Superconvergence of linear finite elements on simplicial meshes

Chen, Jie

2011

Chen, J. (2011). Superconvergence of linear finite elements on simplicial meshes. Doctoral thesis, Nanyang Technological University, Singapore.

<https://hdl.handle.net/10356/50615>

<https://doi.org/10.32657/10356/50615>

**SUPERCONVERGENCE OF LINEAR FINITE
ELEMENTS ON SIMPLICIAL MESHES**

CHEN JIE

School of Physical and Mathematical Sciences

A thesis submitted to the Nanyang Technological University
in partial fulfillment of the requirement for the degree of
Doctoral of Philosophy

2011

Acknowledgements

First and foremost, I am gratefully indebted, and wish to express my sincere appreciation and respect to my dissertation advisor, Prof. Desheng Wang, for persevering with me throughout the time it took me to complete this research and write the dissertation.

Many people on the faculty and staff of the School of Physical and Mathematical Sciences at Nanyang Technological University assisted and encouraged me in various ways during my course of studies. In particular, I appreciate the management and leadership of Prof. San Ling, Prof. Yeow Meng Chee, Prof. Bernhard Schmidt and Prof. Chaoping Xing. I am also appreciative of the help from the IT and Admin. staff.

I am grateful to Prof. Xue-Cheng Tai, Prof. Lilian Wang, Prof. Viet Ha Hoang and Prof. Song Heng Chan for the stimulating lectures and seminars. I am grateful as well to my coauthors Prof. Haijun Wu, Prof. Qiang Du, Prof. Yunqing Huang and Prof. Xiaoping Xie for their patient instruction and good-natured support.

Last, but definitely not least, I am deeply indebted to my parents for their blessings and selfless support; To my wife for her patience, moral support, and encouragement during my study.

Contents

ACKNOWLEDGEMENTS	2
SUMMARY	6
1 PRELIMINARIES	9
1.1 Polynomials Spaces	10
1.2 Function Spaces	11
1.2.1 Continuous Function Spaces	11
1.2.2 Lebesgue Spaces	11
1.2.3 Sobolev Spaces	12
1.3 Polynomial Approximation Theory	13
1.3.1 Bramble-Hilbert Lemma	14
1.3.2 Interpolation Error Estimates	15
2 FINITE ELEMENT ANALYSIS	16
2.1 Introduction	16
2.2 The Finite Element Method	17
2.2.1 Weak Formulation	18
2.2.2 Ritz-Galerkin Approximation	19
2.2.3 Basic Aspects of the Finite Element Method	21
2.2.4 Affine equivalence of Finite Elements	22
2.3 The Construction of Finite Element Spaces	23
2.3.1 One-dimensional Finite Elements	24
2.3.2 Triangular Finite Elements	25

2.3.3	Tetrahedral Finite Elements	27
2.4	A Priori Error Estimates	29
2.4.1	Error Estimates of Finite Elements Interpolations	29
2.4.2	Error Estimates of Finite Elements Solutions	30
3	SUPERCONVERGENCE TECHNIQUES IN FEM	32
3.1	Superconvergence by Local Symmetry	33
3.2	Generalized "Computer-based" Method	35
3.3	Superconvergence by Post-processing	38
3.3.1	Superconvergence Patch Recovery	38
3.3.2	Polynomial-Preserving Recovery	40
4	LOCAL ERROR EXPANSION FORMULA AND SUPERCONVER-	
	GENCE ON PAR6	42
4.1	Preliminaries	43
4.2	Local error expansion formula in n dimensional space	45
4.3	Par6 pattern: the optimal Centroidal Voronoi tessellation in three di- mensional spaces	50
4.4	Superconvergence on Par6	52
4.4.1	Superconvergence between the finite element solution and linear interpolant	54
4.4.2	Superconvergence between the gradient recovered by SPR and true gradient	62
4.5	Numerical substantiation	67
5	LINEAR FINITE ELEMENT SUPERCONVERGENCE ON UN-	
	STRUCTURED SIMPLICIAL MESHES	69
5.1	Introduction	69
5.2	Superconvergence between the finite element solution and linear inter- polant in three dimensional spaces	71
5.3	Numerical substantiation	85
5.4	Preliminary exploration on superconvergence in high dimensional space	92

5.5	Appendix	96
6	ADAPTIVE TETRAHEDRAL MESH GENERATION BY CON- FORMING CENTROIDAL VORONOI-DELAUNAY TESSELLA- TIONS FOR FINITE ELEMENT METHODS	100
6.1	Introduction	100
6.2	A posterior error estimator for linear finite element methods	103
6.2.1	A posterior error estimator based on the residual error	104
6.2.2	A posterior error estimator based on superconvergent patch re- covery	105
6.3	Mesh generation and optimization	108
6.3.1	Centroidal Voionoi tessellations and Delaunay tetrahedronlization	108
6.3.2	Algorithms for CCVDTs	110
6.3.3	Equidistribution of energy	114
6.3.4	Sliver elimination and local optimization	116
6.4	Adaptive finite element algorithm based on CCVDT	119
6.4.1	Modification of density function	119
6.4.2	Adaptive algorithm based on CCVDT	121
6.5	Numerical examples	123
6.5.1	Experiment 1	123
6.5.2	Experiment 2	124
6.5.3	Comparison among different refinement strategies	136

Summary

In 1960's, it has been observed that at some special a priori points, the convergence rate of finite element approximation or its derivatives is higher than what is globally possible. This phenomenon has been termed as superconvergence. The notion "superconvergence" is now used in a much broader sense. The finite element solution or its derivatives can be recovered by means of various post-processing techniques and obtain an increase in accuracy. This is also called superconvergence and the initial case (without post-processing) is referred to as natural superconvergence.

This interesting and important phenomenon brought a new study field of the finite element theory. During this almost fifty years' period more than 1000 papers have been written on this subject. Many methods with/without post-processing have been introduced. Moreover, superconvergence phenomena have been used in various fields of engineering and sciences. Nowadays, superconvergence is still a dynamically developing field of research. By using the MathSciNet search engine, we observed that, in the last 10 years, the number of mathematical publications on this subject is steady from 30 to 50. It should be noted that there are also large amount of engineering papers devoted to this topic, e.g. most of the papers related to superconvergence patch recovery (SPR) method are published on engineering journals.

In this dissertation work, we focus on the linear finite element superconvergence on unstructured simplicial meshes for the second order elliptic problems. First of all, we find the gradients recovered from linear finite element solutions by SPR (or Modified SPR) enjoy the superconvergent property on high quality unstructured meshes in three-dimensional spaces, especially on centroidal Voronoi-Delaunay tessellations (CVDT), where Modified SPR (MSPR) is a recovery method raised to overcome

the influence of slivers. Second, to analyze this phenomenon a local error expansion formula is deduced. Since the normal component of the gradients of the test functions is discontinuous, it is difficult to combine elementwise error estimates together. Thus this element error expansion formula involves only the tangential derivative of the test function on the edges. This local error expansion formula holds in n ($n \geq 3$)-dimensional spaces not only in three-dimensional spaces, which makes the superconvergence analysis in higher dimensional spaces possible. Third, before we go the general unstructured meshes, we first analyze the superconvergence on Par6 patterns, which is considered as the optimal CVDT meshes in three-dimensional spaces. Fourth, we analyze the superconvergent property on unstructured simplicial meshes and prove that the finite element solutions are superconvergent to the linear interpolations of true solutions in H^1 norm with an order $O(h^{(1+\rho)})$ ($0 \leq \rho \leq \alpha$) on three-dimensional simplicial meshes where the lengths of each pair of opposite edges in most tetrahedrons differ only by $O(h^{(1+\alpha)})$. At last, as a direct application of superconvergent property, an adaptive finite element methods by conforming centroidal Voronoi-Delaunay tessellations (CCVDT) is introduced.

Since we focus on the three-dimensional problem, which is more meaningful for real world application, it makes our research more difficult and brings us some of problems that will not appear in lower dimensions, such as the loss of orthogonality, the loss of symmetry in geometry and the influence of "slivers". Brandts and Křížek wrote the paper "History and future of superconvergence in three-dimensional finite elements methods" to explain the difficulties in this field in 2000. We overcame these difficulties and achieved the superconvergent results in three-dimensional spaces finally. To realize this purpose, some new methods and skills were raised, for instance, the analytical method which is effective in high dimensions, the modified superconvergent patch recovery method (MSPR) and a simpler but effective method to eliminate the slivers and so on.

There are six chapters in this report. Chapter 1 contains preliminaries of function spaces and approximation theories. In Chapter 2, we present a standard definition and a priori error estimates of finite element methods for later reference. In Chapter 3, we introduce some superconvergence techniques. Close attention is paid to those

methods which are related to our approach. The local error expansion formula and the superconvergence analysis on Par6 patterns are presented in Chapter 4. The superconvergence on unstructured simplicial meshes is analyzed in Chapter 5, where an edge pair condition i.e. the lengths of each pair of opposite edges in most tetrahedrons differ only by $O(h^{(1+\alpha)})$ is raised and numerous examples show that CVDT meshes satisfy the edge pair condition with α no smaller than 0.5. In Chapter 6, an adaptive finite element method by CCVDT is introduced.

Many interesting as well as challenging problems arose during my dissertation research. For example, What are the geometric conditions for superconvergence in four and higher dimensional spaces? Whether is the Gersho's conjecture true or not in three-dimensional spaces? If it is true, can the Lloyd iteration lead a CVDT mesh to Par6 pattern when the number of generators goes to infinity? These will be my future research topics.

Chapter 1

PRELIMINARIES

This chapter contains material from algebra and analysis that will be of use in the later portion of the report. It is presented here for ready reference.

Throughout this report, n stands for the spatial dimension. We denote by Ω a domain in the n -dimensional Euclidean spaces $\mathbb{R}^n$, i.e., a bounded open connected subset of $\mathbb{R}^n$ with a Lipschitz continuous boundary. We let $\mathbf{x} = (x_1, \dots, x_n)$ denote a typical point in $\mathbb{R}^n$ and let $|\mathbf{x}| = (x_1^2 + \dots + x_n^2)^{1/2}$ denote the Euclidean norm of $\mathbf{x}$.

We will use the standard multi-index notation. Denote by $\mathbb{N}_0$ the set of nonnegative integers. A multi-index is an n -tuple $\alpha = (\alpha_1, \dots, \alpha_n) \in \mathbb{N}_0^n$. The length of α is given by $|\alpha| = \sum_{i=1}^n \alpha_i$. We also define $\alpha! = \alpha_1! \cdots \alpha_n!$.

For an m -times differentiable function v and any $\alpha \in \mathbb{N}_0^n$ with $|\alpha| \leq m$, we denote by $D^\alpha v(\mathbf{x})$ the weak partial derivative $\partial^{|\alpha|} v(\mathbf{x}) / \partial x_1^{\alpha_1} \cdots \partial x_n^{\alpha_n}$, which is referred as the α th weak derivative.

The rest of this chapter is organized as the following. In Section 1.1, notations of polynomial spaces are introduced. Section 1.2 is devoted to the notations and standard results in function spaces. In Section 1.3, Bramble-Hilbert lemma and a theorem of interpolation error estimates are presented.

1.1 Polynomials Spaces

We introduce some notations and properties of polynomial spaces of several variables in this section.

For $\alpha \in \mathbb{N}_0^n$ and $\mathbf{x} = (x_1, \dots, x_n)$, a monomial in variables $x_1, \dots, x_n$ is a product

$$\mathbf{x}^\alpha = x_1^{\alpha_1} \cdots x_n^{\alpha_n}. \quad (1.1)$$

Here the total degree (or degree) of $\mathbf{x}^\alpha$ is $|\alpha|$. A polynomial p in n variables of degree at most m is a linear combination of monomials,

$$p(\mathbf{x}) = \sum_{|\alpha| \leq m} c_\alpha \mathbf{x}^\alpha, \quad (1.2)$$

where the coefficients c_α are in $\mathbb{R}$.

Let Π_m^n be the vector space of n -variable polynomials of total degree less than or equal to m ; i.e.,

$$\Pi_m^n = \text{Span} \left\{ \prod_{j=1}^n x_j^{i_j} \mid 0 \leq i_1, \dots, i_n \leq m, 0 \leq \sum_{j=1}^n i_j \leq m \right\}. \quad (1.3)$$

We sometimes write $\Pi_m^n(x_1, \dots, x_n)$ to specify the n variables. Let Q_m^n be the space of n -variable polynomials such that the degree of every variable is not greater than m ; that is

$$Q_m^n = \text{Span} \left\{ \prod_{j=1}^n x_j^{i_j} \mid 0 \leq i_1, \dots, i_n \leq m \right\}. \quad (1.4)$$

A polynomial is called homogenous if all the monomials appearing in it have the same degree. Denote by $\mathcal{P}_m^n$ the space of all homogenous polynomials on $\mathbb{R}^n$ of degree m .

1.2 Function Spaces

In this section, we introduce function spaces that are used in the weak (variational) formulation of partial differential equations. We shall follow standard notations as regards function spaces, norms, etc.

1.2.1 Continuous Function Spaces

Define $C(\Omega)$ the space of real valued continuous functions on Ω . For any nonnegative integer m , define the space $C^m(\Omega)$ as the space of all the real valued functions that are m times continuously differentiable on Ω . Those functions in $C^m(\Omega)$ are called smooth functions. Analogously, $C^m(\overline{\Omega})$ is defined, which is a Banach space equipped with the norm

$$\|v\|_{C^m(\overline{\Omega})} = \max_{|\alpha| \leq m} \sup_{\mathbf{x} \in \Omega} |D^\alpha v(\mathbf{x})|.$$

It is algebraically clear that $C^m(\overline{\Omega}) \subseteq C^m(\Omega)$.

Clearly, $C(\Omega)$ is the special case of $C^m(\Omega)$ when $m = 0$. Another important case of $C^m(\Omega)$ is $m = \infty$, which is the space of infinitely differentiable functions on Ω . Moreover, the space of infinitely differentiable functions with a compact support in Ω is denoted by $\mathcal{D}(\Omega)$. The dual space $\mathcal{D}'(\Omega)$ of $\mathcal{D}(\Omega)$ is the space of distributions on Ω .

