k(\sigma_n) = \delta_{l,m,n}^{i,j,k} \quad (3.20a)$$

$$\int_{(\xi_l, [\eta_{m-1}, \eta_m], \sigma_n)} \text{lel}^{i,j,k}(\xi, \eta, \sigma) d\mathbf{r} = \ell^i(\xi_l) \left(\int_{\eta_{m-1}}^{\eta_m} e^j(\eta) d\eta \right) \ell^k(\sigma_n) = \delta_{l,m,n}^{i,j,k} \quad (3.20b)$$

$$\int_{(\xi_l, \eta_m, [\sigma_{n-1}, \sigma_n])} \text{lle}^{i,j,k}(\xi, \eta, \sigma) d\mathbf{r} = \ell^i(\xi_l) \ell^j(\eta_m) \left(\int_{\sigma_{n-1}}^{\sigma_n} e^k(\sigma) d\sigma \right) = \delta_{l,m,n}^{i,j,k} \quad (3.20c)$$

The discrete function space $EP_{N-1}(\Omega_{\text{ref}})$ spanned by the edge polynomials can be expressed as

$$\begin{aligned} EP_{N-1}(\Omega_{\text{ref}}) &= \text{span} \left(\{ \text{ell}^{i,j,k}(\xi, \eta, \sigma) | i \in \{1, 2, \dots, N\}, j, k \in \{0, 1, \dots, N\} \} \right) \\ &\quad \times \text{span} \left(\{ \text{lel}^{i,j,k}(\xi, \eta, \sigma) | j \in \{1, 2, \dots, N\}, i, k \in \{0, 1, \dots, N\} \} \right) \\ &\quad \times \text{span} \left(\{ \text{lle}^{i,j,k}(\xi, \eta, \sigma) | k \in \{1, 2, \dots, N\}, i, j \in \{0, 1, \dots, N\} \} \right) \end{aligned} \quad (3.21)$$

Face polynomials

Similarly, the face polynomials are defined as

$$\{ \text{lee}^{i,j,k}(\xi, \eta, \sigma) | i \in \{0, 1, \dots, N\}, j, k \in \{1, 2, \dots, N\} \} \quad (3.22a)$$

$$\{ \text{ele}^{i,j,k}(\xi, \eta, \sigma) | j \in \{0, 1, \dots, N\}, i, k \in \{1, 2, \dots, N\} \} \quad (3.22b)$$

$$\{ \text{eel}^{i,j,k}(\xi, \eta, \sigma) | k \in \{0, 1, \dots, N\}, i, j \in \{1, 2, \dots, N\} \} \quad (3.22c)$$

in which

$$\text{lee}^{i,j,k}(\xi, \eta, \sigma) = \ell^i(\xi) e^j(\eta) e^k(\sigma) \quad (3.23a)$$

$$\text{ele}^{i,j,k}(\xi, \eta, \sigma) = e^i(\xi) \ell^j(\eta) e^k(\sigma) \quad (3.23b)$$

$$\text{eel}^{i,j,k}(\xi, \eta, \sigma) = e^i(\xi) e^j(\eta) \ell^k(\sigma) \quad (3.23c)$$

The Kronecker delta property of face polynomials are expressed as surface integrals,

$$\begin{aligned} \int_{(\xi_l, [\eta_{m-1}, \eta_m], [\sigma_{n-1}, \sigma_n])} \text{lee}^{i,j,k}(\xi, \eta, \sigma) d\Gamma \\ = \ell^i(\xi_l) \left(\int_{\eta_{m-1}}^{\eta_m} e^j(\eta) d\eta \right) \left(\int_{\sigma_{n-1}}^{\sigma_n} e^k(\sigma) d\sigma \right) = \delta_{l,m,n}^{i,j,k} \end{aligned} \quad (3.24a)$$

$$\begin{aligned} \int_{([\xi_{l-1}, \xi_l], \eta_m, [\sigma_{n-1}, \sigma_n])} \text{ele}^{i,j,k}(\xi, \eta, \sigma) d\Gamma \\ = \left(\int_{\xi_{l-1}}^{\xi_l} e^i(\xi) d\xi \right) \ell^j(\eta_m) \left(\int_{\sigma_{n-1}}^{\sigma_n} e^k(\sigma) d\sigma \right) = \delta_{l,m,n}^{i,j,k} \end{aligned} \quad (3.24b)$$

$$\begin{aligned} \int_{([\xi_{l-1}, \xi_l], [\eta_{m-1}, \eta_m], \sigma_n)} \text{eel}^{i,j,k}(\xi, \eta, \sigma) d\Gamma \\ = \left(\int_{\xi_{l-1}}^{\xi_l} e^i(\xi) d\xi \right) \left(\int_{\eta_{m-1}}^{\eta_m} e^j(\eta) d\eta \right) \ell^k(\sigma_n) = \delta_{l,m,n}^{i,j,k} \end{aligned} \quad (3.24c)$$

The discrete function space $FP_{N-1}(\Omega_{\text{ref}})$ spanned by the face polynomials can be defined as

$$\begin{aligned} FP_{N-1}(\Omega_{\text{ref}}) &= \text{span} \left(\{ \text{lee}^{i,j,k}(\xi, \eta, \sigma) | i \in \{0, 1, \dots, N\}, j, k \in \{1, 2, \dots, N\} \} \right) \\ &\quad \times \text{span} \left(\{ \text{ele}^{i,j,k}(\xi, \eta, \sigma) | j \in \{0, 1, \dots, N\}, i, k \in \{1, 2, \dots, N\} \} \right) \\ &\quad \times \text{span} \left(\{ \text{eel}^{i,j,k}(\xi, \eta, \sigma) | k \in \{0, 1, \dots, N\}, i, j \in \{1, 2, \dots, N\} \} \right) \end{aligned} \quad (3.25)$$

Volume polynomials

The volume polynomials are defined as

$$\{ \text{eee}^{i,j,k}(\xi, \eta, \sigma) | i, j, k \in \{1, 2, \dots, N\} \} \quad (3.26)$$

in which

$$\text{eee}^{i,j,k}(\xi, \eta, \sigma) = e^i(\xi) e^j(\eta) e^k(\sigma) \quad (3.27)$$

The Kronecker delta property of volume polynomials can be expressed as volume integral,

$$\begin{aligned} & \int_{([\xi_{l-1}, \xi_l], [\eta_{m-1}, \eta_m], [\sigma_{n-1}, \sigma_n])} \text{eee}^{i,j,k}(\xi_l, \eta_m, \sigma_n) dV \\ &= \left(\int_{\xi_{l-1}}^{\xi_l} e^i(\xi) d\xi \right) \left(\int_{\eta_{m-1}}^{\eta_m} e^j(\eta) d\eta \right) \left(\int_{\sigma_{n-1}}^{\sigma_n} e^k(\sigma) d\sigma \right) = \delta_{l,m,n}^{i,j,k} \end{aligned} \quad (3.28)$$

Again, these volume polynomials span a discrete function space $\text{VP}_{N-1}(\Omega_{\text{ref}})$, which is defined as

$$\text{VP}_{N-1}(\Omega_{\text{ref}}) = \text{span} \left(\{ \text{eee}^{i,j,k}(\xi, \eta, \sigma) | i, j, k \in \{1, 2, \dots, N\} \} \right) \quad (3.29)$$

3.2.2. Coordinate transformation

Recall the pushforward operator $\Phi : \mathcal{M} \mapsto \mathcal{N}$ and the pullback operator $\Phi^* : \Lambda^k(\mathcal{N}) \mapsto \Lambda^k(\mathcal{M})$ that are defined in section 2.1.3, and they are now applied to perform the coordinate transformation on the basis polynomials. Consider a basis function $\varphi_0(x_0)$ defined on a reference domain $x_0 \in \Omega_{\text{ref}}$, and another function $\varphi(x)$ defined on the arbitrary general domain $x \in \Omega$ with the following mappings,

$$\varphi_0 : \Omega_{\text{ref}} \mapsto \mathbb{R} \quad (3.30a)$$

$$\varphi : \Omega \mapsto \mathbb{R} \quad (3.30b)$$

and the pushforward and pullback operators with the mappings

$$\Phi : \Omega_{\text{ref}} \mapsto \Omega \quad (3.31a)$$

$$\Phi^* : \varphi \mapsto \varphi_0 \quad (3.31b)$$

This gives the coordinate transformation as

$$\varphi(x) = \varphi(\Phi(x_0)) = (\Phi^* \varphi)(x_0) = \varphi_0(x_0) \quad (3.32)$$

which clearly illustrates the naming that Φ pushes forward the coordinate from Ω_{ref} to Ω , and Φ^* pulls back the function from φ to φ_0 .

The basis polynomials introduced in the previous section are defined on the reference domain $\Omega_{\text{ref}} = [-1, 1]^3$ with the coordinate systems (ξ, η, σ) , and the general coordinate (x, y, z) is defined on Ω , the transformation can then be expressed as

$$(x, y, z) = \Phi(\xi, \eta, \sigma) = (\Phi_x(\xi, \eta, \sigma), \Phi_y(\xi, \eta, \sigma), \Phi_z(\xi, \eta, \sigma)) \quad (3.33)$$

of which, the Jacobian matrix $\mathcal{J}$ can be defined as

$$\mathcal{J} = \begin{bmatrix} \frac{\partial x}{\partial \xi} & \frac{\partial x}{\partial \eta} & \frac{\partial x}{\partial \sigma} \\ \frac{\partial y}{\partial \xi} & \frac{\partial y}{\partial \eta} & \frac{\partial y}{\partial \sigma} \\ \frac{\partial z}{\partial \xi} & \frac{\partial z}{\partial \eta} & \frac{\partial z}{\partial \sigma} \end{bmatrix} \quad (3.34)$$

and the Jacobian of this mapping is then denoted as $\det(\mathcal{J})$. The metric matrix can be found by

$$\mathcal{G} = \mathcal{J}^\top \mathcal{J} = \begin{bmatrix} g_{1,1} & g_{1,2} & g_{1,3} \\ g_{2,1} & g_{2,2} & g_{2,3} \\ g_{3,1} & g_{3,2} & g_{3,3} \end{bmatrix} \quad (3.35)$$

the determinant of which is then the metric of this mapping as

$$g = \det(\mathcal{G}) = [\det(\mathcal{J})]^2 \quad (3.36)$$

As for the inverse transformation, its Jacobian matrix is just the inverse of $\mathcal{J}$ as

$$\mathcal{J}^{-1} = \begin{bmatrix} \frac{\partial \xi}{\partial x} & \frac{\partial \xi}{\partial y} & \frac{\partial \xi}{\partial z} \\ \frac{\partial \eta}{\partial x} & \frac{\partial \eta}{\partial y} & \frac{\partial \eta}{\partial z} \\ \frac{\partial \sigma}{\partial x} & \frac{\partial \sigma}{\partial y} & \frac{\partial \sigma}{\partial z} \end{bmatrix} \quad (3.37)$$

of which, the inverse Jacobian is just the reciprocal of Jacobian of equation (3.34)

$$\det(\mathcal{J}^{-1}) = \frac{1}{\det(\mathcal{J})} \quad (3.38)$$

and the its inverse $\mathcal{G}^{-1}$ is then

$$\mathcal{G}^{-1} = (\mathcal{J}^{-1})^\top \mathcal{J}^{-1} = \begin{bmatrix} g^{1,1} & g^{1,2} & g^{1,3} \\ g^{2,1} & g^{2,2} & g^{2,3} \\ g^{3,1} & g^{3,2} & g^{3,3} \end{bmatrix} \quad (3.39)$$

Therefore, the transformation from Ω_{ref} to Ω can then be implemented as the followings [39, 19].

Node polynomials

$$\begin{aligned} \text{lll}_\Phi^{i,j,k}(x, y, z) &= \text{lll}_\Phi^{i,j,k}(\Phi(\xi, \eta, \sigma)) = \text{lll}^{i,j,k}(\xi, \eta, \sigma), \\ &\text{for } i, j, k \in \{0, 1, \dots, N\} \end{aligned} \quad (3.40)$$

Edge polynomials

$$\begin{aligned} \text{ell}_\Phi^{i,j,k}(x, y, z) &= (\mathcal{J}^{-1})^\top \begin{bmatrix} \text{ell}^{i,j,k}(\Phi^{-1}(x, y, z)) \\ 0 \\ 0 \end{bmatrix}, \\ &\text{for } i \in \{1, 2, \dots, N\}, j, k \in \{0, 1, \dots, N\} \end{aligned} \quad (3.41)$$

$$\begin{aligned} \text{lel}_\Phi^{i,j,k}(x, y, z) &= (\mathcal{J}^{-1})^\top \begin{bmatrix} 0 \\ \text{lel}^{i,j,k}(\Phi^{-1}(x, y, z)) \\ 0 \end{bmatrix}, \\ &\text{for } j \in \{1, 2, \dots, N\}, i, k \in \{0, 1, \dots, N\} \end{aligned} \quad (3.42)$$

$$\begin{aligned} \text{lle}_\Phi^{i,j,k}(x, y, z) &= (\mathcal{J}^{-1})^\top \begin{bmatrix} 0 \\ 0 \\ \text{lle}^{i,j,k}(\Phi^{-1}(x, y, z)) \end{bmatrix}, \\ &\text{for } k \in \{1, 2, \dots, N\}, i, j \in \{0, 1, \dots, N\} \end{aligned} \quad (3.43)$$

The transformed edge polynomials also satisfy the Kronecker delta property over line integrals as expressed by equation (3.20c).

Face polynomials

$$\begin{aligned} \text{lee}_\Phi^{i,j,k}(x, y, z) &= \frac{\mathcal{J}}{\sqrt{g}} \begin{bmatrix} \text{lee}^{i,j,k}(\Phi^{-1}(x, y, z)) \\ 0 \\ 0 \end{bmatrix}, \\ &\text{for } i \in \{0, 1, \dots, N\}, j, k \in \{1, 2, \dots, N\} \end{aligned} \quad (3.44)$$

$$\begin{aligned} \text{ele}_\Phi^{i,j,k}(x, y, z) &= \frac{\mathcal{J}}{\sqrt{g}} \begin{bmatrix} 0 \\ \text{ele}^{i,j,k}(\Phi^{-1}(x, y, z)) \\ 0 \end{bmatrix}, \\ &\text{for } j \in \{0, 1, \dots, N\}, i, k \in \{1, 2, \dots, N\} \end{aligned} \quad (3.45)$$

$$\begin{aligned} \text{eel}_\Phi^{i,j,k}(x, y, z) &= \frac{\mathcal{J}}{\sqrt{g}} \begin{bmatrix} 0 \\ 0 \\ \text{eel}^{i,j,k}(\Phi^{-1}(x, y, z)) \end{bmatrix}, \\ &\text{for } j \in \{0, 1, \dots, N\}, i, k \in \{1, 2, \dots, N\} \end{aligned} \quad (3.46)$$

The transformed face polynomials also satisfy the Kronecker delta property over surface integrals as expressed by equation (3.24c).

Volume polynomials

$$\begin{aligned} \text{eee}_{\Phi}^{i,j,k}(x, y, z) &= \text{eee}_{\Phi}^{i,j,k}(\Phi(\xi, \eta, \sigma)) = \frac{1}{\sqrt{g}} \text{eee}^{i,j,k}(\xi, \eta, \sigma), \\ &\text{for } i, j, k \in \{1, 2, \dots, N\} \end{aligned} \quad (3.47)$$

Again, the transformed volume polynomials satisfy the Kronecker delta property over volume integrals as expressed by equation (3.28).

3.2.3. Reconstruction

Now the previously discussed de Rham complex equation (2.38) can be written by the discrete function spaces (equations (3.17), (3.21), (3.25) and (3.29)) as following [39],

$$\begin{array}{ccc} \text{NP}_N(\Omega_{\text{ref}}) & \subset & H^1(\Omega_{\text{ref}}) \\ \downarrow \nabla & & \downarrow \nabla \\ \text{EP}_{N-1}(\Omega_{\text{ref}}) & \subset & H(\text{curl}; \Omega_{\text{ref}}) \\ \downarrow \nabla \times & & \downarrow \nabla \times \\ \text{FP}_{N-1}(\Omega_{\text{ref}}) & \subset & H(\text{div}; \Omega_{\text{ref}}) \\ \downarrow \nabla \cdot & & \downarrow \nabla \cdot \\ \text{VP}_{N-1}(\Omega_{\text{ref}}) & \subset & L^2(\Omega_{\text{ref}}) \end{array}$$

Node polynomials

A node polynomial $\psi^h \in \text{NP}_N(\Omega_{\text{ref}})$ can be used to represent scalar physical quantities that should be placed at vertices, and it is reconstructed as

$$\psi^h(\xi, \eta, \sigma) = \sum_{i=0}^N \sum_{j=0}^N \sum_{k=0}^N \Psi_{i,j,k} \text{lll}^{i,j,k}(\xi, \eta, \sigma) \quad (3.48)$$

in which $\Psi_{i,j,k}$ is the degrees of freedom associated to the node elements. Notice that the obtained data result ψ^h as well as DoF $\Psi_{i,j,k}$ here are technically one-dimensional arrays, while the actual dimension of the problem to be solved could be equal to or higher than one. Therefore re-ordering and re-shaping of the data into certain higher dimension is needed. As mentioned before, the topology of the grid cares only about connections among each geometric elements, to which, it is recommended to chose a easily maintained and user friendly indexing. In this paper, the implementation of reshaping of DoF and reconstructed function follows the Fortran order of indexing. An example of two-dimensional reshaping is shown in figure 3.3, in which ξ is the primary axis and η the secondary. Both data array

	η	
	$\rightarrow$	
ξ	$\downarrow$	
		0 4 8
		1 5 9
		2 6 10
		3 7 11

Figure 3.3: Fortran indexing of array.

elements and geometric elements (nodes, edges, etc.) are numbered along the primary axis first, then the secondary, and this order of indexing can be easily applied to higher dimensions. An advantage of this ordering is that in programming, it is easy to fetch the data by a natural indexing, such as

`psi_324 = psi[3][2][4]`

which fetches the 3rd element in the primary axis, the 2nd in the secondary and the 4th in the tertiary.

Edge polynomials

An edge polynomial $\omega^h \in \text{EP}_{N-1}(\Omega_{\text{ref}})$ that can represent vector quantities placed over edges is reconstructed as

$$\omega^h(\xi, \eta, \sigma) = \begin{bmatrix} \sum_{i=1}^N \sum_{j=0}^N \sum_{k=0}^N w_{i,j,k}^\xi \text{ell}^{i,j,k}(\xi, \eta, \sigma) \\ \sum_{i=0}^N \sum_{j=1}^N \sum_{k=0}^N w_{i,j,k}^\eta \text{lel}^{i,j,k}(\xi, \eta, \sigma) \\ \sum_{i=0}^N \sum_{j=0}^N \sum_{k=1}^N w_{i,j,k}^\sigma \text{lle}^{i,j,k}(\xi, \eta, \sigma) \end{bmatrix} \quad (3.49)$$

Notice that the resulted ω^h consists of three scalar components. The lengths of DoF's w^ξ , w^η and w^σ along each axis could vary and depend on the quality of the grid of that certain axis.

Face polynomials

Similar to the edge polynomial, the face polynomial $u^h \in \text{FP}_{N-1}(\Omega_{\text{ref}})$ represents vector quantities that should be placed on face geometry, and is reconstructed as

$$u^h(\xi, \eta, \sigma) = \begin{bmatrix} \sum_{i=0}^N \sum_{j=1}^N \sum_{k=1}^N u_{i,j,k}^\xi \text{lee}^{i,j,k}(\xi, \eta, \sigma) \\ \sum_{i=1}^N \sum_{j=0}^N \sum_{k=1}^N u_{i,j,k}^\eta \text{ele}^{i,j,k}(\xi, \eta, \sigma) \\ \sum_{i=1}^N \sum_{j=1}^N \sum_{k=0}^N u_{i,j,k}^\sigma \text{eel}^{i,j,k}(\xi, \eta, \sigma) \end{bmatrix} \quad (3.50)$$

Volume polynomials

Finally the volume polynomial $f^h \in \text{VP}_{N-1}(\Omega_{\text{ref}})$ that represents those volumetric scalar quantities is reconstructed as

$$f^h(\xi, \eta, \sigma) = \sum_{i=1}^N \sum_{j=1}^N \sum_{k=1}^N f_{i,j,k} \text{eee}^{i,j,k}(\xi, \eta, \sigma) \quad (3.51)$$

3.2.4. Incidence matrices in 3-dimension

The concept of incidence matrix introduced in section 3.1.3 can now be extended into 3-dimension, and its topological property would still be well preserved. These matrices are used to mimic the 3 major vector operators, i.e. the gradient ∇ , curl $\nabla \times$ and divergence $\nabla \cdot$, which would connect the 4 polynomials constructed in section 3.2.3 along a de Rham complex.

Incidence matrix of gradient $\mathbb{E}_{(\nabla)}$

The top view of an example of a single-layer thick 3D mesh of shape $2 \times 2 \times 1$ is shown in figure 3.4. Consider a node polynomial ψ^h and an edge polynomial ω^h , and the gradient is applied as

$$\omega^h = \nabla \psi^h \quad (3.52)$$

By the gradient theorem, the line integral can be used to find that, for example, at e1 in figure 3.4 the expansion coefficients $w_1 = \Psi_2 - \Psi_1$, i.e. the difference of boundary nodes of that certain edge. This makes it possible to construct a matrix $\mathbb{E}_{(\nabla)}$ similar to equation (3.12) that consists of only -1 , 0 and 1 , and relates the expansion coefficients of node polynomials Ψ and those of edge polynomials w algebraically at the discrete level as

$$w = \mathbb{E}_{(\nabla)} \Psi \quad (3.53)$$

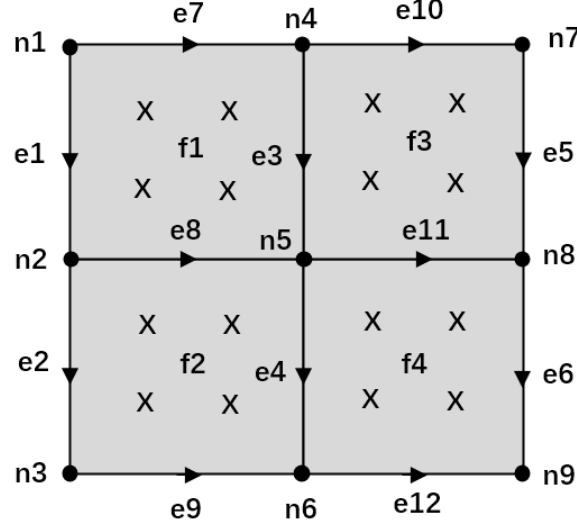


Figure 3.4: Top view of $2 \times 2 \times 1$ mesh, in which n , e and f indicate nodes, edges and faces respectively. The cross X indicates that the orientation of the face points inward.

$\mathbb{E}_{(V)}$ related to figure 3.4 is explicitly expressed as following,

$$\begin{bmatrix} -1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -1 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 1 \\ -1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 1 \end{bmatrix} \quad (3.54)$$

Note that the interval between -1 and 1 in each row is a result of the local numbering of nodes and edges in figure 3.4.

Incidence matrix of curl $\mathbb{E}_{(V \times)}$

Similarly, consider an edge polynomial ω^h and a face polynomial u^h , and the curl is applied as

$$u^h = \nabla \times \omega^h \quad (3.55)$$

By the Stokes' integral theorem, the algebraic relation on, for example, $f1$ in figure 3.4, can be expressed as $u_1 = -w_1 + w_3 + w_7 - w_8$, i.e. the summation of all 4 edges of the corresponding face's boundary, where the consistent orientation makes a positive contribution while the different one makes negative. This again allows to build an incidence matrix $\mathbb{E}_{(V \times)}$, which relates the expansion coefficients of edge polynomials ω and those of face polynomials u algebraically as

$$u = \mathbb{E}_{(V \times)} \omega \quad (3.56)$$

$\mathbb{E}_{(V \times)}$ related to figure 3.4 is explicitly expressed as following,

$$\begin{bmatrix} -1 & 0 & 1 & 0 & 0 & 0 & 1 & -1 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 1 & 0 & 0 & 0 & 1 & -1 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & 1 & 0 & 0 & 0 & 0 & 1 & -1 & 0 \\ 0 & 0 & 0 & -1 & 0 & 1 & 0 & 0 & 0 & 0 & 1 & -1 \end{bmatrix} \quad (3.57)$$

Incidence matrix of divergence $\mathbb{E}_{(\nabla)}$

Finally, consider a face polynomial u^h and a volume polynomial f^h , and a very simple cube mesh as shown in figure 3.5, which consists of 1 volume and 6 faces, while edges and nodes are ignored in this

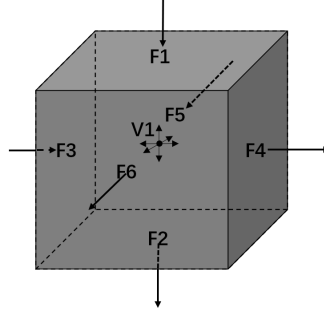


Figure 3.5: A cube mesh, in which the orientations of the volume V1 and all 6 faces F1-6 point outward.

illustration. The divergence is now applied as

$$f^h = \nabla \cdot u^h \quad (3.58)$$

By the Gauss integral theorem, the algebraic relation over the volume and faces can be expressed as $f_1 = -u_1 + u_2 - u_3 + u_4 - u_5 + u_6$. Again its the summation of all 6 boundary faces of the corresponding volume, where the same orientation makes a positive contribution while the opposite one makes negative. The resulted incidence matrix $\mathbb{E}_{(\nabla)}$ relates the expansion coefficients of face polynomials u and those of the volume polynomials f as

$$f = \mathbb{E}_{(\nabla)} u \quad (3.59)$$

The full matrix in this case is simply

$$\begin{bmatrix} -1 & 1 & -1 & 1 & -1 & 1 \end{bmatrix} \quad (3.60)$$

3.2.5. Double de Rham complex

The function spaces of mimetic polynomials and incidence matrices together resemble the double de Rham complex expressed in equation (2.56), as follows [39].

$$\begin{array}{ccccccc} 0 \rightarrow H^1(\Omega) & \xrightarrow{\nabla} & H(\text{curl}; \Omega) & \xrightarrow{\nabla \times} & H(\text{div}; \Omega) & \xrightarrow{\nabla \cdot} & L^2(\Omega) \rightarrow 0 \\ \updownarrow & & \updownarrow & & \updownarrow & & \updownarrow \\ 0 \leftarrow H^1(\Omega) & \xleftarrow{\tilde{\nabla} \cdot} & H(\text{curl}; \Omega) & \xleftarrow{\tilde{\nabla} \times} & H(\text{div}; \Omega) & \xleftarrow{\tilde{\nabla}} & L^2(\Omega) \leftarrow 0 \end{array} \quad (3.61)$$

The primary operators on the top complex are purely topological and metric free that resemble the exterior derivative and its discrete counterpart coboundary operator, while the adjoint operators on the bottom complex resembles the codifferential, which are induced by equation (2.55) and on $\mathbb{R}^3$ by integration by parts. Recall that the codifferential is defined by the Hodge star operator by equation (2.54), thus it introduces metrics by the L^2 inner product as

$$\langle \alpha^{(k)}, \beta^{(k)} \rangle_{L^2} = \int_M \alpha^{(k)} \wedge \star \beta^{(k)} \quad (3.62)$$

This would lead to a scheme of mixed FEM on single grid [27, 1, 29, 24], and will be implemented in chapter 4.