1.2.2 Lebesgue Spaces

For $1 \leq p \leq \infty$, define the Lebesgue spaces $L^p(\Omega)$ to be the class of real valued Lebesgue measurable functions on Ω which are p -integrable. For $v \in L^p(\Omega)$, $1 \leq p < \infty$, define the norm to be

$$\|v\|_{L^p(\Omega)} = \left(\int_{\Omega} |v(\mathbf{x})|^p d\mathbf{x} \right)^{1/p}. \quad (1.5)$$

For $v \in L^\infty(\Omega)$ define the norm

$$\|v\|_{L^\infty(\Omega)} = \text{ess sup}_{\mathbf{x} \in \Omega} |v(\mathbf{x})|, \quad (1.6)$$

where $\text{ess sup}_{\mathbf{x} \in \Omega} |v(\mathbf{x})|$ is the essential supremum of v on Ω . It is well-known that $L^p(\Omega)$ is a Banach space.

1.2.3 Sobolev Spaces

For any integer $m \geq 0$, and any $1 \leq p \leq \infty$, the Sobolev space $W^{k,p}(\Omega)$ is the set of all the functions $v \in L^p(\Omega)$ such that for each multi-index $\alpha \in \mathbb{N}_0^n$ with $|\alpha| \leq m$, the α th weak derivative $D^\alpha v$ exists and $D^\alpha v \in L^p(\Omega)$.

The Sobolev space $W^{k,p}(\Omega)$ is a Banach space with the norm

$$\begin{aligned} \|v\|_{W^{k,p}(\Omega)} &= \left(\sum_{|\alpha| \leq k} \|D^\alpha v\|_{L^p(\Omega)}^p \right)^{1/p}, \quad 1 \leq p < \infty, \\ \|v\|_{W^{k,\infty}(\Omega)} &= \max_{|\alpha| \leq k} \|D^\alpha v\|_{L^\infty(\Omega)}. \end{aligned}$$

Moreover, the standard seminorm over $W^{k,p}(\Omega)$ is

$$\begin{aligned} |v|_{W^{k,p}(\Omega)} &= \left(\sum_{|\alpha|=k} \|D^\alpha v\|_{L^p(\Omega)}^p \right)^{1/p}, \quad 1 \leq p < \infty, \\ |v|_{W^{k,\infty}(\Omega)} &= \max_{|\alpha|=k} \|D^\alpha v\|_{L^\infty(\Omega)}. \end{aligned}$$

It is clear from the definitions above that $W^{0,p}(\Omega) \equiv L^p(\Omega)$.

When $p = 2$, people usually write $H^k(\Omega) = W^{k,2}(\Omega)$. The Sobolev space $H^k(\Omega)$ is a Hilbert space with the inner product

$$(u, v)_k = \int_{\Omega} \sum_{|\alpha| \leq k} D^\alpha u(\mathbf{x}) D^\alpha v(\mathbf{x}) \, d\mathbf{x}, \quad u, v \in H^k(\Omega). \quad (1.7)$$

For $m \in \mathbb{N}$, the space $H_0^m(\Omega)$ is the closure of $\mathcal{D}(\Omega)$ in $H^m(\Omega)$. The dual space of

$H_0^m(\Omega)$ is denoted by $H^{-m}(\Omega)$, provided with the norm

$$\|u\|_{H^{-m}(\Omega)} = \sup_{v \in H_0^m(\Omega)} \frac{\langle u, v \rangle}{|v|_{H^m(\Omega)}},$$

where $\langle \cdot, \cdot \rangle$ stands the duality pairing between $H^{-m}(\Omega)$ and $H_0^m(\Omega)$.

We quote the following Sobolev embedding results, which are important in theory of partial differential equations. See [1, 2, 3] for details.

Theorem 1.1. *Let Ω be a nonempty Lipschitz domain in $\mathbb{R}^n$. Let $1 \leq p \leq q$, $m \geq 1$, and $k \leq m$. Then the following statements are valid.*

- (a) *If $kp < n$, then $W^{m,p}(\Omega) \hookrightarrow W^{m-k,q}(\Omega)$ for $q \leq \frac{np}{n-kp}$;*
- (b) *If $kp = n$, then $W^{m,p}(\Omega) \hookrightarrow W^{m-k,q}(\Omega)$ for $q \leq \infty$;*
- (c) *If $kp > n$, then $W^{m,p}(\Omega) \hookrightarrow C^{m-k}(\overline{\Omega})$.*

Here, $V \hookrightarrow W$ means that the space V is continuous embedded in W ; i.e., $V \subseteq W$ and $\|v\|_W \leq C \|v\|_V$ for all $v \in V$.

Before ending this section, we introduce Green's formula for later reference. The formula presented here is extended to functions from Sobolev spaces. Assuming $u \in H^2(\Omega)$ and $v \in H^1(\Omega)$, then it follows that

$$-\int_{\Omega} \Delta u v \, d\mathbf{x} = \int_{\Omega} \nabla u \cdot \nabla v \, d\mathbf{x} - \int_{\partial\Omega} \frac{\partial u}{\partial \mathbf{n}} v \, d\Gamma, \quad (1.8)$$

where $\partial u / \partial \mathbf{n}$ is the outward normal derivative of u , $d\Gamma$ is the Lebesgue measure on the boundary $\partial\Omega$.

1.3 Polynomial Approximation Theory

The Bramble-Hilbert lemma is a fundamental result on multivariate polynomial approximation. It is frequently applied in the analysis of finite element methods (FEM).

In this section, we first present the lemma and one of its applications. Then we provide the estimates of the interpolation error, which will lead the error estimates of finite element approximations.

1.3.1 Bramble-Hilbert Lemma

Recall the basic definitions of multivariate Taylor series [4]. The classical Taylor polynomial of order m (degree $m - 1$) of a function $u \in C^{m-1}(\Omega)$ at $\mathbf{x} \in \Omega$ about the point $\mathbf{y} \in \Omega$ is given by

$$T_y^m u(\mathbf{x}) = \sum_{|\alpha| < m} \frac{1}{\alpha!} D^\alpha u(\mathbf{y}) (\mathbf{x} - \mathbf{y})^\alpha.$$

For a ball $B(\mathbf{x}, r) \subset\subset \Omega$, the Taylor polynomial of order m (degree $m - 1$) of u averaged over $B(\mathbf{x}, r)$ is defined as

$$Q^m u(\mathbf{x}) = \int_{B(\mathbf{x}, r)} T_y^m u(\mathbf{x}) \phi(\mathbf{y}) \, d\mathbf{y},$$

where ϕ is a cut-off function supported in $\overline{B(\mathbf{x}, r)}$. Then, the following important result is obtained [4, 5].

Lemma 1.2 (Bramble-Hilbert lemma). *Let Ω be star-shaped with respect to some ball $B(\mathbf{x}, r)$ and let $u \in W^{m,p}(\Omega)$. If $1 < p < \infty$ and $m > o/p$, or $p = 1$ and $m \geq o$, then*

$$\|u - Q^m u\|_{L^\infty(\Omega)} \leq C \lambda^{m-o/p} |u|_{W^{m,p}(\Omega)},$$

where $\lambda = \text{diam}(\Omega)$, C is a constant independent of λ and u . In particular, for $p \geq 1$, we have

$$|u - Q^m u|_{W^{k,p}(\Omega)} \leq C \lambda^{m-k} |u|_{W^{m,p}(\Omega)}, \quad k = 0, 1, \dots, m,$$

where λ and C are as above.

The following inequality is an application of Bramble-Hilbert lemma.

Lemma 1.3 (Friedrichs inequality). *Suppose Ω is star-shaped with respect to some ball $B(\mathbf{x}, r)$. Then for all $u \in W^{1,p}(\Omega)$,*

$$\|u - \bar{u}\|_{W^{1,p}(\Omega)} \leq C |u|_{W^{1,p}(\Omega)},$$

where $\bar{u} = \frac{1}{|\Omega|} \int_{\Omega} u(\mathbf{x}) \, d\mathbf{x}$, $|\Omega|$ is the Lebesgue measure of Ω .

Remark 1.4. The Friedrichs inequality is essential in the proof of coercivity for the Neumann problem for the Laplacian operator. The reader is referred to [4] for detailed proof.

1.3.2 Interpolation Error Estimates

Let $\hat{T}$ be a convex polygonal domain in $\mathbb{R}^n$, $\hat{P}$ be a polynomial space over $\hat{T}$ with $\dim \hat{P} = N$. We choose a set of points $\{\hat{\mathbf{x}}_i\}_{i=1}^N$ in $\hat{T}$. Assume that the basis function $\{\hat{\varphi}_i\}_{i=1}^N$ of $\hat{P}$ associated with $\{\hat{\mathbf{x}}_i\}_{i=1}^N$ constitute a unisolvent system on $\hat{T}$ (i.e., the only linear combination of the $\hat{\varphi}_i$ s that vanishes on N distinct points of $\hat{T}$ vanishes identically [6]), with the property $\hat{\varphi}_i(\hat{\mathbf{x}}_j) = \delta_{ij}$. Define an interpolation operator by

$$\hat{I} : C(\hat{T}) \rightarrow \hat{P}, \quad \hat{I}\hat{u} = \sum_{i=1}^N \hat{u}(\hat{\mathbf{x}}_i) \hat{\varphi}_i. \quad (1.9)$$

The unisolvence of the system $\{\hat{\varphi}_i\}_{i=1}^N$ guarantees that the pointwise interpolation operator (1.9) is well defined. It follows that any function $\hat{u} \in \hat{P}$ is uniquely determined by its values at the points $\{\hat{\mathbf{x}}_i\}_{i=1}^N$.

We quote the following estimates for the interpolation error over $\hat{T} \subset \mathbb{R}^n$, $n = 1, 2$, or 3 .

Theorem 1.5. *Let $m, o \in \mathbb{N}_0$ with $m > 0, m + 1 \geq o$, and $\Pi_m^n(\hat{T}) \subseteq \hat{P}$. Let $\hat{I}$ be the operator defined in (1.9). Then there exists a constant C such that*

$$\left| \hat{u} - \hat{I}\hat{u} \right|_{H^o(\hat{T})} \leq C \left| \hat{u} \right|_{H^{m+1}(\hat{T})} \quad \forall \hat{u} \in H^{m+1}(\hat{T}).$$

Remark 1.6. Notice that the embedding result $H^{m+1}(\hat{T}) \hookrightarrow C(\hat{T})$, provided $m > 0$ (Theorem 1.1), and the Bramble-Hilbert lemma are essential in the proof of Theorem 1.5, cf. [4, 7].

Chapter 2

FINITE ELEMENT ANALYSIS

2.1 Introduction

The finite element method is the most extensively used numerical method for solving elliptic boundary value problems.

The foundation of the FEM is traced to the work of Galerkin in the method of weighted residuals, and to Rayleigh and Ritz in variational methods. The major shortcoming of the classical Ritz-Galerkin methods is the requirement that the trial functions used apply to the entire solution domain, which usually produces a dense stiffness matrix.

The notation of piecewise defined trial functions, which is fundamental to the FEM, was introduced by Courant. In [8], finite-dimensional piecewise linear approximations of the variational method over a network of triangles is discussed. The basis functions are chosen such that their supports are "small" and the support of each basis function intersect a "small" number of supports of the other basis functions, which involved a basic concept underlying the FEM. Since then, engineers and mathematicians have proposed a variety of FEM and developed systematic mathematical theory of FEM. For a historical survey, the reader is referred to [9].

The FEM is attractive for solving complex problems since it has many distinct intrinsic properties. One of the advantages of the FEM is the natural way in which it deals with complicated domains and nonuniform meshes. In principle, the FEM can

be applied to domains of arbitrary shape with quite arbitrary boundary conditions. Generally, finite element schemes are stable in appropriate norms, and insensitive to singularities or distortions of the mesh, in contrast to classical difference methods. Moreover, the FEM usually leads to a linear system of sparse coefficient matrix (i.e. most of its entries are zeros), which, comparing with a dense coefficient matrix, is less costly to form and more efficiently to solve with.

On the other hand, because of the extensive work on the mathematical foundations done during the nineteen seventies and eighties, the FEM now enjoys a rich and solid mathematical basis. In particular, techniques for determining a priori and a posteriori estimates provides an important part of the theory of the FEM, and makes it possible to the analysis of important engineering and physical problems in many numerical and experimental studies.

There are numerous textbooks, handbooks, and monographs devoted to mathematical analysis of the FEM, e.g. [4, 10, 11, 12, 13, 14, 15]. A summary of various results for the FEM will be given in this chapter. The materials are only chosen to meet the need for later development. We shall follow a standard approach to introduce the FEM.

The outline of the rest of this chapter is as follows. In Section 2.2, the concept and the basic characteristics of the FEM are described. Some finite elements are developed in Section 2.3. Error estimates of finite element interpolations and finite element solutions of elliptic boundary value problems are discussed in Section 2.4

2.2 The Finite Element Method

Let Ω be a domain in $\mathbb{R}^n$ with Lipschitz-continuous boundary $\partial\Omega$. Consider the elliptic boundary value problem

$$\left\{ \begin{array}{ll} -\Delta u(\mathbf{x}) &= f(\mathbf{x}) \quad \text{in } \Omega, \\ u(\mathbf{x}) &= 0 \quad \text{on } \Gamma_{\text{Dirichlet}}, \\ \partial u(\mathbf{x})/\partial \mathbf{n} &= g(\mathbf{x}) \quad \text{on } \Gamma_{\text{Neumann}}, \end{array} \right. \quad (2.1)$$

where $f \in L^2(\Omega)$ and $g \in L^2(\Gamma_{\text{Neumann}})$ are given; $\Gamma_{\text{Dirichlet}}$ and Γ_{Neumann} are two disjoint sets such that $\Gamma_{\text{Dirichlet}} \cup \Gamma_{\text{Neumann}} = \partial\Omega$ and $\mathbf{n}$ is the unit outer norm vector of $\partial\Omega$.

2.2.1 Weak Formulation

To treat the homogenous boundary condition of (2.1) on the $\Gamma_{\text{Dirichlet}}$, we introduce a space between $H_0^1(\Omega)$ and $H^1(\Omega)$

$$V(\Omega) = \{v \in H^1(\Omega) \mid v \equiv 0 \text{ on } \Gamma_{\text{Dirichlet}}\}, \quad (2.2)$$

which is equipped with a standard $H^1(\Omega)$ norm.