4

Numerical Experiment

In this chapter, the MSEM will be implemented and tested by solving the Poisson's equation and the Stokes' equations. The Poisson's equation is a good simple example of scalar PDE to test the solver, and it will be solved in section 4.1. The Stokes' equations to be discussed in section 4.3, however, include the term of vector Laplacian $\nabla^2 \mathbf{u}$, thus it is beneficial to also study the Poisson's equation in the vector form, which is presented in section 4.2. In addition, the mimetic polynomials introduced in section 3.2 are designed for 3-dimensional cases, which practically consumes enormous computational effort, and it is hard to visualize the results over volumes. Therefore, in this paper, the following problems will be solved in a pseudo-2D domain, i.e. there will be only one layer of volume mesh along the third axis, imaging the mesh depicted in figure 3.5 expanding along faces F4-6 to form a pseudo-2D plane.

4.1. Scalar Poisson's equation

The scalar Poisson's equation is presented as

$$\nabla \cdot (k \nabla \varphi) = -f \quad (4.1)$$

in which φ and f are scalar fields defined on a square domain Ω .

4.1.1. Discretization of the weak form

By introducing an intermediate vector variable $\mathbf{u} = k \nabla \varphi$, equation (4.1) can now be formulated as

$$\mathbf{u} = k \nabla \varphi \quad (4.2a)$$

$$\nabla \cdot \mathbf{u} = -f \quad (4.2b)$$

To discretize equation (4.2), recall the dual de Rham complex equation (3.61), and it is preferable to apply the primal metric-free divergence operator and its adjoint gradient operator. This is because that physically speaking, the divergence describes the conservation of quantity of the system, and thus its structure is better to be preserved. Such scheme results in

$$\mathbf{u} = k \tilde{\nabla} \varphi \quad (4.3a)$$

$$\nabla \cdot \mathbf{u} = -f \quad (4.3b)$$

This means that $\mathbf{u} \in H(\text{div}; \Omega)$ and $f, \varphi \in L^2(\Omega)$.

The weak form of equation (4.3) now can be expressed by introducing test functions $\mathbf{v} \in H(\text{div}; \Omega)$ and $\phi \in L^2(\Omega)$ as

$$\langle \mathbf{v}, k^{-1} \mathbf{u} \rangle_{\Omega} = \langle \mathbf{v}, \tilde{\nabla} \varphi \rangle_{\Omega} \quad (4.4a)$$

$$\langle \phi, \nabla \cdot \mathbf{u} \rangle_{\Omega} = -\langle \phi, f \rangle_{\Omega} \quad (4.4b)$$

By the definition of the dual gradient operator that is adjoint to the primal divergence operator, the right-hand side of equation (4.4a) can be rearranged to give

$$\langle \mathbf{v}, k^{-1} \mathbf{u} \rangle_{\Omega} = -\langle \nabla \cdot \mathbf{v}, \varphi \rangle_{\Omega} + \int_{\Gamma} \varphi (\mathbf{v} \cdot \mathbf{n}) d\Gamma \quad (4.5)$$

where $\mathbf{n}$ is the unit normal vector at the boundary Γ . This step transfers equation (4.4a) from the dual complex to the primal one.

This leads to discretized equations as

$$\langle \mathbf{v}^h, k^{-1} \mathbf{u}^h \rangle_{\Omega} + \langle \nabla \cdot \mathbf{v}^h, \varphi^h \rangle_{\Omega} = \int_{\Gamma} \hat{\varphi} (\mathbf{v}^h \cdot \mathbf{n}) d\Gamma \quad (4.6a)$$

$$\langle \phi^h, \nabla \cdot \mathbf{u}^h \rangle_{\Omega} = -\langle \phi^h, f^h \rangle_{\Omega} \quad (4.6b)$$

in which polynomials $\mathbf{u}^h, \mathbf{v}^h \in \text{FP}_{N-1}(\Omega)$ and $\varphi^h, \phi^h \in \text{VP}_{N-1}(\Omega)$.

The L^2 -inner product is handled by the mass matrices[39], and the differential operator is handled by the incidence matrices. Thus equation (4.6) can be formulated algebraically as

$$\mathbf{v}^T \mathbf{M}_F^k \mathbf{u} + \mathbf{v}^T \mathbf{E}_{(\nabla \cdot)}^T \mathbf{M}_V \varphi = \mathbf{v}^T \mathbf{b} \quad (4.7a)$$

$$\phi^T \mathbf{M}_V \mathbf{E}_{(\nabla \cdot)} \mathbf{u} = -\phi^T \mathbf{M}_V \mathbf{f} \quad (4.7b)$$

where the vector $\mathbf{b}$ corresponds to the given boundary conditions. equation (4.7) can further be used to build the final linear system,

$$\begin{bmatrix} \mathbf{M}_F^k & \mathbf{E}_{(\nabla \cdot)}^T \mathbf{M}_V \\ \mathbf{M}_V \mathbf{E}_{(\nabla \cdot)} & \mathbf{0} \end{bmatrix} \begin{bmatrix} \mathbf{u} \\ \varphi \end{bmatrix} = \begin{bmatrix} \mathbf{b} \\ -\mathbf{M}_V \mathbf{f} \end{bmatrix} \quad (4.8)$$

in which the system matrix on the left-hand side is symmetric.

The boundary condition is a tricky part, and thus for simplicity in this paper we do the followings. Instead of solving an Poisson equation of given arbitrary source term f and boundary conditions, we seek for an already-known neat solution φ plus a neat boundary condition. The solution is designed to be

$$\varphi(x, y, z) = (1 - \cos(2\pi x))e^{-x} \cdot (1 - \cos(2\pi y))e^{-y} \quad (4.9)$$

which is defined on the domain $\Omega = [-1, 1] \times [-1, 1]$, and the corresponding source term f is calculated by Poisson equation itself. The visualizations of both φ and f are presented in figures 4.1 and 4.2. This solution equation (4.9) has a clear exact boundary condition $\varphi(\partial\Omega) = 0$. This makes it easy to implement the zero boundary condition into the final system matrix, where certain rows corresponding to $\partial\varphi$ would contain a single 1 while the rest being 0 to result in $\partial\varphi = 0$. Furthermore, as mentioned before, a pseudo-2D case is used, and thus a periodic boundary condition is applied to the top and bottom boundaries by explicitly excluding the top and bottom boundary faces, i.e. imaging along the z -axis as in figures 4.1 and 4.2 through the paper. This concludes the linear system equation (4.8), and it is ready to be solved.

4.1.2. Numerical results

In the following cases, the factor k will be set to constant 1. The solutions of φ and $\mathbf{u}$ are presented as in figures 4.3 to 4.5, in which the degrees of the polynomials are $N_x = N_y = 20$ along both x - and y -axes.

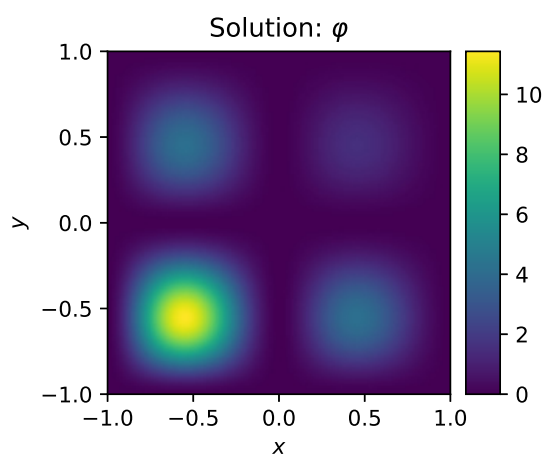


Figure 4.1: The designed exact solution of the Poisson's equation, with exact zero boundary conditions.

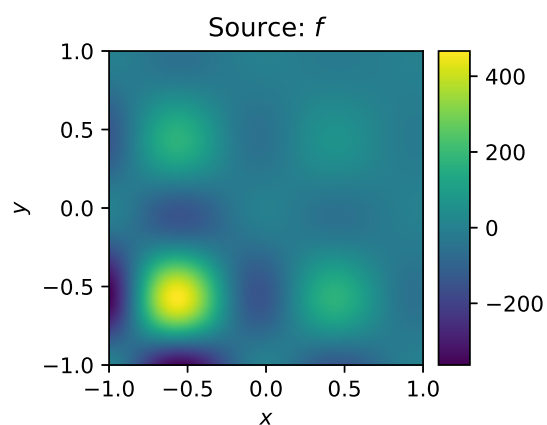


Figure 4.2: The source term of the Poisson's equation corresponding to the given known solution.

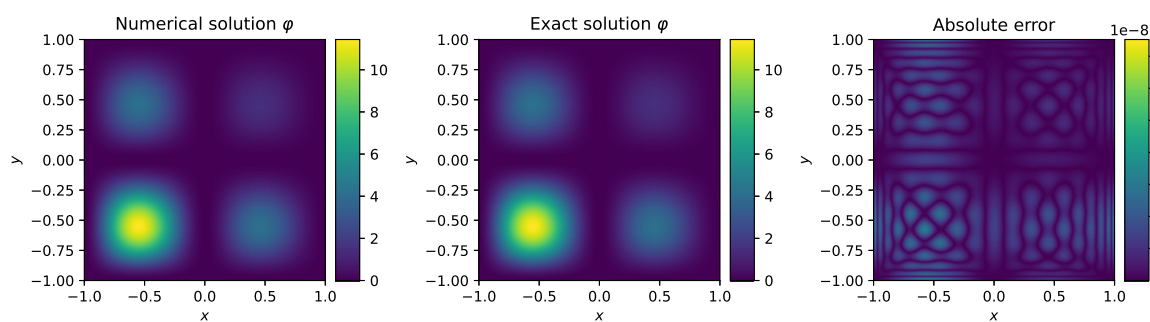


Figure 4.3: Solution ϕ of the scalar Poisson's equation.

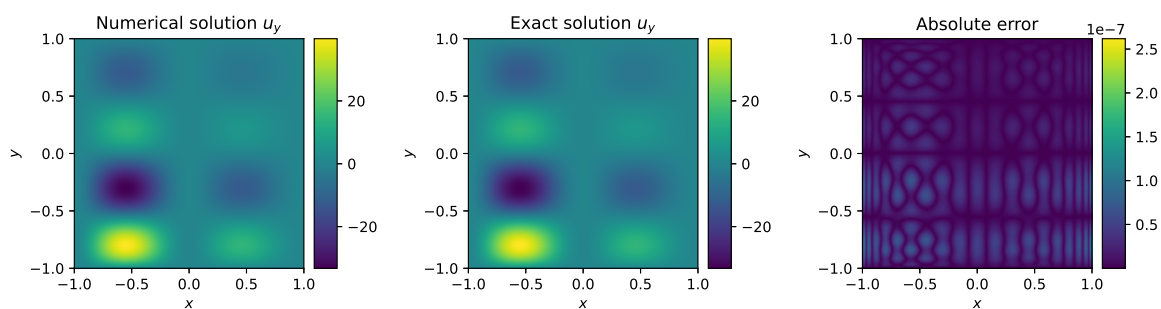


Figure 4.5: Solution u_y of the scalar Poisson's equation.

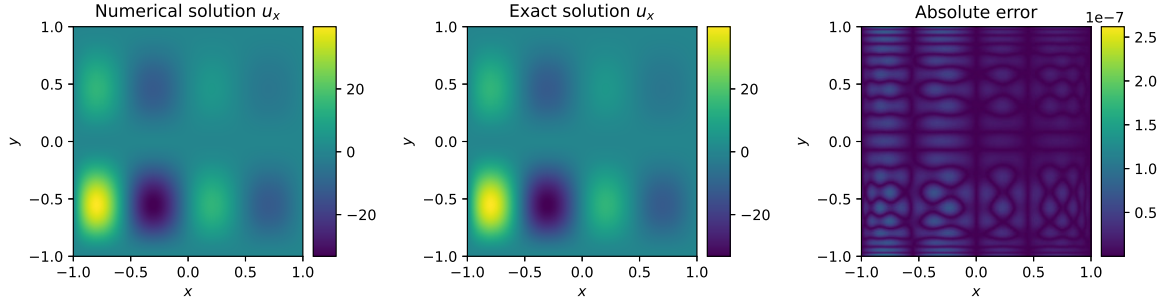


Figure 4.4: Solution u_x of the scalar Poisson's equation.

The accuracy of MSEM is investigated by the L_2 error of the result as

$$\|\varphi^h\|_{L_2} = \sqrt{\int_{\Omega} (\varphi - \varphi_{\text{exact}})^2 d\Omega} \quad (4.10)$$

in which φ is the reconstructed numerical solution by polynomials, and the integral is computed by Simpson's rule. The results are plotted in figure 4.6, in which, the results of two components of $\mathbf{u}$ are

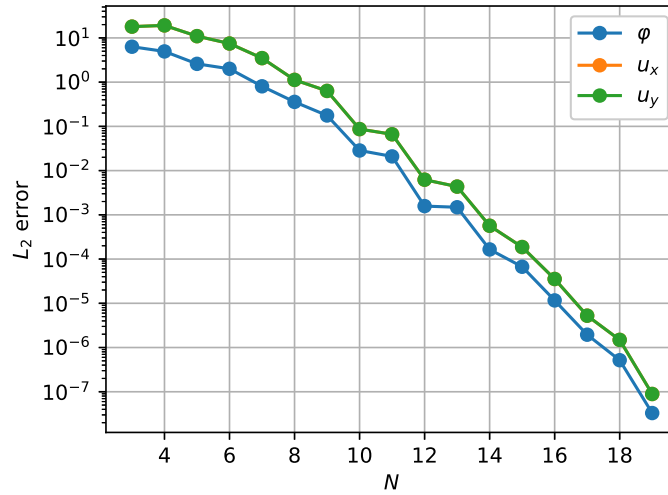


Figure 4.6: The L_2 error of the numerical solutions of scalar Poisson's equation.

identical and thus overlap on each other. It shows that the L_2 error roughly converges exponentially to the polynomial degrees of both solutions φ and $\mathbf{u}$. It is worth noting that some staircases are observed, and this can be explained by the modal behavior of the basis polynomials that reconstruct the source function f , where locally an improving of the polynomial degrees does not yield a more accurate reconstruction of f . Non-rigorously speaking, this is similar to an aliasing effect that both polynomials of N and $(N + 1)$ degrees miss-samples certain features of the source function f .

4.2. Vector Poisson's equation

The vector Poisson's equation is presented as

$$\nabla^2 \mathbf{u} = -\mathbf{f} \quad (4.11)$$

in which both $\mathbf{u}$ and $\mathbf{f}$ are vector fields, and the equation is defined on a square domain Ω .

4.2.1. Discretization of the weak form

By introducing an intermediate variable $p = \nabla \cdot \mathbf{u}$ and applying the vector Laplacian $\nabla^2 \mathbf{u} = \nabla(\nabla \cdot \mathbf{u}) - \nabla \times (\nabla \times \mathbf{u})$, equation (4.11) can be rearranged into

$$p = \nabla \cdot \mathbf{u} \quad (4.12a)$$

$$\nabla p - \nabla \times (\nabla \times \mathbf{u}) = -\mathbf{f} \quad (4.12b)$$

To discretize equation (4.12), again recall the dual de Rham complex equation (3.61). In this case, the term $\nabla \times (\nabla \times \mathbf{u})$ is a tricky one, and it is considered better to assign the inner curl operator to the primal one while the outer curl to the dual. Thus it is chosen that $\mathbf{u} \in H(\text{curl}; \Omega)$ and $p \in H^1(\Omega)$, $\mathbf{f} \in H(\text{curl}; \Omega)$. Consequently, the divergence operator is assigned to be the dual one. This rewrites equation (4.12) as

$$p = \tilde{\nabla} \cdot \mathbf{u} \quad (4.13a)$$

$$\nabla p - \tilde{\nabla} \times (\nabla \times \mathbf{u}) = -\mathbf{f} \quad (4.13b)$$

Introducing the test functions $q \in H^1(\Omega)$ and $\mathbf{v} \in H(\text{curl}; \Omega)$, the weak form of equation (4.13a) can be written as

$$\langle q, p \rangle_\Omega = \langle q, \tilde{\nabla} \cdot \mathbf{u} \rangle_\Omega \quad (4.14)$$

in which, the dual divergence operator on the right-hand side can be transformed to by the primal gradient, giving

$$\langle q, p \rangle_\Omega = -\langle \nabla q, \mathbf{u} \rangle_\Omega + \int_{\partial\Omega} q(\mathbf{u} \cdot \mathbf{n}) d\Gamma \quad (4.15)$$

where $\mathbf{n}$ is unit normal vector at the boundary and Γ is the boundary condition.

Again, for simplicity, in this case the boundary condition is set to be $\Gamma_u = \mathbf{0}$, eliminating the boundary term in equation (4.15). Thus, the weak form of equation (4.13a) becomes

$$\langle q, p \rangle_\Omega + \langle \nabla q, \mathbf{u} \rangle_\Omega = 0 \quad (4.16)$$

The weak form of equation (4.13b) can be written as

$$\langle \mathbf{v}, \nabla p \rangle_\Omega - \langle \mathbf{v}, \tilde{\nabla} \times (\nabla \times \mathbf{u}) \rangle_\Omega = -\langle \mathbf{v}, \mathbf{f} \rangle_\Omega \quad (4.17)$$

in which the dual curl operator in the second term on the left-hand side can be transformed by its primal one as

$$\langle \mathbf{v}, \tilde{\nabla} \times (\nabla \times \mathbf{u}) \rangle_\Omega = \langle \nabla \times \mathbf{v}, \nabla \times \mathbf{u} \rangle_\Omega - \int_{\partial\Omega} (\mathbf{v} \cdot (\nabla \times \mathbf{u} \times \mathbf{n})) d\Gamma \quad (4.18)$$

The boundary condition $\Gamma_u = \mathbf{0}$ again eliminates the last term in equation (4.18), and the weak form of equation (4.13b) eventually becomes

$$\langle \mathbf{v}, \nabla p \rangle_\Omega - \langle \nabla \times \mathbf{v}, \nabla \times \mathbf{u} \rangle_\Omega = -\langle \mathbf{v}, \mathbf{f} \rangle_\Omega \quad (4.19)$$

Both equations (4.16) and (4.19) lead to the discretized equations of equation (4.13) as

$$\langle q^h, p^h \rangle_\Omega + \langle \nabla q^h, \mathbf{u}^h \rangle_\Omega = 0 \quad (4.20a)$$

$$\langle \mathbf{v}^h, \nabla p^h \rangle_\Omega - \langle \nabla \times \mathbf{v}^h, \nabla \times \mathbf{u}^h \rangle_\Omega = -\langle \mathbf{v}^h, \mathbf{f}^h \rangle_\Omega \quad (4.20b)$$

in which $\mathbf{v}^h, \mathbf{u}^h, \mathbf{f}^h \in \text{EP}_{N-1}(\Omega)$ and $q^h, p^h \in \text{NP}_N(\Omega)$. The linear system can be built by the mass matrices and incidence matrices, giving

$$\mathbf{q}^\top \mathbf{M}_N \mathbf{p} + (\mathbf{E}_{(\nabla)} \mathbf{q})^\top \mathbf{M}_E \mathbf{u} = 0 \quad (4.21a)$$

$$\mathbf{v}^\top \mathbf{M}_E (\mathbf{E}_{(\nabla)} \mathbf{p}) - (\mathbf{E}_{(\nabla \times)} \mathbf{v})^\top \mathbf{M}_F (\mathbf{E}_{(\nabla \times)} \mathbf{u}) = -\mathbf{v}^\top \mathbf{M}_E \mathbf{f} \quad (4.21b)$$

and finally the linear system becomes

$$\begin{bmatrix} \mathbf{M}_N & \mathbf{E}_{(\nabla)}^\top \mathbf{M}_E \\ \mathbf{M}_E \mathbf{E}_{(\nabla)} & -\mathbf{E}_{(\nabla \times)}^\top \mathbf{M}_F \mathbf{E}_{(\nabla \times)} \end{bmatrix} \begin{bmatrix} \mathbf{p} \\ \mathbf{u} \end{bmatrix} = \begin{bmatrix} \mathbf{0} \\ -\mathbf{M}_E \mathbf{f} \end{bmatrix} \quad (4.22)$$

in which, the term relating to the boundary condition has been eliminated during the previous derivations, and note that the system matrix is again symmetric.

4.2.2. Numerical results

Similar to the previous case of solving the scalar Poisson's equation, for simplicity, a known solution of zero boundary condition $\mathbf{u} = \mathbf{0}$ is designed, and the corresponding source term $\mathbf{f}$ is calculated to solve the equation numerically. As a result, the numerical solutions of the vector Poisson's equation and the designed exact solutions are illustrated in figures 4.7 to 4.9. The degree of polynomials in this case is 20.

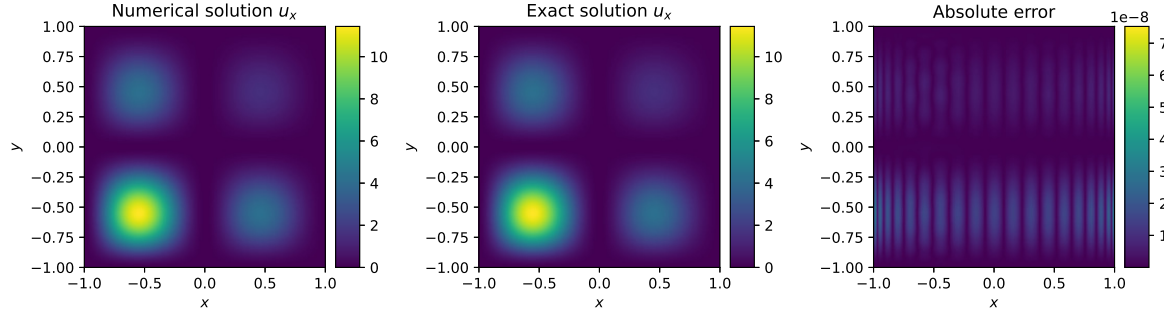


Figure 4.7: Solution u_x of the vector Poisson's equation.

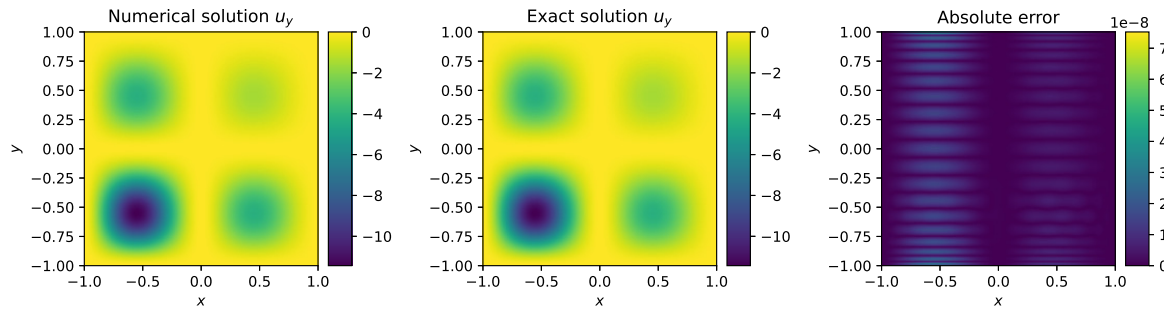


Figure 4.8: Solution u_y of the vector Poisson's equation.

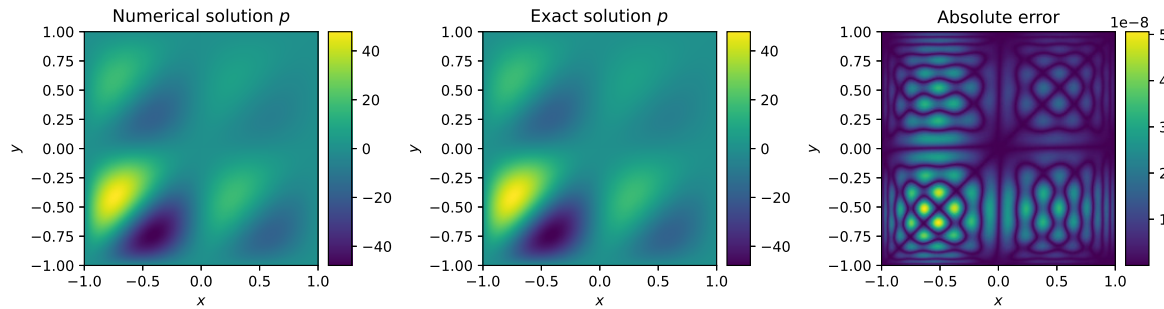


Figure 4.9: Solution $p = \nabla \cdot \mathbf{u}$ of the vector Poisson's equation.