Multiply (2.1) by an arbitrary function $v \in V(\Omega)$ and integrate over Ω . A direct application of the Green's formula (1.8) yields a new problem: Find $u \in V(\Omega)$ such that

$$B(u, v) = F(v) \quad \forall v \in V(\Omega), \quad (2.3)$$

where the bilinear form $B(\cdot, \cdot)$ and linear form $f(\cdot)$ are defined as

$$B(u, v) = \int_{\Omega} \nabla u \cdot \nabla v \, d\Omega, \quad (2.4)$$

$$F(v) = \int_{\Omega} f v \, d\Omega + \int_{\Gamma_{\text{Neumann}}} g v \, d\Gamma. \quad (2.5)$$

Equation (2.3) is known as the weak (or variational) formulation of (2.1).

Remark 2.1. Notice that, in this special case, the bilinear form $B(\cdot, \cdot)$ defines an inner product over the space V and the induces a norm $\|v\|_E = \sqrt{a(v, v)}$ (energy norm), which is equivalent to the standard $H^1(\Omega)$ norm. Moreover, V is a Hilbert space.

Remark 2.2. The bilinear form $B(\cdot, \cdot)$ in (2.4) is continuous (or bounded), i.e. $\exists C \in \mathbb{R}$ such that

$$|B(v, w)| \leq C \|v\|_{H^1(\Omega)} \|w\|_{H^1(\Omega)} \quad \forall v, w \in V(\Omega),$$

and coercive (or V-elliptic) on $V(\Omega)$ (see Remark 1.4), i.e. $\exists \alpha > 0$ such that

$$|B(v, v)| \geq \alpha \|v\|_{H^1(\Omega)}^2 \quad \forall v \in V(\Omega).$$

The following Lax-Milgram lemma guarantees both existence and the uniqueness of the solution to the weak problem (2.3). See its proof in, e.g., [12].

Theorem 2.3 (Lax-Milgram lemma). *Let V be a Hilbert space, $B(\cdot, \cdot) : V \times V \rightarrow \mathbb{R}$ be a continuous coercive bilinear form, and let $F : V \rightarrow \mathbb{R}$ be a continuous linear form. Then, there exists a unique $u \in V$ such that*

$$B(u, v) = F(v) \quad v \in V.$$

Remark 2.4. Clearly, a classical solution $u \in C^2(\Omega) \cap C^1(\overline{\Omega})$ of the boundary value problem (2.1) is also the solution $u \in V(\Omega)$ of the weak formulation (2.3). Conversely, a weak solution of the problem (2.3) with sufficient smoothness is also the classical solution of the problem (2.1).

2.2.2 Ritz-Galerkin Approximation

Let $\mathcal{S}_N \subset V(\Omega)$ be an N -dimensional subspace. We project the problem (2.3) onto $\mathcal{S}_N$. The weak problem reduces to: Find $u_h \in \mathcal{S}_N$ such that

$$B(u_h, v_h) = F(v_h) \quad \forall v_h \in \mathcal{S}_N. \tag{2.6}$$

Applying the Lax-Milgram lemma (Theorem 2.3), one concludes that the problem (2.6) has a unique solution. In addition, if $\{\varphi_i\}_{i=1}^N$ is a basis of $\mathcal{S}_N$, the solution can be expressed as

$$u_h(\mathbf{x}) = \sum_{j=1}^N u_j \varphi_j(\mathbf{x}),$$

where u_j s are unknown coefficients.

Take $v_h \in \mathcal{S}_N$ in (2.6) each of the basis function φ_i . Then solving (2.6) is equivalent

to solving a finite dimensional linear system

$$\mathbf{A}\mathbf{u} = \mathbf{f}, \quad (2.7)$$

where $\mathbf{u} = [u_1, \dots, u_N]^T \in \mathbb{R}^N$ is the unknown vector, $\mathbf{A} = [B(\varphi_j, \varphi_i)] \in \mathbb{R}^{N \times N}$ is referred to as the stiffness matrix, $\mathbf{f} = [F(\varphi_1), \dots, F(\varphi_N)]^T \in \mathbb{R}^N$ is the load vector. The solution of the problem (2.6) can be found by solving a matrix equation system. This solution approach is called the Galerkin method.

Remark 2.5. Note that the bilinear form $B(\cdot, \cdot)$ in (2.4) is symmetric, i.e.

$$B(v, w) = B(w, v) \quad \forall v, w \in V(\Omega).$$

In this case, it can be easily shown that the weak problem (2.3) is equivalent to a minimization problem [12]: Find $u \in V(\Omega)$ such that

$$J(u) = \inf_{v \in V(\Omega)} J(v),$$

where the energy function $J : V(\Omega) \rightarrow \mathbb{R}$ is defined by

$$J(v) = \frac{1}{2}B(v, v) - F(v).$$

Moreover, it is equally straightforward to shown that the finite-dimensional minimization problem: Find $u_h \in \mathcal{S}_N$ such that

$$J(u_h) = \inf_{v \in \mathcal{S}_N} J(v) \quad (2.8)$$

is equivalent to the approximation problem (2.6). The method (2.8) is called the Ritz method. From the above discussion, it is clear that the Galerkin method is more general than the Ritz method, and they are equivalent when both methods are applicable. Because of this, the Galerkin method is also called the Ritz-Galerkin method.

Remark 2.6. The Ritz-Galerkin method provides a general framework for numerical

approximation of the variational problem (2.3). From the above discussion, we see that in applying the method it is very important to choose appropriate basis functions as well as finite-dimensional subspaces. The classical Ritz-Galerkin method was applied mainly with the use of global polynomials or global trigonometric polynomials, which can lead to severely ill-conditioned linear systems.

The FEM is a special case of the Ritz-Galerkin method. It uses basis functions with "small" supports so that the conditioning of the resulting linear system can be moderately maintained.

Céa lemma provides an estimation of errors for the Ritz-Galerkin method.

Theorem 2.7 (Céa lemma). *Let V be a Hilbert space with norm $\|\cdot\|_V$, $\mathcal{S}_N$ be a subspace of V . Assume $B(\cdot, \cdot)$ is continuous coercive bilinear form on V , F is a continuous linear form. Let $u \in V$ be the solution of the problem (2.3). Then for the Ritz-Galerkin approximation problem (2.6), we have*

$$\|u - u_h\|_V \leq \frac{C}{\alpha} \inf_{v_h \in \mathcal{S}_N} \|u - v_h\|_V,$$

where C is the continuity constant and α is the coercivity constant of $B(\cdot, \cdot)$.

2.2.3 Basic Aspects of the Finite Element Method

According to [12], a finite element method is a Ritz-Galerkin method characterized by three basic aspects in the construction of the space $\mathcal{S}_N$.

Aspect I. *A triangulation or a mesh $\mathcal{T}_h$ is established over the set $\overline{\Omega}$, which partitions the domain into a finite number of subsets T with the following properties:*

1. $\overline{\Omega} = \cup_{T \in \mathcal{T}_h} T$;
2. each $T \in \mathcal{T}_h$ is closed with a nonempty and connected interior $\overset{\circ}{T}$ and a Lipschitz-continuous boundary ∂T ;
3. for distinct $T_1, T_2 \in \mathcal{T}_h$, one has $\overset{\circ}{T}_1 \cap \overset{\circ}{T}_2 = \emptyset$.

Once a triangulation $\mathcal{T}_h$ is established over the domain $\overline{\Omega}$, one establishes a finite element space (FES), which is a finite-dimensional space of functions defined over

the set $\bar{\Omega}$. For the problems considered in this work, the space $\mathcal{S}_N \subset V$ is the FES corresponding to the triangulation $\mathcal{T}_h$.

Aspect II. *The spaces $P_T = \{v_h|_T \mid v_h \in \mathcal{S}_N\}$, $T \in \mathcal{T}_h$ are finite-dimensional, which contain polynomials or "nearly polynomials".*

Aspect III. *There exists a "canonical" basis (denoted by $\{\varphi_i\}_{i=1}^{|\mathcal{S}_N|}$) in the space $\mathcal{S}_N$ whose corresponding basis functions have small supports, and these basis functions can be easily described.*

Let Σ_N be a set of linear forms $\{\sigma_i\}_{i=1}^{|\mathcal{S}_N|}$ defined over the space $\mathcal{S}_N$ so that

$$\sigma_j(\varphi_i) = \delta_{ij} \quad 1 \leq i, j \leq |\mathcal{S}_N| \quad \text{and} \quad p = \sum_{i=1}^N \sigma_i(p) \varphi_i \quad \forall p \in \mathcal{S}_N.$$

The linear forms $\{\sigma_i\}_{i=1}^{|\mathcal{S}_N|}$ are called the degrees of freedom. It is straightforward to conclude that the number of the degrees of freedom equals the dimension of the FES $\mathcal{S}_N$. We shall also denote by Σ_T the set of local degrees of freedom defined over P_T .

The three-tuple (T, P_T, Σ_T) defines a finite element (FE). As an abuse of terminology, the set T itself is often referred to as a FE, or an element. The basis functions $\{\varphi_i\}_{i=1}^{|\mathcal{S}_N|}$ in $\mathcal{S}_N$ are also called the shape functions in engineering literature.

For an arbitrary element $T \in \mathcal{T}_h$, it is standard to refer to $h_K = \text{diam}(K)$ as the mesh size of T , and, when $n > 1$, denote by ρ_T the radius of the largest inscribed ball in T . The ratio h_T/ρ_T indicates the flatness of the element.

In particular, a family $\mathcal{T}_h$ of finite elements (FE) is said to be regular if there exists a constant σ such that $h_T/\rho_T \leq \sigma$ for all element $T \in \mathcal{T}_h$. Finite elements considered in this work are all regular.

These three basic aspects are characteristic of the FEM in its simplest form. For features of more general FEM, the reader is referred to the literatures, e.g. [4, 10, 11, 12, 13, 14, 15].

2.2.4 Affine equivalence of Finite Elements

Definition 2.8. *Two finite elements (T, P, Σ) and $(\hat{T}, \hat{P}, \hat{\Sigma})$ are said to be affine-equivalent if there exists an invertible affine mapping $F_T : \hat{T} \rightarrow T$ of the form $F_T(\hat{\mathbf{x}}) =$*

$\mathbf{B}_T \hat{\mathbf{x}} + \mathbf{b}_T$, such that

$$F_T(\hat{T}) = T, \quad \hat{P} = P \circ F_T, \text{ and } \hat{\Sigma}(v_h \circ F_T) = \Sigma(v_h) \quad \forall v_h \in P.$$

Here, $\mathbf{B}_T$ is invertible $n \times n$ matrix and $\mathbf{b}_T$ is a translation vector.

A family of FE is called an affine family if all its FE are affine-equivalent to a single FE $(\hat{T}, \hat{P}, \hat{\Sigma})$, which is called the reference finite element of the family. Whereas, a FE (T, P, Σ) associated with $T \in \mathcal{T}_h$ is termed as a physical finite element. The choice for the reference FE will be specified for several FE families in Section 2.3.

The next theorem shows a crucial relationship between affine-equivalent finite elements.

Theorem 2.9. *Let (T, P, Σ) and $(\hat{T}, \hat{P}, \hat{\Sigma})$ be two affine-equivalent finite elements associated with the affine mapping F_T described in Definition 2.8. Let $\hat{\varphi}_i$, $1 \leq i \leq N_{\hat{T}}$, denote the basis functions of the (reference) finite element $(\hat{T}, \hat{P}, \hat{\Sigma})$. Then the functions $\varphi_i = \hat{\varphi}_i \circ F_T^{-1}$, $1 \leq i \leq N_{\hat{T}}$, are the basis functions of the finite element (T, P, Σ) .*

Theorem 2.9 indicates that, for an affine family of FE, the FES $\mathcal{S}_N$ is completely described by the reference FE $(\hat{T}, \hat{P}, \hat{\Sigma})$ and the family of affine mappings $\{F_T \mid T \in \mathcal{T}_h\}$. In practical implementations, most of the work involved in the computation of the stiffness matrix of the linear system (2.7) is performed on the reference FE, not on a generic physical FE.

Remark 2.10. Not all FE families are affine-equivalent. Counter examples can be found in, e.g., [12]. However, those FE lie out of the range of our interests in this report. We will from now on only consider affine-equivalent families of FE.

2.3 The Construction of Finite Element Spaces

In this section, we will introduce several families of piecewise polynomial finite element spaces for problems posed in $\mathbb{R}^n$, $n = 1, 2$, or 3 , which will be studied in later Chapters.

We follow the approaches in [14], and formulate hierarchical shape functions for some FE.

2.3.1 One-dimensional Finite Elements

Assume that, in example problem (2.1), we have the domain $\Omega = (a, b)$ and a homogenous Dirichlet boundary condition at the end point a . In this case,

$$V(a, b) = \{v \in H^1(a, b) \mid v(a) = 0\}.$$

For a natural $N > 1$, we make a partition $\mathcal{T}_h$ of the domain Ω which consists of N subintervals (elements) $T_i = [x_{i-1}, x_i]$, $1 \leq i \leq N$, where $a = x_0 < x_1 < \dots < x_N = b$. The points x_i , $0 \leq i \leq N$, are called nodes.

We use continuous piecewise linear functions and let

$$\mathcal{V}_h = \{v_h \in V(a, b) \cap C[a, b] \mid v_h|_{T_i} \in \Pi_1^1(T_i), 1 \leq i \leq N\}.$$

A set of "hat functions" $\varphi_i \in \mathcal{V}_h$ with $\varphi_i(x_j) = \delta_{ij}$, $1 \leq i, j \leq N$, are employed for a basis of the FES $\mathcal{V}_h$. See Figure 2.1. Clearly, the number of total degrees of freedom is N . Notice that each shape function φ_i associates with a node x_i , $1 \leq i \leq N$, which thus is called a nodal shape function.

Remark 2.11. The FES defined above is affine-equivalent. In fact, if we choose the reference element as $\hat{T} = [-1, 1]$, then it is mapped to the element $T_i = [x_{i-1}, x_i]$, $1 \leq i \leq N$, through the function

$$F_{T_i} : \hat{T} \rightarrow T_i; \quad x = F_{T_i}(\xi) = \frac{x_i - x_{i-1}}{2}\xi + \frac{x_i + x_{i-1}}{2}. \quad (2.9)$$

From now on, we will use the Roman letter(s) x (and y, z as necessary) to denote the standard Euclidean coordinate(s) in physical elements, and use the Greek letter(s) ξ (η and ζ) for the coordinate(s) in reference elements.

Figure 2.1: Piecewise linear basis functions.

2.3.2 Triangular Finite Elements

We shall introduce hierarchical bases for Lagrangian FE in this subsection. See [14] for more details.

Let the equilateral triangle with vertices $n_1 : (-1, 0)$, $n_2 : (1, 0)$, $n_3 : (0, \sqrt{3})$ be the reference finite element for triangular FE and $d_{i,j}$ is referred as the side/edge with end points n_i and n_j . See Figure 2.2.