Again the L_2 error is calculated by equation (4.10), and is illustrated in figure 4.10, in which the results of the velocity in both directions are again identical and overlap. The convergence trend is almost the same as that of the result of the scalar Poisson's equation as in figure 4.6.

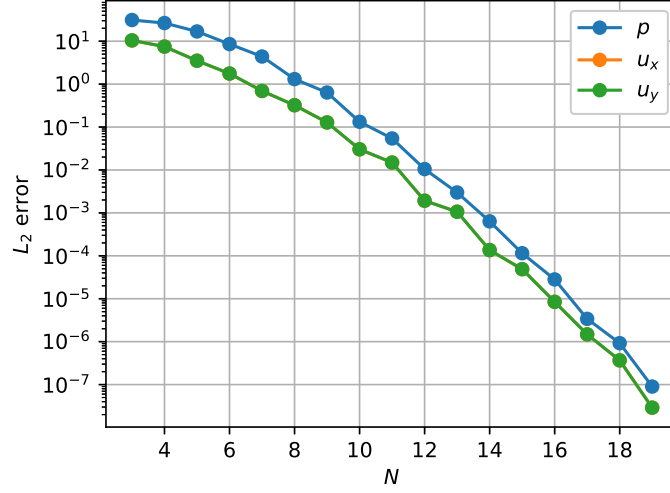


Figure 4.10: The L_2 error of the numerical solutions of vector Poisson's equation.

4.3. Stokes' equations

The Stokes' equations describe an incompressible Newtonian fluid, and are expressed as follows,

$$\mu \nabla^2 \mathbf{u} - \nabla p + \mathbf{f} = \mathbf{0} \quad (4.23a)$$

$$\nabla \cdot \mathbf{u} = 0 \quad (4.23b)$$

in which $\mathbf{u}$, p and $\mathbf{f}$ are the velocity field, pressure field and body force field respectively, and μ is the dynamic viscosity. equation (4.23a) is the momentum equation and equation (4.23b) indicates that the flow field is divergence free (incompressibility).

4.3.1. Discretization of the weak form

By applying the vector Laplacian,

$$\nabla^2 \mathbf{u} = \nabla(\nabla \cdot \mathbf{u}) - \nabla \times (\nabla \times \mathbf{u}) \quad (4.24)$$

equation (4.23a) can be rearranged into

$$\mu \nabla \times (\nabla \times \mathbf{u}) + \nabla p = \mathbf{f} \quad (4.25)$$

given the divergence-free condition $\nabla \cdot \mathbf{u} = 0$. Then an intermediate term of vorticity $\boldsymbol{\omega} = \nabla \times \mathbf{u}$ is introduced into equation (4.23), which can thus be rearranged as

$$\boldsymbol{\omega} = \nabla \times \mathbf{u} \quad (4.26a)$$

$$\mu \nabla \times \boldsymbol{\omega} + \nabla p = \mathbf{f} \quad (4.26b)$$

$$\nabla \cdot \mathbf{u} = 0 \quad (4.26c)$$

To discretize equation (4.26), the divergence operator is chosen to be the primal one, and thus $\mathbf{u} \in H(\text{div}; \Omega)$. Consequently, for equation (4.26a), the curl operator is assigned as the dual one, and $\boldsymbol{\omega} \in H(\text{curl}; \Omega)$. Thus the curl operator in equation (4.26b) should be the primal one while the gradient is thus the dual one, with $p \in L^2(\Omega)$, and $\mathbf{f} \in H(\text{div}; \Omega)$. equation (4.26) now is expressed on the dual complex as

$$\boldsymbol{\omega} = \tilde{\nabla} \times \mathbf{u} \quad (4.27a)$$

$$\mu \nabla \times \boldsymbol{\omega} + \tilde{\nabla} p = \mathbf{f} \quad (4.27b)$$

$$\nabla \cdot \mathbf{u} = 0 \quad (4.27c)$$

The test functions are introduced as $\mathbf{v} \in H(\text{div}; \Omega)$, $\boldsymbol{\xi} \in H(\text{curl}; \Omega)$ and $q \in L^2(\Omega)$.

The weak form of the right-hand side of equation (4.27a) is again found by the adjoint operator of curl as

$$\langle \boldsymbol{\xi}, \tilde{\nabla} \times \mathbf{u} \rangle_{\Omega} = \langle \nabla \times \boldsymbol{\xi}, \mathbf{u} \rangle_{\Omega} - \int_{\partial\Omega} \boldsymbol{\xi} \cdot (\mathbf{u} \times \mathbf{n}) d\Gamma \quad (4.28)$$

Thus the weak form of equation (4.27a) can be found as

$$\langle \boldsymbol{\xi}, \boldsymbol{\omega} \rangle_{\Omega} = \langle \nabla \times \boldsymbol{\xi}, \mathbf{u} \rangle_{\Omega} - \int_{\partial\Omega} \boldsymbol{\xi} \cdot (\mathbf{u} \times \mathbf{n}) d\Gamma \quad (4.29)$$

The weak form of the dual gradient term in equation (4.27b) is found by the primal divergence as

$$\langle \mathbf{v}, \tilde{\nabla} p \rangle_{\Omega} = -\langle \nabla \cdot \mathbf{v}, p \rangle_{\Omega} + \int_{\partial\Omega} p(\mathbf{v} \cdot \mathbf{n}) d\Gamma \quad (4.30)$$

Thus the weak form of equation (4.27b) becomes

$$\langle \mathbf{v}, \mu \nabla \times \boldsymbol{\omega} \rangle_{\Omega} - \langle \nabla \cdot \mathbf{v}, p \rangle_{\Omega} = \langle \mathbf{v}, \mathbf{f} \rangle_{\Omega} - \int_{\partial\Omega} p(\mathbf{v} \cdot \mathbf{n}) d\Gamma \quad (4.31)$$

Lastly, the weak form of equation (4.27c) is simply

$$\langle q, \nabla \cdot \mathbf{u} \rangle_{\Omega} = 0 \quad (4.32)$$

The discretized equations of equation (4.27), therefore, can be expressed as

$$\langle \boldsymbol{\xi}^h, \boldsymbol{\omega}^h \rangle_{\Omega} - \langle \nabla \times \boldsymbol{\xi}^h, \mathbf{u}^h \rangle_{\Omega} = - \int_{\partial\Omega} \boldsymbol{\xi}^h \cdot (\mathbf{u}^h \times \mathbf{n}) d\Gamma \quad (4.33a)$$

$$\langle \mathbf{v}^h, \mu \nabla \times \boldsymbol{\omega}^h \rangle_{\Omega} - \langle \nabla \cdot \mathbf{v}^h, p^h \rangle_{\Omega} = \langle \mathbf{v}^h, \mathbf{f}^h \rangle_{\Omega} - \int_{\partial\Omega} p^h(\mathbf{v}^h \cdot \mathbf{n}) d\Gamma \quad (4.33b)$$

$$\langle q^h, \nabla \cdot \mathbf{u}^h \rangle_{\Omega} = 0 \quad (4.33c)$$

in which, $\boldsymbol{\omega}^h, \boldsymbol{\xi}^h \in \text{EP}_{N-1}(\Omega)$, $\mathbf{u}^h, \mathbf{v}^h \in \text{FP}_{N-1}(\Omega)$ and $p^h, q^h \in \text{VP}_{N-1}(\Omega)$.

4.3.2. Boundary conditions

Note that in equations (4.33a) and (4.33b), there are two boundary integral terms $\int_{\partial\Omega} p^h(\mathbf{v}^h \cdot \mathbf{n}) d\Gamma$ and $\int_{\partial\Omega} \boldsymbol{\xi}^h \cdot (\mathbf{u}^h \times \mathbf{n}) d\Gamma$ for p and $\mathbf{u}$ respectively, and this is where the boundary conditions should be applied. It is worth mentioning that the velocity at the boundary can be decomposed into two parts: the tangential one and the normal one, and the way to implement the boundary conditions on these two is quite different. As mentioned before, the domain is a pseudo 2-dimensional domain, in which there is no gradient of any quantities along the third dimension z , i.e. constant $u_z = 0$ and $\nabla_z p = 0$. Thus the degree of polynomial of the third dimension z is also set to minimum 1.

For simplicity, the exact solution used to test the MSEM is designed to be

$$\mathbf{u}(x, y, z) = \begin{bmatrix} -\frac{1}{\pi} \cos(\pi x) \sin(\pi y) \\ \frac{1}{\pi} \sin(\pi x) \cos(\pi y) \\ 0 \end{bmatrix} \quad (4.34a)$$

$$p(x, y, z) = \sin(\pi x) \cdot \cos\left(\frac{\pi}{2} y\right) \quad (4.34b)$$

The velocity field is visualized in figure 4.11 on a square domain of $[-1, 1]^2$. It is strictly divergence free that satisfies equation (4.23b), and on the boundary the flux $\int_{\partial\Omega} \mathbf{u} \cdot \mathbf{n} d\Gamma = 0$ is also satisfied. The tangential velocity of either u_x or u_y at the boundary is strictly zero, while the normal velocity varies. This indicates that at boundaries there is constant $\mathbf{u} \times \mathbf{n} = \mathbf{0}$. The pressure field equation (4.34b) has an

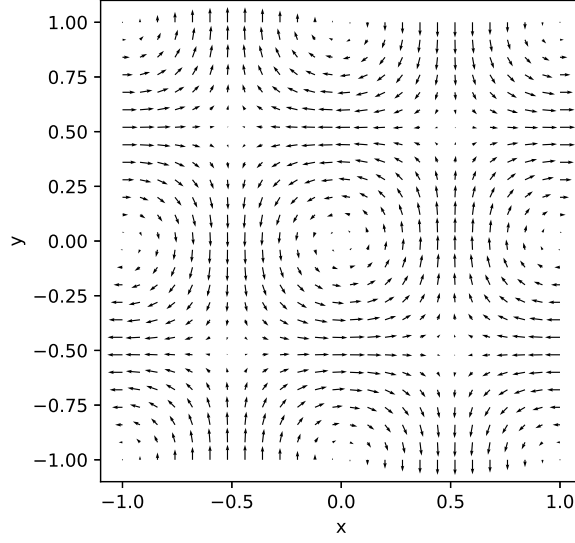


Figure 4.11: Divergence-free velocity field, in which the tangential velocity at the boundary is strictly zero.

average value $\int_{\Omega} p d\Omega$ of 0, and its boundary is constantly normalized to zero. This means that both boundary integral terms can be eliminated from equations (4.33a) and (4.33b), and thus equation (4.33) can be reduced as,

$$\langle \xi^h, \omega^h \rangle_{\Omega} - \langle \nabla \times \xi^h, u^h \rangle_{\Omega} = 0 \quad (4.35a)$$

$$\langle v^h, \mu \nabla \times \omega^h \rangle_{\Omega} - \langle \nabla \cdot v^h, p^h \rangle_{\Omega} = \langle v^h, f^h \rangle_{\Omega} \quad (4.35b)$$

$$\langle q^h, \nabla \cdot u^h \rangle_{\Omega} = 0 \quad (4.35c)$$

By the mass matrices and the incidence matrices, the linear system can be built as

$$\xi^{\top} \mathbf{M}_E \omega - (\mathbf{E}_{(\nabla \times)} \xi)^{\top} \mathbf{M}_F u = 0 \quad (4.36a)$$

$$v^{\top} \mathbf{M}_F^{\mu} \mathbf{E}_{(\nabla \times)} \omega - (\mathbf{E}_{(\nabla \cdot)} v)^{\top} \mathbf{M}_V p = v^{\top} \mathbf{M}_F f \quad (4.36b)$$

$$q^{\top} \mathbf{M}_V \mathbf{E}_{(\nabla \cdot)} u = 0 \quad (4.36c)$$

which is then sorted into

$$\begin{bmatrix} \mathbf{M}_E & -\mathbf{E}_{(\nabla \times)}^{\top} \mathbf{M}_F & \mathbf{0} \\ -\mathbf{M}_F^{\mu} \mathbf{E}_{(\nabla \times)} & \mathbf{0} & \mathbf{E}_{(\nabla \cdot)}^{\top} \mathbf{M}_V \\ \mathbf{0} & \mathbf{M}_V \mathbf{E}_{(\nabla \cdot)} & \mathbf{0} \end{bmatrix} \begin{bmatrix} \omega \\ u \\ p \end{bmatrix} = \begin{bmatrix} \mathbf{0} \\ -\mathbf{M}_F f \\ \mathbf{0} \end{bmatrix} \quad (4.37)$$

of which, if the viscosity μ is set to 1, the system matrix is again symmetric.

However, the boundary condition of the normal velocity should be implemented explicitly. This is done by directly computing the degrees of freedom corresponding to the boundary condition, which is the integral of the normal velocity at the corresponding face at that certain boundary. For example as shown in figure 4.12, the normal velocity $\hat{u}_x$ of the i 'th face at the boundary $y = -1$ is a function of y with varying values. The value of the DoF at this face on the boundary is calculated as

$$u_{x,i} = \iint_{F_{x,i}} \hat{u}_x dy dz \quad (4.38)$$

in which $u_{x,i}$ is the unknown of the linear system associated to the i 'th face geometry in the x direction.

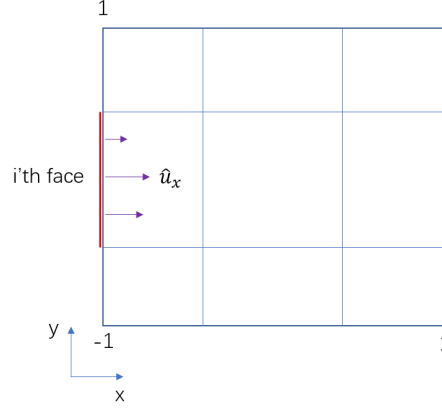


Figure 4.12: Illustration of the application of the boundary condition of normal velocity. The polynomial degrees in both x and y directions are 3, and over the red colored face geometry at the boundary $y = -1$, there is the normal velocity $\hat{u}_x$ in the x direction.

This is then explicitly implemented into the system matrix equation (4.37) as

$$\begin{bmatrix} \dots & \dots & \dots & \dots & \dots \\ \dots & 0 & 1 & 0 & \dots \\ \dots & \dots & \dots & \dots & \dots \end{bmatrix} \begin{bmatrix} \vdots \\ u_{x,i-1} \\ u_{x,i} \\ u_{x,i+1} \\ \vdots \end{bmatrix} = \begin{bmatrix} \vdots \\ \text{rhs}_{u_{x,i-1}} \\ \iint_{F_{x,i}} \hat{u}_x dy dz \\ \text{rhs}_{u_{x,i+1}} \\ \vdots \end{bmatrix} \quad (4.39)$$

in which the the elements in the corresponding row is set to all zero except for the corresponding column, and the desired value is placed on the right-hand side. Then those corresponding columns are moved to the right-hand side.

4.3.3. Numerical results

The source term f of the Stokes' equations equation (4.23) is computed by the previously designed exact solution of $\mathbf{u}$ and p of equations (4.34a) and (4.34b). Additionally with constant $\mu = 1$, and the boundary conditions defined by equations (4.34a) and (4.34b), equation (4.37) is ready to be solved. The degrees of polynomials are $N_x = N_y = 10$, and the solutions of ω_z , $\mathbf{u}$ and p are presented in figures 4.13 to 4.16.

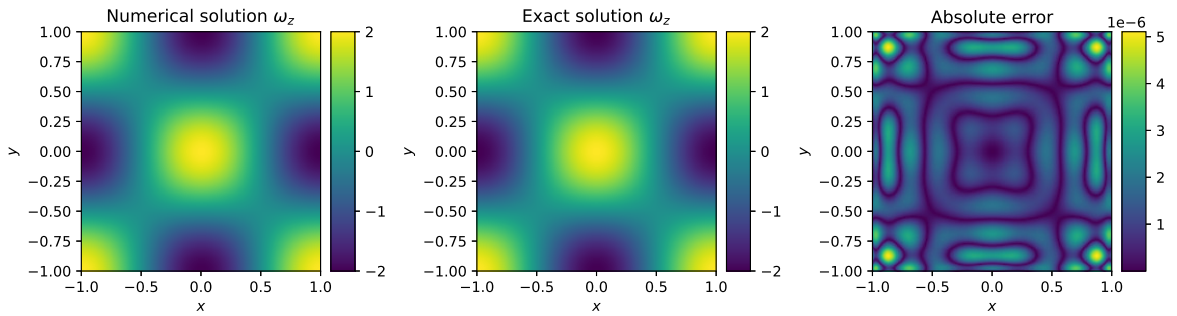


Figure 4.13: Solution ω_z of the Stokes' equations.

The convergence of the solution with respect to the degree of polynomials is presented in the semi-log plot in figure 4.17. It is worth noting that the staircase pattern in the result is much stronger than that presented in figure 4.6, and this can be well explained by the highly periodic patterns in the solution ω , $\mathbf{u}$ and p . Moreover, the convergence trends of the volume, face and edge polynomials with respect to their degrees are much faster than those of the scalar and vector Poisson's equations as in figures 4.6

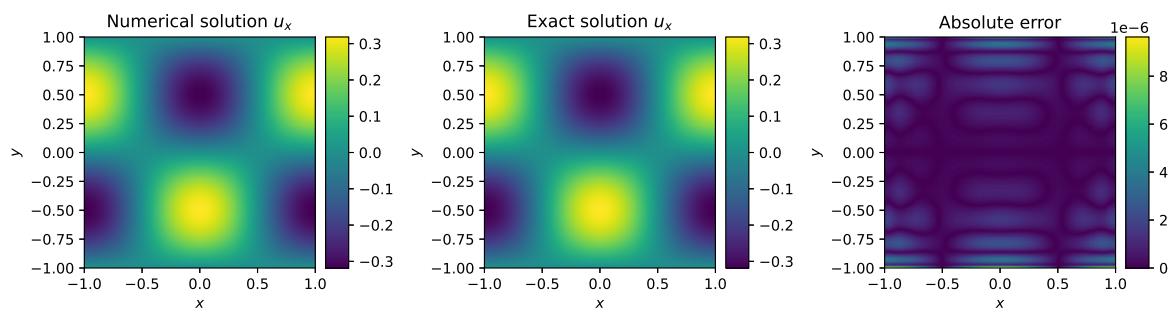


Figure 4.14: Solution u_x of the Stokes' equations.

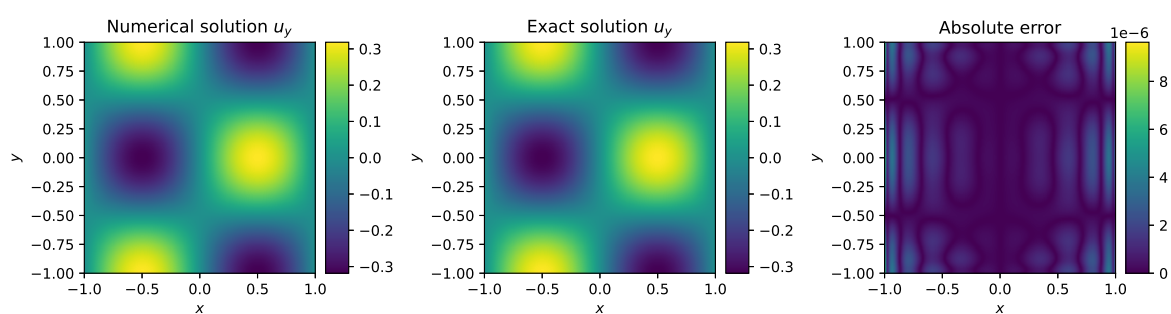


Figure 4.15: Solution u_y of the Stokes' equations.

and 4.10. This could be the result of high gradient presented in the solution used to test the Poisson's equation, where for example in figure 4.4 the solution oscillates from roughly between -30 and 40 in narrow domain $[-1, 0]$, and thus more polynomials are required to properly resolve such rapid changes.

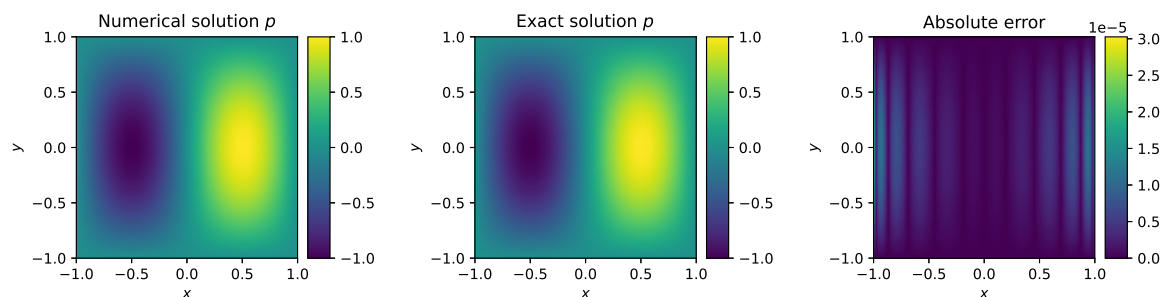


Figure 4.16: Solution p of the Stokes' equations.

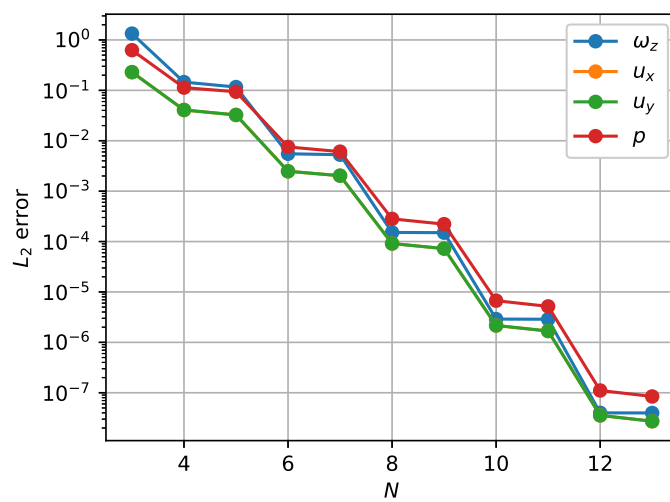


Figure 4.17: The L^2 -error of the numerical solutions of Stokes' equations with respect to the degrees of polynomials.

5

Hybrid Mimetic Spectral Element Method

In the previous chapter, the structure-preserving property and the high-order accuracy of the MSEM has been illustrated. However, all 3 example problems presented in chapter 4 are solved on a single square domain, which leads to a large global matrix. This requires enormous computational efforts and resources. To deal with this, the concept of hybridization is proposed [10, 28, 39] to decompose the single global domain into multiple subdomains. By this, ideally the single problem can be solved parallel for each subdomain, and the sparsity of matrices corresponding to subdomains can be increased to further improve efficiency.

In this chapter, the technique of domain decomposition is introduced in section 5.1, and then it is tested to the scalar Poisson's equation and the Stokes' equations in section 5.2, to examine its performance.

5.1. Domain decomposition

5.1.1. Reenforcement of continuity

Imagine a decomposed pseudo-2D square domain of shape $2 \times 2 \times 1$, i.e. there are 2 subdomains along x - and y -axes respectively, and its top view is illustrated in figure 5.1. The degree of polynomial of all

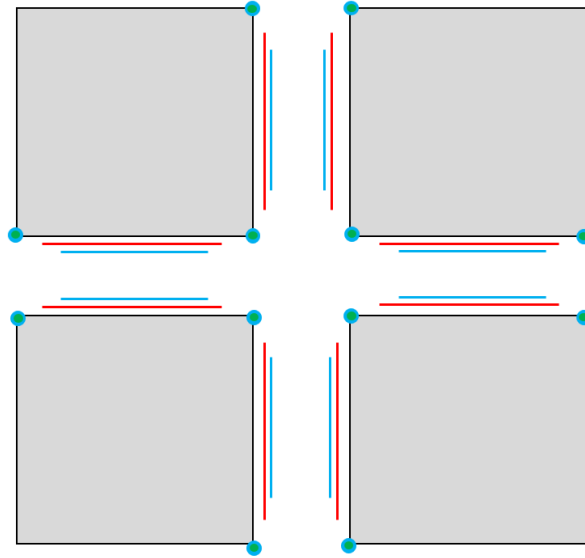


Figure 5.1: Illustration of the top view of a decomposed domain of shape $2 \times 2 \times 1$.

4 subdomains is selected to be $N_x = N_y = N_z = 1$, which results in 8 nodes, 12 edges, 6 faces and 1 volume for each subdomain. At the interfaces among subdomains in figure 5.1, the adjacent faces are marked with red lines, edges with blue lines and dots and nodes with green dots.

Such a subdomain has rare difference from the global domain. If a certain PDE can be solved on the global domain given well defined boundary conditions, it can also be solved as a part of the global solution over the subdomain, provided with the boundary condition that is the exact solution at the decomposed boundary. This is the purpose of hybridization that a single problem can be decomposed into multiple similar sub-problems, which can be solved parallel to improve the efficiency. Additionally, in the case of single domain, the only way to improve the accuracy of the solution is by increasing the degrees of polynomials, as shown in figures 4.6, 4.10 and 4.17, which is called the p -refinement. However, with the domain decomposition, the accuracy can also be improved by increasing the number of subdomains while maintaining the degree of polynomials at low values. This is called the h -refinement, in which h denotes the size of the subdomain.