A basis for an m th order hierarchical Lagrangian FE consists of three categories of shape functions.

1. *Nodal shape functions.* There are three nodal shape functions. Denote by N_i the shape function corresponding to the vertex n_i of $\hat{T}$, and define

$$N_1(\xi, \eta) = \frac{1}{2}(1 - \xi - \frac{\eta}{\sqrt{3}}), \quad (2.10)$$

$$N_2(\xi, \eta) = \frac{1}{2}(1 + \xi - \frac{\eta}{\sqrt{3}}), \quad (2.11)$$

$$N_3(\xi, \eta) = \frac{\eta}{\sqrt{3}}. \quad (2.12)$$

2. *Side modes.* There are $(m - 1)$ side modes associated with each side of $\hat{T}$

Figure 2.2: Triangular finite element.

such that they vanish along the other two sides. For instance, the side modes associated with sides $d_{i,j}$ are:

$$E_i^{1,2}(\xi, \eta) = N_1 N_2 \omega_{i-2}(N_2 - N_1), \quad i = 2, \dots, m, \quad (2.13)$$

where N_i , $i = 1, 2$ are the nodal shape functions defined above, and ω_i are defined as following:

$$\phi_m(x) = \frac{1}{4}(1 - x^2)\omega_{m-2}(x), \quad m = 2, 3, \dots, \quad (2.14)$$

where ϕ_m s are the primitives of the Legendre polynomials. The other side modes are analogous.

3. *Internal modes.* There are $(m-2)(m-1)/2$ internal modes:

$$I_{i,j}(\xi, \eta) = N_1 N_2 N_3 \xi^{i-3} \eta^{j-3}, \quad i, j = 3, \dots, m, \text{ and } i + j \leq m + 3. \quad (2.15)$$

The Lagrangian FES spanned by the shape functions is $\hat{P}^L = \Pi_m^2(\hat{T})$ with $\dim \hat{P}^L = (m+1)(m+2)/2$.

Figure 2.3: Tetrahedral finite element.

2.3.3 Tetrahedral Finite Elements

For tetrahedron, the reference finite element is chosen as $\hat{T} = \{\xi \geq \eta \geq \zeta\}$. The four nodes are $n_1 : (-1, -1, -1)$, $n_2 : (1, -1, -1)$, $n_3 : (1, 1, -1)$, and $n_4 : (1, 1, 1)$. See Figure 2.3. We now develop hierarchical tetrahedral FE.

The tetrahedral FES consists of four groups of shape functions: nodal shape functions, edge modes, face modes, and internal modes. The m th order tetrahedral Lagrangian basis consists:

1. *Nodal shape functions.* There are 4 nodal shape functions.

$$\begin{aligned}
 N_1(\xi, \eta, \zeta) &= \frac{1}{2}(1 - \xi), \\
 N_2(\xi, \eta, \zeta) &= \frac{1}{2}(\xi - \eta), \\
 N_3(\xi, \eta, \zeta) &= \frac{1}{2}(\eta - \zeta), \\
 N_4(\xi, \eta, \zeta) &= \frac{1}{2}(1 + \zeta).
 \end{aligned} \tag{2.16}$$

These are the standard linear shape functions.

2. *Edge modes.* There are $(m - 1)$ edge modes on each side. They are analogous to the side modes defined for the triangular elements (2.13). For example, the edge modes associated with the edge $d_{1,2}$ are

$$E_i^{1,2}(\xi, \eta, \zeta) = N_1 N_2 \omega_i (N_2 - N_1), \quad i = 2, \dots, m, \quad (2.17)$$

where N_j , $j = 1, 2$, are nodal shape functions defined above, ω_i , $i = 2, \dots, m$, are defined in (2.14). The other edge modes are analogous.

3. *Face modes.* There are $(m - 2)(m - 1)/2$ face modes associated with each face, which are analogous to internal modes defined for the triangular elements. For instance, for the face contains the nodes numbered 1, 2, 3, the face modes are:

$$F_{i,j}^{1,2,3}(\xi, \eta, \zeta) = N_1 N_2 N_3 P_{i-3}(N_2 - N_1) P_{j-3}(2N_3 - 1), \quad (2.18)$$

where $i, j = 3, \dots, m$ and $i + j \leq m + 3$, where P_i are Legendre polynomials of degree i , N_j , $j = 1, 2, 3$, are nodal shape functions. The definition of the other edge modes is analogous.

4. *Internal modes.* There are $(m - 3)(m - 2)(m - 1)/6$ internal modes, defined as follows:

$$I_{i,j,k} = N_1 N_2 N_3 N_4 P_{i-4}(N_2 - N_1) P_{j-4}(2N_3 - 1) P_{k-4}(2N_4 - 1), \quad (2.19)$$

where $i, j, k = 4, \dots, m$ and $i + j + k \leq m + 8$.

The m th order tetrahedral Lagrangian finite element space spanned by the above shape functions is

$$\hat{P}^L = \Pi_m^3(\hat{T}),$$

whose dimension is $\dim \hat{P}^L = (m + 1)(m + 2)(m + 3)/6$.

2.4 A Priori Error Estimates

In this section, we first consider some estimates for the finite element interpolation error. By an application of Céa lemma, the error estimates for FE solution for the boundary value problem (2.1) are obtained.

2.4.1 Error Estimates of Finite Elements Interpolations

In §1.3.2, we have presented a theorem for interpolation error estimates. For every FE introduced in Section 2.3, the error estimates Theorem 1.5 is valid on the corresponding reference FE $(\hat{T}, \hat{P}, \hat{\Sigma})$, where the interpolation operator $\hat{I}$ is defined in (1.9) with the associated $\hat{T}, \hat{P}$, and basis $\{\hat{\varphi}_i\}_{i=1}^N$. Therefore, Theorem 1.5 actually provides us interpolation error estimates on the reference element.

Now, over a general physical element (T, P, Σ) , define the interpolation operator I_T by

$$\hat{I}\hat{v}_h = (I_T v_h) \circ F_T \quad \forall v_h \in P, \quad (2.20)$$

where $\hat{v}_h = v_h \circ F_T$, $F_T : \hat{T} \rightarrow T$ is the affine mapping defined in Definition 2.8. Then a similar result follows.

Theorem 2.12. *Let $m, o \in \mathbb{N}_0$ with $m > 0, m + 1 > o$, and $\Pi_m^n(T) \subseteq P$. Let I_T be the operator defined in (2.20). Then there exists a constant C depending only on $\hat{T}$ and $\hat{I}$ such that*

$$|u - I_T u|_{H^o(T)} \leq C \frac{h_T^{m+1}}{\rho_T^o} |u|_{H^{m+1}(T)} \quad \forall u \in H^{m+1}(T).$$

Moreover, if the FE family is regular, then

$$|u - I_T u|_{H^o(T)} \leq C h_T^{m+1-o} |u|_{H^{m+1}(T)} \quad \forall u \in H^{m+1}(T), \quad \forall T \in \mathcal{T}_h.$$

Theorem 2.12 is proved through the use of the reference element $\hat{T}$ [4]. The method

is referred as the reference element technique. In addition, denote

$$h = \max_{T \in \mathcal{T}_h} h_T,$$

which is often termed as the mesh parameter. Define also a global interpolation operator I_h in the FES $\mathcal{S}_N$ by

$$I_h u|_T = I_T u \quad \forall T \in \mathcal{T}_h.$$

Then a global error estimate result is obtained.

Theorem 2.13. *Assume that all the conditions of Theorem 2.12 hold. Then there exists a constant C independent of h such that*

$$\|u - I_h u\|_{H^o(\Omega)} \leq C h^{m+1-o} |u|_{H^{m+1}(\Omega)} \quad \forall u \in H^{m+1}(\Omega). \quad (2.21)$$

We shall note that the (Lagrangian) interpolation is closely related to superconvergence of FEM [121].

2.4.2 Error Estimates of Finite Elements Solutions

Recall that Céa lemma provides an error estimate in norm $\|\cdot\|_V$ for FE approximations of the elliptic problem (2.1). Note also that $I_h v_h = v_h$ for all $v_h \in \mathcal{S}_N$. Combining Theorem 2.7 and Theorem 2.13, the standard a priori error estimates follows

Theorem 2.14. *Let $V(\Omega)$ be the space defined in (2.2), $\mathcal{S}_N \subseteq V(\Omega)$ be a finite element space, $u_h \in \mathcal{S}_N$ be the finite element approximation of (2.1). Assume that all the conditions of Theorem 2.7 and Theorem 2.13 hold. Assume also $u \in H^{m+1}(\Omega)$ for some $m > 0$. Then there exists a constant C independent of h such that*

$$h \|u - u_h\|_{H^1(\Omega)} + \|u - u_h\|_{H^0(\Omega)} \leq C h^{m+1} |u|_{H^{m+1}(\Omega)}.$$

Follow a standard duality argument, one has

Corollary 2.15. *Assume that all assumptions of Theorem 2.14 hold. Assume also that u is sufficiently smooth. Then, for $s \leq m - 1$, we have estimates*

$$\|u - u_h\|_{H^{-s}(\Omega)} \leq Ch^{m+1+s} |u|_{H^{m+1}(\omega)} .$$

Remark 2.16. From Theorem 2.14 we see that the convergence rate of the finite element approximation is one order higher than the convergence rate of its derivatives.

Remark 2.17. Theorem 2.14 illuminates us with three ways of improving convergence rate of FE solutions. In particular, one could

1. Refine the mesh such that the mesh parameter tends to zero, while keeping m fixed. This is the h -version of the FEM.
2. Increase the degree m of the finite element space while keeping the mesh fixed. This is the p -version of the FEM.
3. Let h tend to zero and increase m simultaneously. This is the hp -version of the FEM.

All these versions of FEM are used widely in practice.

Chapter 3

SUPERCONVERGENCE TECHNIQUES IN FEM

In Chapter 2, we have outlined error estimates of FE solutions of the second order boundary value problem (2.1). Theorem 2.14 says that, when a family of polynomial elements of degree m is employed, the optimal convergence rate for solution value is $m + 1$; and the convergence rate for its derivatives is m .

Nonetheless, it has been observed that at some special a priori points, the convergence rate of FE approximation or its derivatives is higher than what is globally possible. This phenomenon has been termed as superconvergence. The notion "superconvergence" is now used in a much broader sense. The FE solution or its derivatives can be recovered by means of various post-processing techniques and obtain an increase in accuracy. This is also called superconvergence. The first case (without post-processing) is usually referred as natural superconvergence.

The superconvergence phenomenon has been observed in 1960's, e.g. Stricklin [17]. The interesting and important phenomenon brought a new study field of the finite element theory. A systematic study concerning with superconvergence of FEM began in 1970's, see, e.g. [18, 19, 20, 21, 22, 23, 24, 25]. Since then, hundreds of books, monographs, and papers on the subject of superconvergence have been published. See [26, 27, 28, 29, 30, 31, 32, 33, 121, 34, 35, 36, 37, 38, 39, 40] for some recent topics and results in superconvergence. For overviews of the field, the reader is referred to

[41, 10, 42, 43, 44, 45, 46] and references therein.

Superconvergence phenomena have been studied for a wide range of problems. Many superconvergence techniques are developed in the last forty years. Please see [47] for a bibliography of superconvergence techniques. In this chapter, we mainly introduce several techniques for superconvergence with and without post-processing which are closely related to our work. In particular, in Section 3.1, we present superconvergence results obtained from the symmetry theory; in Section 3.2, we discuss the main idea of the "computer-based" method. Finally, for superconvergence by post-processing, we introduce the superconvergence patch recovery and the polynomial-preserving recovery techniques in Section 3.3.

3.1 Superconvergence by Local Symmetry

This method is due to Schatz, Sloan, and Wahlbin [48]. Consider an interior node $\mathbf{x}_0 \in \Omega$. Denote $\mathcal{B}_{2r} = \mathcal{B}(\mathbf{x}_0, 2r) \subset \subset \Omega$ and $\mathcal{B}_r = \mathcal{B}(\mathbf{x}_0, r)$, where r is sufficiently large. Let u be the solution of the weak form (2.3), and u_h be a numerical approximation of u in $\mathcal{V}_h^m$ with mesh size h , where $\mathcal{V}_h^m$ is finite element spaces of degree m . Assume that u and u_h satisfy

$$B(u - u_h, v_h) = 0 \quad \forall v_h \in \mathcal{V}_h^{comp}(\Omega), \quad (3.1)$$

where $B(\cdot, \cdot)$ is defined in (2.4), $\mathcal{V}_h^{comp}(\Omega)$ is the set of functions in $\mathcal{V}_h^m$ with compact support in Ω . Clearly, the FE solution u_h of (2.6) satisfies this assumption. Under various conditions given in [49], an L^∞ estimation of the error $u - u_h$ and its derivatives are obtained as following.

Lemma 3.1. *Let u and u_h satisfy (3.1). Assume that $s \geq 0$ and $1 \leq q \leq \infty$. Then there exists a constant C independent of u, u_h, h, r , and $\mathbf{x}_0$ such that*

$$\|u - u_h\|_{L^\infty(\mathcal{B}_r)} \leq C \left(\ln \frac{r}{h} \right)^{\bar{m}} \min_{v_h \in \mathcal{V}_h^m} \|u - v_h\|_{L^\infty(\mathcal{B}_{2r})} + Cr^{-s-n/q} \|u - u_h\|_{W^{-s,q}(\mathcal{B}_{2r})}.$$

Here $\bar{m} = 1$ if $m = 1$, $\bar{m} = 0$ otherwise.

Lemma 3.2. *Suppose the assumption of Lemma 3.1 are satisfied. Then there exists a constant C independent of u, u_h, h, r , and $\mathbf{x}_0$ such that*

$$\begin{aligned} \|u - u_h\|_{W^{1,\infty}(\mathcal{B}_r)} &\leq C \min_{v_h \in \mathcal{V}_h^m} (|u - v_h|_{W^{1,\infty}(\mathcal{B}_{2r})} + r^{-1} \|u - v_h\|_{L^\infty(\mathcal{B}_{2r})}) \\ &\quad + Cr^{-1-s-n/q} \|u - u_h\|_{W^{-s,q}(\mathcal{B}_{2r})}. \end{aligned}$$

Remark 3.3. Lemma 3.1 provides error estimates of function values of u_h , and Lemma 3.2 provides error estimates of its derivatives. Results for analogous but more general cases has been proved in [50].