Therefore, the algebraic system matrix, such as equations (4.8), (4.22) and (4.37), can be applied directly to the subdomain without any boundary conditions being applied yet. The subdomain Ω_i may have two types of boundaries: the those that are also the boundary of the global domain, i.e. $\partial\Omega_i \cap \partial\Omega \neq \emptyset$, and those that are the interfaces between adjacent subdomain, i.e. $\partial\Omega_i \cap \partial\Omega_j \neq \emptyset$. The first case can be implemented in the same way that is used for the single domain presented in chapter 4, with boundary conditions well defined by the PDE problem. The second case is rather a bit tricky, because the boundary conditions at the interfaces between subdomains are unknown, while they should actually be the solutions to be found instead. Furthermore, the solutions at these interfaces should be identical for both adjacent subdomains.

This could be even more complex when more than 2 subdomains share the same quantities of the solution. As shown in figure 5.1, it has been discussed that for MSEM, each variable is assigned to a certain geometry of node, edge, face or volume, thus at the corner of the boundary of the subdomain where 4 or 8 subdomains meet, all geometric entities of the same type of respective subdomains should possess the same degrees of freedom of the solution, if they represent the same geometric entity in the global domain. This especially arises for nodes and edges at the corner, while faces at the interface can only have one neighbor.

To deal with the boundary conditions at the interface, Zhang[39] introduced mimetic trace spaces, by which all geometric entities of the same type at the interface or corner are coupled. However, this results in singularity caused by non-surjective trace matrices relating to nodes and faces, e.g. in figure 5.1 where 4 subdomains meet at the corner, there are 4 edges (blue dots) perpendicular to the paper, and they all should be coupled to give 4 equations, which yields a non-surjective trace matrix $\mathbb{T}_E$ like

$$\mathbb{T}_E = \begin{bmatrix} \cdots & \cdots & \cdots & \cdots & \cdots \\ \cdots & 0 & 1 & 0 & \cdots \\ \cdots & 0 & 1 & 0 & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots \end{bmatrix} \quad (5.1)$$

which is singular.

To solve the singularity, Zhang[39] suggests to introduce an extra dummy degree of freedom to enforce the continuity at the corner. However, in this paper, we try to propose another method to solve this. In simple words, we need $N - 1$ equations to couple N degrees of freedom.

As shown in figure 5.1, the aim is to couple the degrees of freedom of edges of different subdomains at the corner, since they share the same degree of freedom over the global single domain. This explicitly means $\omega_1 = \omega_2 = \omega_3 = \omega_4$, where ω_n denotes the i -th degree of freedom of each edge at the corner, and the numbering here is actually irrelevant. This can be satisfied by 3 linear equations as

$$\omega_1 - \omega_2 = 0 \quad (5.2a)$$

$$\omega_2 - \omega_3 = 0 \quad (5.2b)$$

$$\omega_3 - \omega_4 = 0 \quad (5.2c)$$

in which, again the numbering here is irrelevant as long as 3 equations give 3 non-repeated equality, but a consistent natural numbering is recommended for the implementation. equation (5.2) is expressed as

$$\begin{bmatrix} 1 & -1 & 0 & 0 \\ 0 & 1 & -1 & 0 \\ 0 & 0 & 1 & -1 \end{bmatrix} \begin{bmatrix} \omega_1 \\ \omega_2 \\ \omega_3 \\ \omega_4 \end{bmatrix} = \mathbf{0} \quad (5.3)$$

where the left-hand side matrix is called the reenforce matrix of edges $\mathbf{N}_E$.

The reenforce matrix should be constructed for all kinds of geometry, to which the continuity of degree of freedom is needed. For faces, this is simple, as faces can only meet each other at the interface between 2 subdomains as shown in figure 5.1, and thus 1 equation is required. For edges, it becomes complex as

- Within the interface between 2 subdomains, 2 edges (blue one in figure 5.2) need to be coupled.
- Over the edge of subdomain, where 4 subdomains meet, 4 edges (green one in figure 5.2) need to be coupled.

Additionally, edges should be coupled in both directions. For nodes, it is even more complex as

- Within the interface between 2 subdomains, 2 nodes (blue one in figure 5.2) need to be coupled.
- Over the edge of subdomain, where 4 subdomains meet, 4 nodes (green one in figure 5.2) need to be coupled.
- At the corner of the subdomain, where 8 subdomains meet, 8 nodes (red one in figure 5.2) need to be coupled.

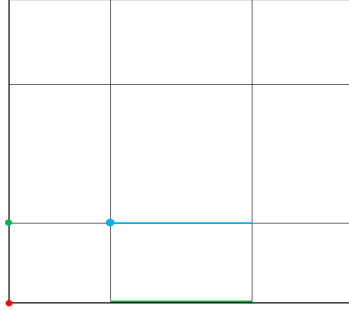


Figure 5.2: Illustration of the surface of the boundary of the subdomain, with degree of freedom $N = 3$.

5.1.2. Linear system of reenforcement

The linear system to apply the reenforcement of the continuity on a decomposed domain is built as following

$$\begin{bmatrix} \mathbf{A} & \mathbf{N}^\top \\ \mathbf{N} & \mathbf{0} \end{bmatrix} \begin{bmatrix} \mathbf{x} \\ \lambda \end{bmatrix} = \begin{bmatrix} \mathbf{rhs} \\ \mathbf{0} \end{bmatrix} \quad (5.4)$$

The matrix $\mathbf{A}$ consists of the system matrices of certain PDE problem, e.g. those in equations (4.8), (4.22) and (4.37), along its diagonal for each individual subdomain with the boundary conditions implemented, giving

$$\mathbf{A} = \begin{bmatrix} \mathbf{A}_1 & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \ddots & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{A}_n \end{bmatrix} \quad (5.5)$$

The reinforcement matrix $\mathbf{N}$ is built by those of each relevant geometry of each subdomain, giving

$$\mathbf{N} = \begin{bmatrix} \begin{bmatrix} \mathbf{N}_{N_1} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{N}_{E_1} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{N}_{F_1} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{N}_{V_1} \end{bmatrix} & \begin{bmatrix} \mathbf{N}_{N_2} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{N}_{E_2} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{N}_{F_2} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{N}_{V_2} \end{bmatrix} & \cdots & \begin{bmatrix} \mathbf{N}_{N_n} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{N}_{E_n} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{N}_{F_n} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{N}_{V_n} \end{bmatrix} \end{bmatrix} \quad (5.6)$$

in which $\mathbf{N}_N$, $\mathbf{N}_E$, $\mathbf{N}_F$ and $\mathbf{N}_V$ are reinforcement matrices for node, edge, face and volume respectively. Note that if certain geometry is not included in the discrete system, corresponding reenforce matrix should be excluded from $\mathbf{N}$ as well.

The unknown $\mathbf{x}$ includes all degrees of freedom to be solved of each subdomain

$$\mathbf{x} = \begin{bmatrix} \mathbf{x}_{N_1} \\ \mathbf{x}_{E_1} \\ \mathbf{x}_{F_1} \\ \mathbf{x}_{V_1} \\ \vdots \\ \mathbf{x}_{N_n} \\ \mathbf{x}_{E_n} \\ \mathbf{x}_{F_n} \\ \mathbf{x}_{V_n} \end{bmatrix} \quad (5.7)$$

in which $\mathbf{x}_N$, $\mathbf{x}_E$, $\mathbf{x}_F$ and $\mathbf{x}_V$ are degrees of freedom associated to node, edge, face and volume. Again, if certain geometry is not included in the discrete system, the corresponding reenforce DoF should be excluded from $\mathbf{x}$.

Finally, the overall right-hand side $\mathbf{rhs}$ consists of the reduction of the body force field or source term given by the PDE in each individual subdomain, and boundary conditions that are implemented in the system matrix $\mathbf{A}_i$ should also be applied correspondingly here at certain rows.

equation (5.4) is a large sparse matrix, which can be solved as a single system. However, the purpose of domain decomposition is to improve the efficiency of finding the solution by breaking the domain into parts, so that each part can be solved parallel. This is achieved by manipulating equation (5.4) by the Schur complement technique. Start from the first row of equation (5.4)

$$\begin{aligned} \mathbf{A}\mathbf{x} + \mathbf{N}^\top \boldsymbol{\lambda} &= \mathbf{rhs} \\ \mathbf{A}^{-1}\mathbf{A}\mathbf{x} + \mathbf{A}^{-1}\mathbf{N}^\top \boldsymbol{\lambda} &= \mathbf{A}^{-1}\mathbf{rhs} \\ \mathbf{N}\mathbf{A}^{-1}\mathbf{A}\mathbf{x} + \mathbf{N}\mathbf{A}^{-1}\mathbf{N}^\top \boldsymbol{\lambda} &= \mathbf{N}\mathbf{A}^{-1}\mathbf{rhs} \\ \mathbf{N}\mathbf{x} + \mathbf{N}\mathbf{A}^{-1}\mathbf{N}^\top \boldsymbol{\lambda} &= \mathbf{N}\mathbf{A}^{-1}\mathbf{rhs} \end{aligned} \quad (5.8)$$

since the second row of equation (5.4) gives $\mathbf{N}\mathbf{x} = \mathbf{0}$, equation (5.8) becomes

$$\mathbf{N}\mathbf{A}^{-1}\mathbf{N}^\top \boldsymbol{\lambda} = \mathbf{N}\mathbf{A}^{-1}\mathbf{rhs} \quad (5.9)$$

The size of the Lagrange multiplier $\boldsymbol{\lambda}$ is equal to the total number of equations that couple the reenforced degrees of freedom, and thus system equation (5.9) is much smaller compared to the original system. Furthermore, the inverse $\mathbf{A}^{-1}$ can be determined efficiently by finding the inverse of each individual $\mathbf{A}_i$ in parallel. Eventually, with $\boldsymbol{\lambda}$ being solved, the unknowns $\mathbf{x}$ can be directly calculated by

$$\mathbf{x} = \mathbf{A}^{-1}(\mathbf{rhs} - \mathbf{N}\boldsymbol{\lambda}) \quad (5.10)$$

5.2. Numerical experiment

The Poisson's equation discussed in section 4.1 can now be solved on a decomposed domain. The discretization scheme used for this problem does not involve edge geometry but only face and volume. Thus it is used to test the feasibility and integrity of the linear system equation (5.4), and individual modules used to implement the hMSEM. The single domain is decomposed into 5, 10, 15, and finally to 200 subdomains along a single dimension, which results in the minimum size of the subdomain being 0.01. The degrees of mimetic polynomials are tested for $N = 1, 2, 3$.

The convergence regarding to h -refinement is shown in figure 5.3, in which the L^2 -errors of the solutions are plotted in log-log plot against the size of the subdomain h . The results show clear straight lines, in which the slopes are equal to the degrees N of mimetic polynomials.

The Stokes' equations discussed in section 4.3 are discretized over edges, faces and volumes for vorticity, velocity and pressure. The convergence regarding to h -refinement is shown in figure 5.4. Again the results show a consistent convergence rate to the degrees of mimetic polynomials.

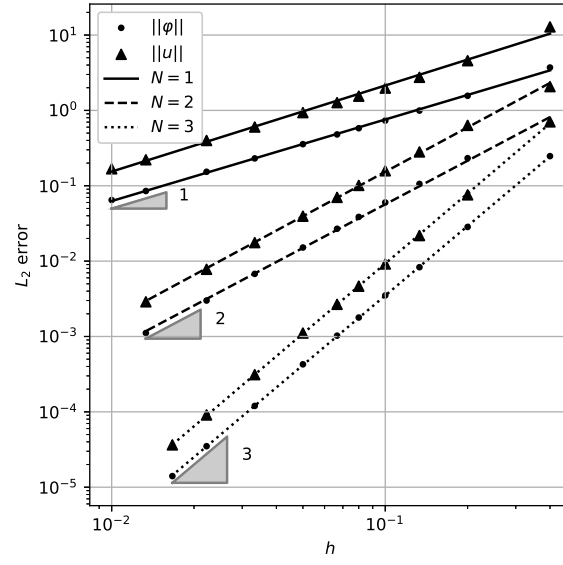


Figure 5.3: L^2 -error of the solutions to the scalar Poisson's equation.

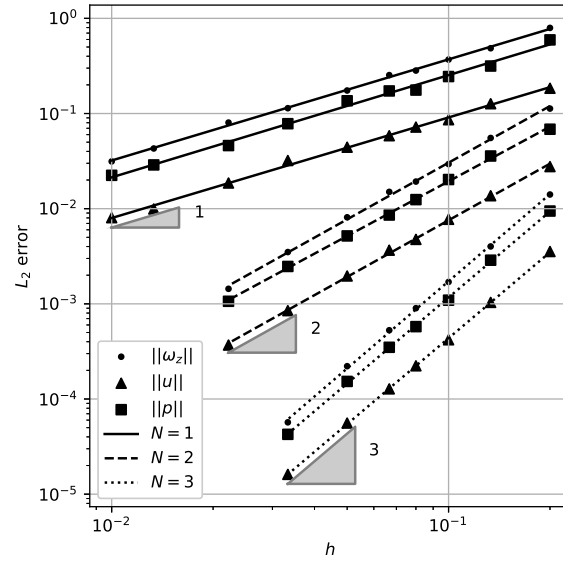


Figure 5.4: L^2 -error of the solutions to the Stokes' equations.