The point $\mathbf{x}_0$ is called a local symmetry point, if $v_h \in \mathcal{V}_h^m(\mathcal{B}_r)$, then

$$\bar{v}_h \equiv v_h(\mathbf{x}_0 - (\mathbf{x} - \mathbf{x}_0)) \in \mathcal{V}_h^m(\mathcal{B}_r). \quad (3.2)$$

Also assume that

$$\min_{v_h \in \mathcal{V}_h^m} (\|w - v_h\|_{L^\infty(\mathcal{B}_{r/2})} + h|w - v_h|_{W^{1,\infty}(\mathcal{B}_{r/2})}) \leq Ch^{m+1} |w|_{W^{m+1,\infty}(\mathcal{B}_r)}. \quad (3.3)$$

Then a superconvergent result of function values follows.

Theorem 3.4. *Assume that the condition of Lemma 3.1 hold and that $u - u_h$ satisfies (3.1). Assume that $\|u - u_h\|_{W^{-s,q}(\Omega)} \leq Ch^{m+1+\tau}$ with $\tau > 0$, and the symmetry assumption (3.2) with $r = h^\sigma, \sigma = \tau/(s + n/q + 1) \leq 1$. Furthermore, if m is even, if approximation assumption (3.3), and if $u \in W^{m+2,\infty}(\mathcal{B}_r)$, then there exists a constant C independent of $\mathbf{x}_0$ and h such that*

$$|(u - u_h)(\mathbf{x}_0)| \leq Ch^{m+1+\sigma}.$$

Analogously, one has analogous superconvergent results of derivatives.

Theorem 3.5. *Assume that the condition of Lemma 3.2 hold and that $u - u_h$ satisfies (3.1). Assume also that $\|u - u_h\|_{W^{-s,q}(\Omega)} \leq Ch^{m+\tau'}$ with $\tau' > 0$, and the symmetry assumption (3.2) with $r = h^{\sigma'}, \sigma' = \tau'/(s + n/q + 2) \leq 1$. Furthermore, if m is odd, if approximation assumption (3.3), and if $u \in W^{m+2,\infty}(\mathcal{B}_r)$, then there exists a constant*

C independent of $\mathbf{x}_0$ and h such that

$$\left| \nabla u(\mathbf{x}_0) - \hat{\nabla} u_h(\mathbf{x}_0) \right| \leq Ch^{m+\sigma'},$$

where $\hat{\nabla} u_h(\mathbf{x}_0) = \frac{1}{2} \left(\lim_{\varepsilon \rightarrow 0+} \nabla u_h(\mathbf{x}_0 + \varepsilon \beta) + \lim_{\varepsilon \rightarrow 0-} \nabla u_h(\mathbf{x}_0 + \varepsilon \beta) \right)$, β is any unit vector in $\mathbb{R}^n$.

Remark 3.6. Comparing with Theorem 2.14, one gets the following conclusions. When m is even, the convergence rate of FE approximations of function values at the local symmetry points is σ order higher than the global rate. On the other hand, when m is odd, the convergence rate of its derivatives is σ' order higher than the global rate.

Remark 3.7. As we shall see later, local symmetry assumption is a sufficient condition for superconvergence, but not necessary. In fact, there are many superconvergent points which are not local symmetry points.

3.2 Generalized "Computer-based" Method

The method was developed by Babuška *et al.* [51] in finding derivative superconvergent points. Here we outline the method by following the description provided by Wahlbin [45]. The framework is generalized for problems of dimension $n = 1, 2$, or 3 .

The main hypotheses in [51] are: (a) there is no roundoff error; (b) the mesh is locally translation invariant; (c) the solution is sufficiently smooth locally and the pollution error is under control.

Assume that the FE mesh in Ω is locally translation invariant near $\mathbf{x}_0$. To be more precise, we suppose that the FE partition in Ω is based on a translation invariant uniform n -cell mesh near $\mathbf{x}_0$, in which each n -cell contains one or more elements.

Denote a cell centered at $\mathbf{x}_0 = (x_1, \dots, x_n) \in \Omega$ with side $2l$ as $c(\mathbf{x}_0, l) = \{y \in \Omega \mid |y_i - x_i| \leq l, i = 1, \dots, n\}$. Let $c(\mathbf{x}_0, h)$ be the master cell. Let $\Omega_1 = c(\mathbf{x}_0, H)$ and $\Omega_0 = c(\mathbf{x}_0, 2H)$ be two regions in Ω with $H = h^\delta, 0 < \max(\delta, n\delta/2) < 1$. For simplicity, assume that the $2h$ -periodic extensions of the master cell $c(\mathbf{x}_0, h)$ fit these two regions exactly.

Let u be sufficiently smooth, u_h be the polynomial FE approximation of u of degree m . Assume u and u_h satisfy (3.1). For $m \geq 1$, assume also that

$$\|u - u_h\|_{L^\infty(\Omega_0)} \leq Ch^{m+1-L}, \quad (3.4)$$

with $L \geq 0$ and $\max(L + \delta, L + n\delta/2) < 1$. This assumption implies that pollution effects from outside of the domain Ω_0 have been properly controlled and the error loss is of order h^L . Moreover, for $m > 1$, we may assume that

$$\|u - u_h\|_{W^{-1,\infty}(\Omega_0)} \leq Ch^{m+2-\Lambda}, \quad (3.5)$$

with $\Lambda \geq 0$ and $\Lambda + \delta < 1$.

Let Q denote the $(m+1)$ th order Taylor expansion of u at $\mathbf{x}_0$. Then

$$\|u - Q\|_{W^{s,\infty}(\Omega_0)} \leq Ch^{m+2-s}, \quad 0 \leq s \leq m+2. \quad (3.6)$$

Let I_h be the standard interpolation operator into $\mathcal{V}_h^m(\Omega_0)$, and set $\rho = Q - I_h Q$. Let $\mathcal{V}_h^\pi(c(\mathbf{x}_0, h))$ denote the $2h$ -periodic functions in $\mathcal{V}_h^m(c(\mathbf{x}_0, h))$. Define a projection operator $PP(\rho) \in \mathcal{V}_h^\pi(c(\mathbf{x}_0, h))$ by

$$\int_{c(\mathbf{x}_0, h)} (\rho - PP(\rho)) \, d\Omega = 0 \quad (3.7)$$

$$B_{c(\mathbf{x}_0, h)}(\rho - PP(\rho), v_h) = 0 \quad \forall \mathcal{V}_h^\pi(c(\mathbf{x}_0, h)). \quad (3.8)$$

Also denote $H^{1,\pi}(\Omega_0)$ the $2h$ -periodic functions in $H^1(\Omega_0)$. The key observation in [51] is that ρ is in $H^{1,\pi}(\Omega_0)$. Moreover, one has [45]

Lemma 3.8. *For all $\varrho \in H^{1,\pi}(\Omega_0)$, we have*

$$B(\varrho - PP(\varrho), v_h) = 0 \quad \forall v_h \in \mathcal{V}_h^{comp}(\Omega_0). \quad (3.9)$$

Clearly, ρ satisfies (3.9). Put $\omega = \rho - PP(\rho)$. We have the following local estimates of error in derivatives, which is a generalization of the corresponding theorem in [51]. See also [45].

Theorem 3.9. *For $m \geq 1$, we have*

$$\frac{\partial}{\partial x_i}(u - u_h)(\mathbf{x}) = \frac{\partial \omega}{\partial x_i}(\mathbf{x}) + R_i(\mathbf{x}), \quad i = 1, \dots, n, \quad \mathbf{x} \in \Omega_1,$$

where

$$\|R_i\|_{L^\infty(\Omega_1)} \leq C(h^{m+\delta} + h^{m+1-L-\delta} + h^{m+1-L-n\delta/2}).$$

Theorem 3.9 provides estimates of errors for derivatives of FE solutions. An analogue theorem of errors in function values is established as following.

Theorem 3.10. *For $m > 1$, we have*

$$(u - u_h)(\mathbf{x}) = \omega(\mathbf{x}) + R(\mathbf{x}), \quad \mathbf{x} \in \Omega_1,$$

where

$$\|R\|_{L^\infty(\Omega_1)} \leq Ch^{m+1+\delta} + Ch^{m+2-\Lambda-\delta}.$$

Remark 3.11. Theorem 3.9 and 3.10 for two-dimensional cases are proved in [51, 45] and [52], respectively.

Remark 3.12. The condition $m > 1$ is essential in Theorem 3.10. Since the assumption (3.5) does not hold in general when $m = 1$.

Remark 3.13. Theorem 3.9 states that the major part of the FE approximation error in the derivatives is measured by $\partial\omega/\partial x_i(\mathbf{x})$, since the convergence rate of the remainder is of an order $\min(\delta, 1 - L - \delta, 1 - L - n\delta/2)$ higher than the global convergence rate, provided $\max(L + n\delta/2, L + \delta) < 1$. Similarly, Theorem 3.10 indicates that, for $m > 1$, ω gives the main error in function values. The convergence rate of the remainder is of an order $\min(\delta, 1 - \Lambda - \delta)$ higher than the global rate, provided $\Lambda + \delta < 1$.

Remark 3.14. Notice that ρ is $2h$ -periodic. Therefore, the task of finding superconvergent points can be narrowed down in the master cell, or equivalently in a reference

cell $T = [-1, 1]^n$. The superconvergent points of x_i -derivative (resp. function value) are those points $\hat{\mathbf{x}}$ such that $\partial\omega/\partial x_i(\hat{\mathbf{x}}) = 0$ (resp. $\omega(\hat{\mathbf{x}}) = 0$). We conclude from Remark 3.13 that to identify the m th order FE superconvergent points in T , it is equivalent to find the critical points and zeros of some periodic piecewise polynomials ω of degree $m + 1$ in T such that

$$\int_T \omega \, dT = 0, \quad \int_T \nabla \omega \cdot \nabla v_h \, dT = 0 \quad \forall v_h \in \mathcal{V}_m^\pi(T), \quad (3.10)$$

where $\mathcal{V}_m(T)$ and $\mathcal{V}_m^\pi(T)$ are the FE local space and the periodic FE local space of order m defined on the reference cell T , respectively.

Remark 3.15. As described in Remark 3.14, Theorem 3.9 and 3.10 reduce the problem of finding superconvergent points to the problem of finding intersections of certain polynomial contours. In [51], the actual derivative superconvergent points were located by computer programs without explicitly constructing those polynomials. That is why the method is referred as the "computer-base" method.

3.3 Superconvergence by Post-processing

The local symmetry theory and the computer-based method provide natural superconvergence results in an interior subdomain (local superconvergence). There are various post-processing techniques which increase accuracy in the whole domain (global superconvergence), cf. e.g. [10, 47, 53, 54]. In this section, we briefly introduce the superconvergent patch recovery (SPR) and the polynomial-preserving recovery (PPR) techniques.

3.3.1 Superconvergence Patch Recovery

The SPR procedure was introduced by Zienkiewicz and Zhu in 1992 [55, 56, 57]. It has been recommended as one of the best procedures which is simple to implement [41, 58].

The SPR is utilized for derivatives (gradients and stresses). Suppose that the

derivatives sampled at certain points in an element of degree m possess the superconvergent property and have errors of order $O(h^{m+1})$. The idea of the SPR is to involve a smoothing of the sampled values by a polynomial of degree m within a patch of elements for which the number of sampling points is greater than the number of parameters in the polynomial. This polynomial is made to fit the superconvergent sample points in a least square manner, which hence has superconvergent accuracy everywhere.

For instance, consider an element patch that shares a common vertex (assembly point). We recover the i th component u_i of the gradient ∇u from the m th degree FE solution $u_h, i = 1, \dots, n$. Select a set of sampling points $\{\mathbf{x}^k\}_{k=1}^M$ in the patch, at which superconvergence of the corresponding derivative occurs. Writing the recovered solution as

$$(G_h u_h)_i = \mathbf{p}(\mathbf{x}) \mathbf{a}_i = [1, x_1, \dots, x_n, x_1^2, \dots, x_n^m] [a_{i,1}, a_{i,2}, \dots, a_{i,\Gamma_m^n}]^T$$

and minimize (least square fit)

$$\sum_{k=1}^M [(u_h)_i(\mathbf{x}^k) - \mathbf{p}(\mathbf{x}^k) \mathbf{a}_i]^2,$$

where G_h is the gradient recovery operator, $(G_h u_h)_i$ is the i th component of the recovered gradient $G_h u_h$, $(u_h)_i$ is the x_i -derivative of the FE solution u_h , Γ_m^n is the dimension of $\prod_m^n$, and $M > \Gamma_m^n$. $(G_h u_h)_i$ is obtained with the coefficient vector

$$\mathbf{a}_i = \mathbf{A}_i^{-1} \mathbf{b}_i,$$

where

$$\begin{aligned} \mathbf{A}_i &= \sum_{k=1}^M \mathbf{p}_i(\mathbf{x}^k)^T \mathbf{p}_i(\mathbf{x}^k), \\ \mathbf{b} &= \sum_{k=1}^M \mathbf{p}_i(\mathbf{x}^k)^T (u_h)_i(\mathbf{x}^k). \end{aligned}$$

Then superconvergence of u_i is achieved throughout each element.

The effectiveness of superconvergence by the SPR has been mathematically proved [46, 59, 60, 61, 62]. Moreover, under particular conditions, two order increase of convergence rate can be obtained [63, 64, 65] for derivatives. This phenomena is termed as ultra-convergence.

The SPR can be extended to produce superconvergent function values. In this case, the recovered polynomials should be one degree higher than those used for the shape functions.

Many investigators have modified the procedure by increasing the functional where the least square fit is performed to include satisfaction of discrete equilibrium equations or boundary conditions, etc. See, e.g. [66, 67].

We shall note that the SPR technique described above depends on the knowledge of superconvergence property of the FE solutions and the availability of the optimal sampling points. We notice also that, when superconvergent points do not in fact exist, a recovery by equilibration of patches (REP) technique has been presented to achieve superconvergence [68, 69]. However, mathematical proof for effectiveness of REP is required. Therefore, for high degree element, we need to study natural superconvergence to apply SPR.

3.3.2 Polynomial-Preserving Recovery

Zhang and Naga have recently proposed a new recovery technique, the polynomial preserving recovery [70, 71, 72, 73].

Given a finite element space of degree m , instead of fitting a polynomial of degree m to gradients at the sampling points on element patches as the SPR does, the PPR fits a polynomial of degree $m + 1$ to solution values at some nodal points, and then takes derivatives to obtain recovered gradient at each assembly points. The PPR is superconvergent for FES of any order. They showed that the PPR possesses all known superconvergence and ultra-convergence properties of the SPR method, and is applicable to arbitrary grids with cost comparable to the SPR. In computer implementation, there is no significant difference between least-squares fitting a polynomial

of degree m or degree $m+1$, compared with the overall cost in finite element solution.

Chapter 4

LOCAL ERROR EXPANSION FORMULA AND SUPERCONVERGENCE ON PAR6

In this chapter, our first development is to deduce a local error expansion formula that is uniform in n dimensional space ($n \geq 3$). The degenerative form for two dimensional space can be found in [26]. Since the normal component of the gradients of the test functions is discontinuous, it is difficult to combine elementwise error estimates together. Thus following the idea in [26], we derive an element error expansion formula that involves only the tangential derivative of the test function on the edges.

We then take the step by giving the theoretical analysis of superconvergence property on a particular centroidal Voronoi tessellation (CVT) structure: Par6 tessellation. The details of Par6 are presented in section 4.2. Following the pioneer work [74, 75], we first present the result that the gradient of the linear finite element approximation u_h is superconvergent to the gradient of the piecewise linear interpolant u_I of the solution u . More precisely, we have

$$\|u_h - u_I\|_{1,\Omega} \lesssim h^2 \|u\|_{3,\infty,\Omega}.$$

Here the convergence order is approximately $1/2$ higher than general cases on general CVT meshes because of the highly symmetric structure of Par6 tessellation. The low order terms in the asymptotic expansion of the local error are totally canceled on Par6 structure. The errors on the boundary are also treated in this estimation. The second major part of this proof is that the gradient recovered by SPR is superconvergent to true gradient, that is to say

$$\|\nabla u - G_h u_h\|_{0,\Omega} \lesssim h^2 \|u\|_{3,\infty,\Omega},$$

where G_h is the SPR recovery operator. Both the superconvergence and the gradient recovery results are for a non-self-adjoint and possibly indefinite problem.

The rest of this chapter is organized as follows. The notations that will be used in this chapter are introduced in Section 4.1. A local error expansion formula in n -dimensional space is deduced in Section 4.2. A detailed introduction of Par6 tessellation is given in Section 4.3. The theoretical proof of superconvergence property on Par6 tessellation is presented in Section 4.4. And in Section 4.5, numerical example is presented to verify the theoretical result.

4.1 Preliminaries

The non-self-adjoint and possibly indefinite problem is considered: find $u \in H^1(\Omega)$ such that

$$B(u, v) = \int_{\Omega} (\mathcal{D} \nabla u + \mathbf{b}u) \cdot \nabla v + cuv \, dx = f(v) \quad (4.1)$$

for all $v \in H^1(\Omega)$. Here $\mathcal{D}$ is a $n \times n$ symmetric positive definite matrix, $\mathbf{b}$ a vector, and c a scalar, and $f(\cdot)$ is a linear functional. We assume that all the coefficient functions are smooth.

In order to insure that (4.1) has a unique solution, we assume that the eigenvalues of $\mathcal{D}$ satisfy $0 < \mu < \lambda_{\min} < \lambda_{\max} < \nu$ uniformly in Ω . Let $\mathcal{V}_h \subset H^1(\Omega)$ be the space of continuous piecewise linear polynomials associated with a quasi-uniform triangulation

Figure 4.1: The vertex-first projection of a 4-simplex.

$\mathcal{T}_h$, and consider the approximate problem: find $u_h \in \mathcal{V}_h$ such that

$$B(u_h, v_h) = f(v_h) \quad (4.2)$$

for all $v_h \in \mathcal{V}_h$. Here $\mathcal{V}_h$ denotes piecewise linear finite element spaces and this holds for the rest of this thesis. The following result is standard in FEM

$$\|u - u_h\|_{1,\Omega} \leq \frac{\nu}{\mu} \inf_{v_h \in \mathcal{V}_h} \|u - v_h\|_{1,\Omega}.$$

We define the piecewise constant matrix function $\mathcal{D}_\tau$ in terms of the diffusion matrix D as follows:

$$\mathcal{D}_{\tau ij} = \frac{1}{|\tau|} \int_{\tau} \mathcal{D}_{ij} \, dx.$$

Note that $\mathcal{D}_\tau$ is symmetric and positive definite.

We consider a n -simplex τ in n dimensional space ($n \geq 3$) with $n + 1$ nodes denoted by $\{\mathbf{p}_k\}_{k=1}^{n+1}$ and the corresponding coordinates are $(x_{1k}, x_{2k}, \dots, x_{nk})$ for $k = 1, 2, \dots, n + 1$. A 4-simplex is shown in Figure 4.1. Let e_{ij} denote the oriented edges

of element τ from $\mathbf{p}_i$ to $\mathbf{p}_j$ and $\mathbf{t}_{ij}, d_{ij}$ the corresponding unit tangent vectors and edge length, respectively. Let $\mathbf{F}_k$ denote the facet opposite vertex $\mathbf{p}_k$, which is a hyperplane in n dimensional space, and the outer normal vector $\mathbf{n}_k$ of $\mathbf{F}_k$ is defined by

$$\begin{aligned}\mathbf{n}_k \cdot (\mathbf{p}_l - \mathbf{p}_m) &= 0, \text{ for } m \in \{1, 2, \dots, n+1\}, l = 1, 2, \dots, n+1, l \neq k, m \\ |\mathbf{n}_k| &= 1.\end{aligned}$$

The volume of the n -simplex is given by

$$n!V = \left| \det \begin{pmatrix} 1 & x_{11} & x_{21} & \cdots & x_{n1} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & x_{1(n+1)} & x_{2(n+1)} & \cdots & x_{n(n+1)} \end{pmatrix} \right|.$$

Thus the barycentric coordinates $\{\varphi_k\}_{k=1}^{n+1}$ are defined by

$$\varphi_k = \frac{n!V_k}{n!V} = \frac{V_k}{V}, \quad (4.3)$$

where V_k is defined by replacing the k th row of V with $(1, x_1, x_2, \dots, x_n)$. Let $\mathcal{D}_\tau$ be a constant symmetric $n \times n$ matrix defined on τ . We define $\xi_{ij} = \mathbf{n}_i \cdot \mathcal{D}_\tau \mathbf{n}_j$. Since $\mathcal{D}_\tau$ is symmetric, $\xi_{ij} = \xi_{ji}$.

4.2 Local error expansion formula in n dimensional space

In this section, we derive a local error expansion formula in n dimensional space, where n is the dimension of the space.

Lemma 4.1.

$$\nabla \phi \cdot \mathcal{D}_\tau \mathbf{n}_k = \sum_{l=1, l \neq k}^{n+1} \frac{\xi_{kl}}{\mathbf{n}_l \cdot \mathbf{t}_{kl}} \frac{\partial \phi}{\partial \mathbf{t}_{kl}}.$$

Proof. It follows

$$\mathcal{D}_\tau \mathbf{n}_k = \sum_{l=1, l \neq k}^{n+1} \frac{\mathbf{n}_l \cdot \mathcal{D}_\tau \mathbf{n}_k}{\mathbf{n}_l \cdot \mathbf{t}_{kl}} \mathbf{t}_{kl}.$$

In the above formula, $\mathbf{n}_l, \mathbf{n}_k, \mathbf{t}_{kl}$ can be expressed with the vertex coordinates explicitly and $\mathcal{D}_\tau$ is a constant matrix in n -simplex τ . Thus it is a directly computational result. $\square$

The following two Lemmas are analogous to the results in [75, Lemma 2.2 and Lemma 2.3].

Lemma 4.2. *Let ϕ_q be a quadratic polynomial and ϕ_I the continuous piecewise linear interpolant for ϕ_q on τ . Then for a constant vector $\mathbf{t}$,*

$$\int_\tau \nabla(\phi_I - \phi_q) \cdot \mathbf{t} = \frac{1}{2} \sum_{k=1}^{n+1} \mathbf{n}_k \cdot \mathbf{t} \int_{\mathbf{F}_k} \sum_{i,j=1, i < j}^{n+1} d_{ij}^2 \varphi_i \varphi_j \frac{\partial^2 \phi_q}{\partial \mathbf{t}_{ij}^2}.$$

Proof. By the Taylor expansion,

$$(\phi_I - \phi_q) = \frac{1}{2} \sum_{k=1}^{n+1} \varphi_k(\mathbf{x} - \mathbf{p}_k) \cdot \nabla^2 \phi_q(\mathbf{x} - \mathbf{p}_k).$$

Noticing the identity $\mathbf{x} - \mathbf{p}_k = \sum_{i=1, i \neq k}^{n+1} \varphi_i e_{ki}$, which is a computational result, holds in n dimensional space, the desired result follows from Green's formula. $\square$

Lemma 4.3. *For a function $\phi \in W^{1,1}(\tau)$ we have*

$$\begin{aligned} \frac{1}{\mathbf{n}_k \cdot \mathbf{t}_{lk}} \int_{\mathbf{F}_l} \varphi_k \varphi_m \phi - \frac{1}{\mathbf{n}_l \cdot \mathbf{t}_{kl}} \int_{\mathbf{F}_k} \varphi_l \varphi_m \phi &= \frac{1}{\mathbf{n}_k \cdot \mathbf{t}_{lk}} \frac{1}{\mathbf{n}_l \cdot \mathbf{t}_{kl}} \int_\tau (\varphi_k + \varphi_l) \varphi_m \frac{\partial \phi}{\partial \mathbf{t}_{kl}}, \\ \frac{1}{\mathbf{n}_k \cdot \mathbf{t}_{lk}} \int_{\mathbf{F}_l} \phi - \frac{1}{\mathbf{n}_l \cdot \mathbf{t}_{kl}} \int_{\mathbf{F}_k} \phi &= \frac{1}{\mathbf{n}_k \cdot \mathbf{t}_{lk}} \frac{1}{\mathbf{n}_l \cdot \mathbf{t}_{kl}} \int_\tau \frac{\partial \phi}{\partial \mathbf{t}_{kl}}, \\ \frac{1}{\mathbf{n}_k \cdot \mathbf{t}_{lk}} \int_{\mathbf{F}_l} \varphi_k \varphi_o &= \frac{1}{\mathbf{n}_l \cdot \mathbf{t}_{kl}} \int_{\mathbf{F}_k} \varphi_l \varphi_m, \end{aligned}$$

where φ_k is the barycentric coordinate of node $\mathbf{p}_k$ defined in (4.3).

Proof. By Green's formula,

$$\begin{aligned}\int_{\tau} \nabla(fu) \cdot \mathbf{t}_{kl} &= \mathbf{n}_k \cdot \mathbf{t}_{kl} \int_{\mathbf{F}_k} fu + \mathbf{n}_l \cdot \mathbf{t}_{kl} \int_{\mathbf{F}_l} fu \\ &= -\mathbf{n}_k \cdot \mathbf{t}_{lk} \int_{\mathbf{F}_k} fu + \mathbf{n}_l \cdot \mathbf{t}_{kl} \int_{\mathbf{F}_l} fu.\end{aligned}$$

Then set $f = (\varphi_k + \varphi_l)\varphi_m$ to get the first identity we want, where we use the facts $f|_{\mathbf{F}_k} = \varphi_l\varphi_m$, $f|_{\mathbf{F}_l} = \varphi_k\varphi_m$ and f is a constant along lines parallel to $\mathbf{t}_{kl}$, since $f = (1 - \sum_{i=1, i \neq k, l}^{n+1} \varphi_i)\varphi_m$. The second identity is obtained by setting $f = 1$.

The third equality is a direct computational result, where o is a vertex index different from k, l, m . The volume of a n -simplex τ is calculated by

$$\begin{aligned}n |\tau| &= |\mathbf{F}_k| |d_{kl}| \mathbf{n}_k \cdot \mathbf{t}_{kl} \\ &= |\mathbf{F}_l| |d_{kl}| \mathbf{n}_l \cdot \mathbf{t}_{lk},\end{aligned}$$

thus

$$|\mathbf{F}_k| \frac{1}{\mathbf{n}_l \cdot \mathbf{t}_{kl}} = |\mathbf{F}_l| \frac{1}{\mathbf{n}_k \cdot \mathbf{t}_{lk}}.$$

As a consequence, the following identity holds

$$\begin{aligned}\frac{1}{\mathbf{n}_l \cdot \mathbf{t}_{kl}} \int_{\mathbf{F}_k} \varphi_l \varphi_m &= \frac{1}{\mathbf{n}_l \cdot \mathbf{t}_{kl}} |\mathbf{F}_k| \frac{1}{n(n+1)} \\ &= \frac{1}{\mathbf{n}_k \cdot \mathbf{t}_{lk}} |\mathbf{F}_l| \frac{1}{n(n+1)} = \frac{1}{\mathbf{n}_k \cdot \mathbf{t}_{lk}} \int_{\mathbf{F}_l} \varphi_k \varphi_o.\end{aligned}$$

□

The following identity for triangle $\triangle_{klm}$ [26] is used in the next lemma.

$$d_{lm}^2 \frac{\partial^2 \phi}{\partial \mathbf{t}_{lm}^2} - d_{km}^2 \frac{\partial^2 \phi}{\partial \mathbf{t}_{km}^2} = (d_{lm}^2 - d_{km}^2) \frac{\partial^2 \phi}{\partial \mathbf{t}_{kl}^2} + 4 |\triangle_{klm}| \frac{\partial^2 \phi}{\partial \mathbf{t}_{kl} \partial \mathbf{n}_{kl,m}}, \quad (4.4)$$

where $\mathbf{n}_{kl,m}$ is the unit outward normal vector of edge $\mathbf{t}_{kl}$ on the supporting plane of triangle $\triangle_{klm}$.