Conclusion and Recommendation for Future Work

6.1. Conclusions

In this thesis, a straightforward method to enforce the continuity between subdomains is proposed for the application of MSEM on decomposed domain, i.e. hybrid MSEM. This method is used especially for problems, in which certain DoF's are associated with edges that causes singularity issue. This method is tested by solving the scalar Poisson's equation and then the Stokes' equations, where the first one has no DoF associated over edges while the second one does. To answer the research questions posed in chapter 1, we may conclude the followings,

1. Can the singularity issue be eliminated while keeping the idea of hMSEM original, i.e. to find an algebraic way?

In section 5.1 we discuss the origin of the singularity, and propose a straightforward brutal constraint to enforce the continuity over the interface between subdomains. This yields non-square reenforcement matrix $\mathbf{N}$ for DoF's that need to be coupled over all 4 geometric entities respectively. Such matrix as well as the corresponding Lagrange multipliers λ has much smaller size compared to the global system, which can be solved independently from the unknowns $\mathbf{x}$. Meanwhile the parallelism of solving the linear system is still maintained, which is the major aim of domain decomposition to improve the computational efficiency.

2. Is it possible to generalize the proposed method to more common problems, e.g. the Stokes' equations?

In section 5.2, this method that constrains the continuity is applied to the scalar Poisson's equation to test the linear system including reenforcement matrices, even though the discretization scheme of this problem does not include unknowns associated over edges. It is then also applied to the Stokes' equations, of which the discretization scheme introduces vorticity as a unknown that is associated to mimetic edge polynomials. The results of both problems show expected convergence rate regarding to h -refinement.

6.2. Recommendation for future work

In this paper, the idea of MSEM is clearly introduced and the relevant mimetic basis polynomials are constructed, as well as the metric-free differential operators. However, the solver is tested over orthogonal grids, while the power of MSEM can also be demonstrated over curvilinear ones [39], where the conservation should be satisfied for vorticity and mass. In this paper, the feasibility of the hybridization is discussed and its convergence is studied, but the conservation of the result is not verified. Therefore, it is recommended that the hybrid method be generalized over curvilinear grids and the conservation be verified.

Another improvement can be made for a more generalized and robust implementation of the boundary conditions of variables assigned on different geometries. In this paper, we mainly focus on the interfaces of the interior domain. The boundary conditions are chosen for simplicity, such that the tangent velocity is zero and the pressure is uniform at the boundary, which leads to the vanishing of the boundary integral terms. Note that here the variables assigned over faces and volumes at the boundary do not need to be coupled between subdomains, but this is required for variables on edges and nodes. Therefore, it is recommended that a complete implementation of the boundary condition be done that handles arbitrary inputs of BC's.

References

- [1] Douglas N Arnold. *Finite Element Exterior Calculus*. Society for Industrial and Applied Mathematics, 2018.
- [2] Douglas N. Arnold. "Spaces of Finite Element Differential Forms". In: *Analysis and Numerics of Partial Differential Equations*. Ed. by Franco Brezzi et al. Springer Milan, 2013, pp. 117–140. ISBN: 978-88-470-2592-9. DOI: 10.1007/978-88-470-2592-9_9.
- [3] Douglas N. Arnold, Richard S. Falk, and Ragnar Winther. "Differential Complexes and Stability of Finite Element Methods I. The de Rham Complex". In: *Compatible Spatial Discretizations*. Ed. by Douglas N. Arnold et al. New York, NY: Springer New York, 2006, pp. 23–46. ISBN: 978-0-387-38034-6.
- [4] Pavel Bochev. "A discourse on variational and geometric aspects of stability of discretizations". In: (Jan. 2003).
- [5] Pavel B. Bochev and James M. Hyman. "Principles of Mimetic Discretizations of Differential Operators". In: *Compatible Spatial Discretizations*. Ed. by Douglas N. Arnold et al. New York, NY: Springer New York, 2006, pp. 89–119. ISBN: 978-0-387-38034-6.
- [6] Alain Bossavit. "On the geometry of electromagnetism". In: *Integration* 6 (Jan. 1998).
- [7] Alain Bossavit. "Solving Maxwell Equations in a Closed Cavity, and the Question of Spurious Modes". In: *Magnetics, IEEE Transactions on* 26 (Apr. 1990), pp. 702–705. DOI: 10.1109/20.106414.
- [8] Franco Brezzi. "On the Existence, Uniqueness and Approximation of Saddle-Point Problems Arising from Lagrangian Multipliers". In: *Revue Francaise D Automatique Informatique Recherche Operationnelle* 8 (Jan. 1974). DOI: 10.1051/m2an/197408R201291.
- [9] Franco Brezzi, Jim Douglas, and L. Marini. "Two Families of Mixed Finite Elements for Second Order Elliptic Problems". In: *Numerische Mathematik* 47 (June 1985), pp. 217–235. DOI: 10.1007/BF01389710.
- [10] Franco Brezzi and Michel Fortin. "Mixed and Hybrid Finite Element Method". In: *Springer Series In Computational Mathematics; Vol. 15* (Jan. 1991), p. 350. DOI: 10.1007/978-1-4612-3172-1.
- [11] Jozef Dodziuk. "Finite-Difference Approach to the Hodge Theory of Harmonic Forms". In: *American Journal of Mathematics* 98 (Apr. 1976). DOI: 10.2307/2373615.
- [12] Harley Flanders. *Differential forms with applications to the Physical Sciences*. Dover publications, 1989.
- [13] T. Frankel. *The geometry of physics: An introduction*. Cambridge University Press, 2011.
- [14] M. Gerritsma. "An introduction to a compatible spectral discretization method". In: *Mechanics of Advanced Materials and Structures* 19.1-3 (2012), pp. 48–67. ISSN: 15376494. DOI: 10.1080/15376494.2011.572237. URL: <https://www.scopus.com/inward/record.uri?eid=2-s2.0-84859206806&doi=10.1080%2f15376494.2011.572237&partnerID=40&md5=5092f291e18ac0d21cf971e3c2eec4de>.
- [15] M. Gerritsma. "Edge functions for spectral element methods". In: *Lecture Notes in Computational Science and Engineering* 76 LNCSE (2011), pp. 199–207. ISSN: 14397358. DOI: 10.1007/978-3-642-15337-2_17. URL: https://www.scopus.com/inward/record.uri?eid=2-s2.0-78651568818&doi=10.1007%2f978-3-642-15337-2_17&partnerID=40&md5=b3562625f25b59c49f50ad094afe3dce.
- [16] Allen Hatcher. *Algebraic Topology*. Cambridge University Press, 2001. ISBN: 9780521795401.
- [17] John David Jackson. *Classical Electrodynamics, 3rd Edition*. Wiley, 1998.
- [18] J.J. Kreeft. "Mimetic spectral element method; a discretization of geometry and physics". In: (2013). DOI: 10.4233/uuid:adbca9e7-08b9-4da3-9174-85c030dd1a15. URL: <https://doi.org/10.4233/uuid:adbca9e7-08b9-4da3-9174-85c030dd1a15>.

- [19] Jasper Kreeft, Artur Palha, and Marc Gerritsma. "Mimetic framework on curvilinear quadrilaterals of arbitrary order". In: (2011). arXiv: 1111.4304 [math.NA]. URL: <https://arxiv.org/abs/1111.4304>.
- [20] W. Massey. *A Basic Course in Algebraic Topology*. Springer, 1991.
- [21] C. Mattiussi. "A reference discretization strategy for the numerical solution of physical field problems". In: *Advances in Imaging and Electron Physics* 121.C (2002), pp. 143–279. ISSN: 10765670. DOI: 10.1016/S1076-5670(02)80027-1. URL: <https://www.scopus.com/inward/record.uri?eid=2-s2.0-50949111246&doi=10.1016%2fS1076-5670%2802%2980027-1&partnerID=40&md5=f9c7186cf26216fa3cf8a1f48674af0a>.
- [22] C. Mattiussi. "The finite volume, finite element, and finite difference methods as numerical methods for physical field problems". In: *Advances in Imaging and Electron Physics* 113.C (2000), pp. 1–146. ISSN: 10765670. DOI: 10.1016/S1076-5670(00)80012-9. URL: <https://www.scopus.com/inward/record.uri?eid=2-s2.0-1542295883&doi=10.1016%2fS1076-5670%2800%2980012-9&partnerID=40&md5=fdca28865d33ba7f3696ef287b4a6f5a>.
- [23] J. Munkres. *Elements of Algebraic Topology*. CRC Press, 1993.
- [24] Jean-Claude Nédélec. "Mixed finite elements in $\mathbb{R}^3$ ". In: *Numerische Mathematik* 35.3 (1980), pp. 315–341.
- [25] Jean-Claude Nédélec. "Mixed Finite Elements in $\mathbb{R}^3$ ". In: *Numerische Mathematik* 35 (Jan. 1980), pp. 315–341. DOI: 10.1007/BF01396415.
- [26] A. Palha and M. Gerritsma. "A mass, energy, enstrophy and vorticity conserving (MEEVC) mimetic spectral element discretization for the 2D incompressible Navier–Stokes equations". In: *Journal of Computational Physics* 328 (2017), pp. 200–220. ISSN: 00219991. DOI: 10.1016/j.jcp.2016.10.009. URL: <https://www.scopus.com/inward/record.uri?eid=2-s2.0-84992428921&doi=10.1016%2fj.jcp.2016.10.009&partnerID=40&md5=ebfa6f03922ed248af295bd844b13cac>.
- [27] Artur Palha et al. "Physics-compatible discretization techniques on single and dual grids, with application to the Poisson equation of volume forms". In: *Journal of Computational Physics* 257 (Apr. 2013). DOI: 10.1016/j.jcp.2013.08.005.
- [28] Theodore Pian and Chang-Chun Wu. "Hybrid and Incompatible Finite Element Methods". In: (Nov. 2005). DOI: 10.1201/9780203487693.
- [29] Pierre-Arnaud Raviart and Jean-Marie Thomas. "A mixed finite element method for 2nd order elliptic problems". In: *Mathematical Aspects of Finite Element Methods* (1977), pp. 292–315.
- [30] K. Sankaran. "Beyond DIV, CURL and GRAD: modelling electromagnetic problems using algebraic topology". In: *Journal of Electromagnetic Waves and Applications* 31.2 (2017), pp. 121–149. ISSN: 09205071. DOI: 10.1080/09205071.2016.1257397. URL: <https://www.scopus.com/inward/record.uri?eid=2-s2.0-84996836113&doi=10.1080%2f09205071.2016.1257397&partnerID=40&md5=432af0eaaad4a5b8ac9950ed94734522>.
- [31] Suyash Shrestha. "Hybridised Mimetic Discretisation and Variational Multiscale Theory for Advection-Dominated Problems". In: (2022).
- [32] P.R. Spalart and V. Venkatakrishnan. "On the role and challenges of CFD in the aerospace industry". In: *Aeronautical Journal* 120.1223 (2016). cited By 93, pp. 209–232. DOI: 10.1017/aer.2015.10. URL: <https://www.scopus.com/inward/record.uri?eid=2-s2.0-84960408743&doi=10.1017%2faer.2015.10&partnerID=40&md5=12cd1169041710e258f41fdb49b29276>.
- [33] M. Spivak. *Calculus on manifolds*. Perseus Books, 1998.
- [34] Enzo Tonti. "On the Mathematical Structure of a Large Class of Physical Theories". In: 1971.
- [35] Enzo Tonti. "The Formal Structure of Physical Theories". In: (Jan. 1975).
- [36] Enzo Tonti. "The reason for analogies between physical theories". In: *Applied Mathematical Modelling* 1 (1976), pp. 37–50.
- [37] Enzo Tonti. "Why starting from differential equations for computational physics?" In: *Journal of Computational Physics* 257 (Jan. 2014), pp. 1260–1290. DOI: 10.1016/j.jcp.2013.08.016.
- [38] T. J. Willmore. *An introduction to differential geometry*. Courier Corporation, 2013.

- [39] Y. Zhang. "Mimetic Spectral Element Method and Extensions toward Higher Computational Efficiency". In: (2022). doi: 10.4233/uuid:a87e7be3-fb08-4706-9676-a6ae43f5aa0d. URL: <https://doi.org/10.4233/uuid:a87e7be3-fb08-4706-9676-a6ae43f5aa0d>.
- [40] Y. Zhang. "Spatially mass-, kinetic energy- and helicity-preserving mimetic discretization of 3D incompressible Euler flows". In: (2016). URL: <http://resolver.tudelft.nl/uuid:d158a27e-b8a9-4677-9775-ed47f01ebfaf>.
- [41] Y. Zhang et al. "A mass-, kinetic energy- and helicity-conserving mimetic dual-field discretization for three-dimensional incompressible Navier-Stokes equations, part I: Periodic domains". In: *Journal of Computational Physics* 451 (2022). issn: 00219991. doi: 10.1016/j.jcp.2021.110868. URL: <https://www.scopus.com/inward/record.uri?eid=2-s2.0-85121810949&doi=10.1016%2fj.jcp.2021.110868&partnerID=40&md5=438d49a8f6b3463914c992f652b6c176>.