Lemma 4.4. *Let ϕ_q be a quadratic polynomial and $v_h \in \mathcal{V}_h$. Then we have*

$$\begin{aligned}
& \int_{\tau} \nabla(\phi_I - \phi_q) \cdot \mathcal{D}_{\tau} \nabla v_h \\
&= \sum_{k,l=1, k \neq l}^{n+1} \frac{\partial v_h}{\partial \mathbf{t}_{kl}} \frac{\xi_{kl}}{4 \mathbf{n}_l \cdot \mathbf{t}_{kl}} \left(\sum_{m=1, m \neq k, l}^{n+1} \int_{\mathbf{F}_k} \varphi_l \varphi_m [(d_{lm}^2 - d_{km}^2) \frac{\partial^2 \phi_q}{\partial \mathbf{t}_{kl}^2} \right. \\
&\quad \left. + 4 |\Delta_{klm}| \frac{\partial^2 \phi_q}{\partial \mathbf{t}_{kl} \partial \mathbf{n}_{kl,m}}] \right).
\end{aligned}$$

Proof. Using Lemma 4.1 and 4.2, we have

$$\begin{aligned}
& \int_{\tau} \nabla(\phi_I - \phi_q) \cdot \mathcal{D}_{\tau} \nabla v_h \\
&= \frac{1}{2} \sum_{k=1}^{n+1} \nabla v_h \cdot \mathcal{D}_{\tau} \mathbf{n}_k \int_{\mathbf{F}_k} \sum_{i,j=1, i < j}^{n+1} d_{ij}^2 \varphi_i \varphi_j \frac{\partial^2 \phi_q}{\partial \mathbf{t}_{ij}^2} \\
&= \sum_{k,l=1, k \neq l}^{n+1} \int_{\mathbf{F}_k} \frac{\partial v_h}{\partial \mathbf{t}_{kl}} \frac{\xi_{kl}}{2 \mathbf{n}_l \cdot \mathbf{t}_{kl}} \sum_{i,j=1, i < j}^{n+1} d_{ij}^2 \varphi_i \varphi_j \frac{\partial^2 \phi_q}{\partial \mathbf{t}_{ij}^2} \\
&= \sum_{k,l=1, k \neq l}^{n+1} \left[\frac{\partial v_h}{\partial \mathbf{t}_{kl}} \frac{\xi_{kl}}{4 \mathbf{n}_l \cdot \mathbf{t}_{kl}} \int_{\mathbf{F}_k} \sum_{i,j=1, i < j}^{n+1} d_{ij}^2 \varphi_i \varphi_j \frac{\partial^2 \phi_q}{\partial \mathbf{t}_{ij}^2} \right. \\
&\quad \left. + \frac{\partial v_h}{\partial \mathbf{t}_{lk}} \frac{\xi_{kl}}{4 \mathbf{n}_k \cdot \mathbf{t}_{lk}} \int_{\mathbf{F}_l} \sum_{i,j=1, i < j}^{n+1} d_{ij}^2 \varphi_i \varphi_j \frac{\partial^2 \phi_q}{\partial \mathbf{t}_{ij}^2} \right] \\
&= \sum_{k,l=1, k \neq l}^{n+1} \left(\sum_{j=1}^{\frac{(n-1)(n-2)}{2}} I_j + \sum_{i=1}^{n-1} I_i \right),
\end{aligned}$$

where

$$\begin{aligned}
I_j &= \frac{\partial v_h}{\partial \mathbf{t}_{kl}} \frac{\xi_{kl}}{4} \left(\frac{1}{\mathbf{n}_l \cdot \mathbf{t}_{kl}} \int_{\mathbf{F}_k} d_{mo}^2 \varphi_m \varphi_o \frac{\partial^2 \phi_q}{\partial \mathbf{t}_{mo}^2} \right. \\
&\quad \left. - \frac{1}{\mathbf{n}_k \cdot \mathbf{t}_{lk}} \int_{\mathbf{F}_l} d_{mo}^2 \varphi_m \varphi_o \frac{\partial^2 \phi_q}{\partial \mathbf{t}_{mo}^2} \right), \text{ for } j = 1, 2, \dots, \frac{(n-1)(n-2)}{2},
\end{aligned}$$

and

$$I_i = \frac{\partial v_h}{\partial \mathbf{t}_{kl}} \frac{\xi_{kl}}{4} \left(\frac{1}{\mathbf{n}_l \cdot \mathbf{t}_{kl}} \int_{\mathbf{F}_k} d_{lm}^2 \varphi_l \varphi_m \frac{\partial^2 \phi_q}{\partial \mathbf{t}_{lm}^2} \right. \\ \left. - \frac{1}{\mathbf{n}_k \cdot \mathbf{t}_{lk}} \int_{\mathbf{F}_l} d_{km}^2 \varphi_k \varphi_m \frac{\partial^2 \phi_q}{\partial \mathbf{t}_{km}^2} \right), \text{ for } i = 1, 2, \dots, n-1.$$

Here we patch the terms in $\int_{\mathbf{F}_k} \sum_{i,j=1, i < j}^{n+1} d_{ij}^2 \varphi_i \varphi_j \frac{\partial^2 \phi_q}{\partial \mathbf{t}_{ij}^2}$ and $\int_{\mathbf{F}_l} \sum_{i,j=1, i < j}^{n+1} d_{ij}^2 \varphi_i \varphi_j \frac{\partial^2 \phi_q}{\partial \mathbf{t}_{ij}^2}$ one on one. For I_j , the subscripts m, o are chosen to be different from k, l , so there are $C_{n-1}^2 = \frac{(n-1)(n-2)}{2}$ terms totally. For I_i , one subscript is fixed to be k on $\int_{\mathbf{F}_l}$ and l on $\int_{\mathbf{F}_k}$ and the other subscript is chosen to be different from k, l , so the total number of terms is $C_{n-1}^1 = n-1$.

By Lemma 4.3 and identity (4.4), we obtain

$$I_j = 0, \\ I_i = \frac{\partial v_h}{\partial \mathbf{t}_{kl}} \frac{\xi_{kl}}{4 \mathbf{n}_l \cdot \mathbf{t}_{kl}} \left(\int_{\mathbf{F}_k} \varphi_l \varphi_m \left[(d_{lm}^2 - d_{km}^2) \frac{\partial^2 \phi_q}{\partial \mathbf{t}_{kl}^2} + 4 |\Delta_{klm}| \frac{\partial^2 \phi_q}{\partial \mathbf{t}_{kl} \partial \mathbf{n}_{kl,m}} \right] \right), \\ = \frac{\partial v_h}{\partial \mathbf{t}_{lk}} \frac{\xi_{kl}}{4 \mathbf{n}_k \cdot \mathbf{t}_{lk}} \left(\int_{\mathbf{F}_l} \varphi_k \varphi_m \left[(d_{km}^2 - d_{lm}^2) \frac{\partial^2 \phi_q}{\partial \mathbf{t}_{lk}^2} + 4 |\Delta_{lkm}| \frac{\partial^2 \phi_q}{\partial \mathbf{t}_{lk} \partial \mathbf{n}_{lk,m}} \right] \right).$$

Hence, the lemma follows. $\square$

Remark 4.5. Noticing here I_i can be written as an integral on facet $\mathbf{F}_k$ or an integral on facet $\mathbf{F}_l$, it allows us to write the local error expansion formula in different forms to eliminate the lowest order terms.

From Lemma 4.4, using the standard scaling argument and the Bramble-Hilbert Lemma on the reference element, we obtain the following result.

Figure 4.2: Par6 tessellation.

Lemma 4.6. *Let $\phi \in H^3(\tau)$, $v_h \in \mathcal{V}_h$, then we have*

$$\begin{aligned}
& \int_{\tau} \nabla(\phi_I - \phi) \cdot \mathcal{D}_{\tau} \nabla v_h \\
&= \sum_{k,l=1,k \neq l}^{n+1} \frac{\partial v_h}{\partial \mathbf{t}_{kl}} \frac{\xi_{kl}}{4\mathbf{n}_l \cdot \mathbf{t}_{kl}} \left(\sum_{m=1,m \neq k,l}^{n+1} \int_{\mathbf{F}_k} \varphi_l \varphi_m [(d_{lm}^2 - d_{km}^2) \frac{\partial^2 \phi}{\partial \mathbf{t}_{kl}^2} \right. \\
&\quad \left. + 4 |\triangle_{klm}| \frac{\partial^2 \phi}{\partial \mathbf{t}_{kl} \partial \mathbf{n}_{kl,m}}] \right) + O(h^3) \|\phi\|_{3,\tau} \|v_h\|_{1,\tau}.
\end{aligned}$$

4.3 Par6 pattern: the optimal Centroidal Voronoi tessellation in three dimensional spaces

Par6 pattern is a assembly which can be repeated indefinitely to fill space [76]. Different from two dimensional case, regular tetrahedrons, unlike equilateral triangles, can not be fitted together to fill space. Par6 assembly is obtained by distorting a cube into a parallelepiped involving a 35.3° rotation of the edges about the y- and z-axis. And then each parallelepiped is divided into six identical tetrahedrons. Furthermore, the four faces of these tetrahedrons are all the same—an isosceles triangle with one edge of length p and the other two of length $\sqrt{3}p/2$. Repeating this assembly to get Par6 tessellation (see Figure 4.2).

Par6 based centroidal Voronoi Tessellation has the lowest energy per unit volume and is the most likely congruent cell predicted by the three-dimensional Gershgorin's conjecture [77]. Given a density function ρ , a tessellation $V = \{V_i\}_1^N$ of the domain

Ω and a set of points $Z = \{z_i\}_1^N$ in Ω , we can define the following cost functional:

$$\mathcal{F}(V, Z) = \sum_{i=1}^N F(V_i, z_i), \quad \text{where } F(V_i, z_i) = \int_{V_i} \rho(x) \|x - z_i\|^2 dx.$$

The energy per unit volume (E_p) for a partition or tessellation $\{V, Z\}$ is then defined by:

$$D(V, Z) = \frac{N^{2/n} \mathcal{F}(V, Z)}{n |\Omega|^{1+2/n}}.$$

Here, n is the dimension of the space, and $|\Omega|$ is the volume of $\Omega = \bigcup_{i=1}^N V_i$.

For a given bounded domain Ω together with a specified density function and a fixed number of generator, an *optimal CVT* is defined as a global minimum of $\mathcal{F}(V, Z)$, while the optimal centroidal Voronoi tessellation in a given Euclidean-dimensional space (e.g., the two-dimensional space), asymptotically speaking, is defined as the CVT which has the lowest energy per unit volume among all CVTs that cover the whole space (as the number of generators going to infinity).

The optimal CVT concept is closely related to the Gersho's conjecture [78], which states that: *asymptotically speaking, all cells of the optimal CVT, while forming a tessellation, are congruent to a basic cell which depends on the dimension.* This claim is trivially true in one dimension. It has been proved for the two-dimensional case [79] with the basic cell being the two-dimensional regular hexagon. Gersho's conjecture remains open for three and higher dimensions [80]. In [81], it was shown that the body-centered-cubic (BCC, see Figure 4.3) lattice based CVT enjoys the lowest energy per unit volume among all possible lattice based CVTs. The BCC based CVTs has the energy per unit volume valued at 0.07854, with the basic cell given by the truncated octahedron.

For nonlattice based or general CVTs, it remains unresolved whether the BCC enjoys the lowest energy per unit volume [80]. One question pertains to the possibility of having the optimal CVT made up by a combination of several types of basic cells. In [77], a series of numerical examples are designed for both lattice and nonlattice

Figure 4.3: Basic Voronoi cell of BCC configuration.

based CVTs. The computed energy per unit volume and other related properties and statistics substantiate the claim of the three-dimensional Gersho's conjecture: *the BCC based CVT enjoys the lowest energy among all three-dimensional CVTs including both lattice and nonlattice CVTs*. Thus, asymptotically speaking, the congruent cell of the optimal CVT is the Voronoi cell of the BCC based tessellation, that is, the truncated octahedron.

4.4 Superconvergence on Par6

In this section, we will use the identity in Lemma 4.6 to analyze the superconvergence property on Par6 mesh. Following the discussion in Section 4.2, we consider the unique shape tetrahedron τ in Par6 illustrated in Figure 4.4. Let $\{\mathbf{p}_k\}_{k=1}^4$ denote four vertices of τ and the corresponding four barycentric coordinates are denoted as $\{\varphi_k\}_{k=1}^4$. We assume τ follow the orientation given by the right-hand rule and $\triangle_{klm}$ is used to denote the face with vertices $\mathbf{p}_k, \mathbf{p}_l$ and $\mathbf{p}_m$. If the orientation of $\triangle_{klm}$, given by the order k, l, m , coincides with the induced orientation from τ , we say $\triangle_{klm}$ has the consistent orientation with τ . F_k is the surface opposite vertex $\mathbf{p}_k$ with the outer normal vector $\mathbf{n}_k$. Let e_{ij} denote the oriented edges of element τ from $\mathbf{p}_i$ to $\mathbf{p}_j$ and $\mathbf{t}_{ij}, d_{ij}$ the corresponding unit tangent vectors and edge length, respectively. Let θ_{kl}

Figure 4.4: A tetrahedron.

be the angle between $\mathbf{t}_{kl}$ and the supporting plane of F_l . In general, $\theta_{kl} \neq \theta_{lk}$. Let $\mathcal{D}_\tau$ be a constant symmetric 3×3 matrix defined on τ . We define $\xi_{ij} = \mathbf{n}_i \cdot \mathcal{D}_\tau \mathbf{n}_j$. Since $\mathcal{D}_\tau$ is symmetric, $\xi_{ij} = \xi_{ji}$.

The following identity is proved in Lemma 4.6 for $v_h \in P_1(\tau)$ and $\phi \in H^3(\tau)$:

$$\begin{aligned}
& \int_\tau \nabla(\phi_I - \phi) \cdot \mathcal{D}_\tau \nabla v_h \\
&= \sum_{k,l=1, k \neq l}^4 \frac{\partial v_h}{\partial \mathbf{t}_{kl}} \frac{\xi_{kl}}{2 \sin \theta_{kl}} [(d_{km}^2 - d_{lm}^2) \int_{F_k} \varphi_l \varphi_m \frac{\partial^2 \phi}{\partial \mathbf{t}_{kl}^2} \\
&\quad - 4 |\Delta_{klm}| \int_{F_k} \varphi_l \varphi_m \frac{\partial^2 \phi}{\partial \mathbf{t}_{kl} \partial \mathbf{n}_{kl,m}}] + O(h^3) \|\phi\|_{3,\tau} \|v_h\|_{1,\tau},
\end{aligned} \tag{4.5}$$

where ϕ_I is the piecewise linear interpolant for ϕ , m is chosen such that Δ_{klm} has the consistent orientation with τ and $\mathbf{n}_{kl,m}$ is the unit outward normal vector of edge $\mathbf{t}_{kl}$ on the supporting plane of triangle Δ_{klm} .

Remark 4.7. Since in three dimensions $\mathbf{n}_l \cdot \mathbf{t}_{kl} = -\sin \theta_{kl}$, there is a difference on sign between three dimensional case and n dimensional case. For ease of illustration, we introduce an orientation on tetrahedron τ so that when the local error is expanded

on edge e_{kl} , m is determined by the orientation. As a result, the constant coefficient of $\frac{\partial v_h}{\partial \mathbf{t}_{kl}}$ is $\frac{1}{2}$ instead of $\frac{1}{4}$.

4.4.1 Superconvergence between the finite element solution and linear interpolant

A superconvergence result between the linear finite element approximation of a model second order elliptic equation and its linear interpolant is given in this section.

Recall the property of Par6 triangulation $\mathcal{T}_h$. The Par6 assembly is obtained by distorting the cube into a parallelepiped with a 35.3° rotation of the edges about the y- and z-axis. Each parallelepiped is divided into six tetrahedrons and all the tetrahedrons in Par6 are the same. Furthermore, the four faces of these tetrahedrons are all the same—an isosceles triangle with one edge of length p and the other two of length $\sqrt{3}p/2 \doteq 0.866p$ (see Figure 4.5).

Definition 4.8. Let $\mathcal{T}_h$ denote the Par6 triangulation and $\mathcal{E} = \mathcal{E}_1 \oplus \mathcal{E}_2$ denote the set of edges in $\mathcal{T}_h$, where $\mathcal{E}_1$ is the set of interior edges and $\mathcal{E}_2$ is set of edges on the boundary. Let Ω_e denote the patch of e , which is the union of tetrahedrons sharing e .

Throughout the report, we use the notation $A \lesssim B$ to represent the inequality $A \leq \text{constant} \times B$, where the constant may depend only on the minimum dihedral angle of the tetrahedrons in the mesh $\mathcal{T}_h$ and the domain Ω . The notation $A \simeq B$ is equivalent to the relationship $|A - B| \lesssim O(h^{1+\alpha})$, which means the difference between A and B is controlled by a high order term.

The following lemma is the key in this chapter.

Lemma 4.9. Let the triangulation $\mathcal{T}_h$ be Par6. Let $\mathcal{D}_\tau$ be a piecewise constant matrix function defined on $\mathcal{T}_h$, whose elements $\mathcal{D}_{\tau ij}$ satisfy

$$|\mathcal{D}_{\tau ij}| \lesssim 1, \quad |\mathcal{D}_{\tau ij} - \mathcal{D}_{\tau' ij}| \lesssim h,$$

Figure 4.5: The Par6 assembly and the tetrahedron in Par6

for $i, j = 1, 2, 3$. Here τ and τ' are tetrahedrons sharing a common edge. Then

$$\left| \sum_{\tau \in \mathcal{T}_h} \int_{\tau} \nabla(u - u_I) \cdot \mathcal{D}_{\tau} \nabla v_h \right| \lesssim h^2 |\log h|^{1/2} \|u\|_{3,\infty,\Omega} |v_h|_{1,\Omega}, \quad (4.6)$$

where $u \in W^{3,\infty}(\Omega)$ and $v_h \in \mathcal{V}_h$.

Proof. Denote, with respect to τ ,

$$\alpha_{klm} = -\frac{\xi_{kl}}{2\sin\theta_{kl}}(d_{km}^2 - d_{lm}^2), \quad \beta_{klm} = \frac{2\xi_{kl}}{\sin\theta_{kl}} |\Delta_{klm}|.$$

Applying identity (4.5),

$$\begin{aligned} & \sum_{\tau \in \mathcal{T}_h} \int_{\tau} \nabla(u - u_I) \cdot \mathcal{D}_{\tau} \nabla v_h \\ &= \sum_{\tau \in \mathcal{T}_h} \sum_{k,l=1, k \neq l}^4 \frac{\partial v_h}{\partial \mathbf{t}_{kl}} \left[\alpha_{klm} \int_{F_k} \varphi_l \varphi_m \frac{\partial^2 u}{\partial \mathbf{t}_{kl}^2} + \beta_{klm} \int_{F_k} \varphi_l \varphi_m \frac{\partial^2 u}{\partial \mathbf{t}_{kl} \partial \mathbf{n}_{kl,m}} \right] \\ &= I_1 + I_2, \end{aligned}$$

where

$$I_i = \sum_{e_{kl} \in \mathcal{E}_i} \sum_{\tau \in \Omega_{e_{kl}}} \frac{\partial v_h}{\partial \mathbf{t}_{kl}} \left[\alpha_{klm} \int_{F_k} \varphi_l \varphi_m \frac{\partial^2 u}{\partial \mathbf{t}_{kl}^2} + \beta_{klm} \int_{F_k} \varphi_l \varphi_m \frac{\partial^2 u}{\partial \mathbf{t}_{kl} \partial \mathbf{n}_{kl,m}} \right],$$

for $i = 1, 2$. In the above formulas, F_k , α_{klm} and β_{klm} are different for different tetrahedrons. The index τ is omitted for the simplification of notation.

As mentioned before, the tetrahedrons contained in Par6 tessellation are all the same and only two types of edges are contained in Par6: edge of length p and edge of length $\sqrt{3}/2p$. From further observation on Par6 assembly shown in Figure 4.5, it can be found that for interior edges, the edge of length p such as e_{AG} is shared by 4 tetrahedrons while the edge of length $\sqrt{3}/2p$, for example e_{AF} , is shared by 6 tetrahedrons. Thus we estimate I_1 in the following way.

For the edge of length p , taking e_{AG} for example, we will pair the tetrahedrons in patch $\Omega_{e_{AG}}$ one to one to cancel the low order terms. In tetrahedron τ_{AEFG} , we have

term

$$\frac{\partial v_h}{\partial \mathbf{t}_{AG}} [\alpha_{AGE} \int_{F_{EFG}} \varphi_G \varphi_E \frac{\partial^2 u}{\partial \mathbf{t}_{AG}^2} + \beta_{AGE} \int_{F_{EFG}} \varphi_G \varphi_E \frac{\partial^2 u}{\partial \mathbf{t}_{AG} \partial \mathbf{n}_{AG,E}}],$$

while in tetrahedron τ_{GCDA} we have

$$\frac{\partial v_h}{\partial \mathbf{t}_{GA}} [\alpha_{GAC} \int_{F_{CDA}} \varphi_A \varphi_C \frac{\partial^2 u}{\partial \mathbf{t}_{GA}^2} + \beta_{GAC} \int_{F_{CDA}} \varphi_A \varphi_C \frac{\partial^2 u}{\partial \mathbf{t}_{GA} \partial \mathbf{n}_{GA,C}}].$$

Noticing $\triangle_{AGE}$ and $\triangle_{GAC}$ are on the same plane, we get $\mathbf{n}_{AG,E} = -\mathbf{n}_{GA,C}$. And since not only the tetrahedrons in Par6 are the same, but also the four faces of these tetrahedrons are all the same, the following inequalities hold:

$$\begin{aligned} \left| \int_{F_{EFG}} \varphi_G \varphi_E \frac{\partial^2 u}{\partial \mathbf{t}_{AG}^2} - \int_{F_{CDA}} \varphi_A \varphi_C \frac{\partial^2 u}{\partial \mathbf{t}_{GA}^2} \right| &\lesssim \|u\|_{3,\infty,\Omega} h^3, \\ \left| \int_{F_{EFG}} \varphi_G \varphi_E \frac{\partial^2 u}{\partial \mathbf{t}_{AG} \partial \mathbf{n}_{AG,E}} - \int_{F_{CDA}} \varphi_A \varphi_C \frac{\partial^2 u}{\partial \mathbf{t}_{GA} \partial \mathbf{n}_{GA,C}} \right| &\lesssim \|u\|_{3,\infty,\Omega} h^3. \end{aligned}$$

Using the elementary identity

$$\left| \int_F f \right| \lesssim h^{-1} \int_\tau |f| + \int_\tau |\nabla f|,$$

we get (for $\mathbf{z} = \mathbf{t}_{AG}$ and $\mathbf{z} = \mathbf{n}_{AG,E}$)

$$\int_{F_{EFG}} \varphi_G \varphi_E \frac{\partial^2 u}{\partial \mathbf{t}_{AG} \partial \mathbf{z}} \frac{\partial v_h}{\partial \mathbf{t}_{AG}} \lesssim h^{-1} \int_\tau |\nabla^2 u| |\nabla v_h| + \int_\tau |\nabla^3 u| |\nabla v_h|. \quad (4.7)$$

Coefficients α and β are estimated by

$$\begin{aligned} |\alpha_{AGE} - \alpha_{GAC}| &= 0, \\ |\beta_{AGE} - \beta_{GAC}| &= \left| \frac{\xi_{AG}}{\cos \theta_{AG}} |\triangle_{AGE}| - \frac{\xi_{GA}}{\cos \theta_{GA}} |\triangle_{GAC}| \right| \\ &= \left| \frac{|\triangle_{AGE}|}{\cos \theta_{AG}} \right| |\xi_{AG} - \xi_{GA}| \\ &\lesssim h^3, \end{aligned} \quad (4.8)$$

Table 4.1: Number of tetrahedrons contained in the boundary edge patch.

Edge type	Edges on the boundary surface	Edges on the corner
length p	2	1
length $\sqrt{3}/2p$	3	depends on position

where $|\mathcal{D}_{\tau ij} - \mathcal{D}_{\tau' ij}| \lesssim h$ has been used. The other pair of tetrahedrons contained in patch $\Omega_{e_{AG}}$, say τ_{ADEG} and τ_{GCFA} , are treated in the same way.

For the edge of length $\sqrt{3}/2p$, such as e_{AF} , we also pair the tetrahedrons in patch $\Omega_{e_{AF}}$ to cancel low order terms. The only difference is that there are 3 pairs to treat in this type of patch.

Thus combining (4.7) with (4.8) and noticing $v_h \in P_1(\tau)$, we estimate I_1 by

$$|I_1| \lesssim h^2 \int_{\Omega} (|\nabla^2 u| + h |\nabla^3 u|) |\nabla v_h| \lesssim h^2 \|u\|_{3,\Omega} |v_h|_{1,\Omega}. \quad (4.9)$$

Now we turn to the estimate for I_2 . If $v_h = 0$ on $\partial\Omega$, then it is easy to see $I_2 = 0$. For the edges on the boundary, say $e \in \mathcal{E}_2$, after carefully observation on Par6 tessellation we show the number of tetrahedrons contained in the patch Ω_e in Table 4.1. For the corner edges of length $\sqrt{3}/2p$, the number of tetrahedrons contained in patch Ω_e depends on the position. Corner edges that appear on position AE and CG are shared by 2 tetrahedrons, while DH and BF are only contained by 1 tetrahedron. We can pair the tetrahedrons in boundary edge patch and treat it same as before. The remaining question is how to estimate the term that can not find a partner. In general case, we define

$$B_{e_{kl}}(u) = \alpha_{klm} \frac{\partial^2 u}{\partial \mathbf{t}_{kl}^2} + \beta_{klm} \frac{\partial^2 u}{\partial \mathbf{t}_{kl} \partial \mathbf{n}_{kl,m}},$$

$$\overline{B_{e_{kl}}}(u) = |e_{kl}|^{-1} \int_{e_{kl}} B_{e_{kl}}(u).$$

Thus

$$I_2 = \sum_{e_{kl} \in \mathcal{E}_2} \sum_{\tau \in \Omega_{e_{kl}}} \int_{F_k} \varphi_l \varphi_m B_{e_{kl}}(u) \frac{\partial v_h}{\partial \mathbf{t}_{kl}}.$$

Since only the terms that can not find a partner are considered, we just need to estimate

$$\begin{aligned}\tilde{I}_2 &= \sum_{e_{kl} \in \partial\Omega} \int_{F_k} \varphi_l \varphi_m B_{e_{kl}}(u) \frac{\partial v_h}{\partial \mathbf{t}_{kl}} \\ &= \sum_{e_{kl} \in \partial\Omega} \int_{F_k} \varphi_l \varphi_m \overline{B_{e_{kl}}}(u) \frac{\partial v_h}{\partial \mathbf{t}_{kl}} - \sum_{e_{kl} \in \partial\Omega} \int_{F_k} \varphi_l \varphi_m (B_{e_{kl}}(u) - \overline{B_{e_{kl}}}(u)) \frac{\partial v_h}{\partial \mathbf{t}_{kl}}.\end{aligned}$$

For the second term, we have

$$\begin{aligned}\left| \sum_{e_{kl} \in \partial\Omega} \int_{F_k} \varphi_l \varphi_m (B_{e_{kl}}(u) - \overline{B_{e_{kl}}}(u)) \frac{\partial v_h}{\partial \mathbf{t}_{kl}} \right| &\lesssim h^3 |u|_{3,\infty,\Omega} \sum_{e_{kl} \in \partial\Omega} \int_{F_k} \left| \frac{\partial v_h}{\partial \mathbf{t}_{kl}} \right| \\ &\lesssim h^{5/2} |u|_{3,\infty,\Omega} |v_h|_{1,\Omega},\end{aligned}\tag{4.10}$$

where the trace inequality has been used.

We now estimate the first term. Let $\mathcal{P}$ to be the set of vertices on $\partial\Omega$. Then we have

$$\begin{aligned}\sum_{e_{kl} \in \partial\Omega} \int_{F_k} \varphi_l \varphi_m \overline{B_{e_{kl}}}(u) \frac{\partial v_h}{\partial \mathbf{t}_{kl}} &= \sum_{e_{kl} \in \partial\Omega} \overline{B_{e_{kl}}}(u) \frac{\partial v_h}{\partial \mathbf{t}_{kl}} \int_{F_k} \varphi_l \varphi_m \\ &= \sum_{e_{kl} \in \partial\Omega} \overline{B_{e_{kl}}}(u) \frac{\partial v_h}{\partial \mathbf{t}_{kl}} \frac{|F_k|}{12} \\ &= \frac{1}{12} \sum_{x \in \mathcal{P}} (\overline{B_{e_{kl}}}(u) - \overline{B_{e'_{kl}}}(u)) v_h(x) \frac{|F_k|}{|e_{kl}|},\end{aligned}$$

where e'_{kl} is a boundary edge of a neighboring tetrahedron τ' .

It is easy to see

$$\begin{aligned}\frac{|F_k|}{|e_{kl}|} &\lesssim h, \\ |\overline{B_{e_{kl}}}(u) - \overline{B_{e'_{kl}}}(u)| &\lesssim h^3 |u|_{3,\infty,\Omega}.\end{aligned}$$

Thus we get

$$\begin{aligned} \left| \sum_{x \in \mathcal{P}} (\overline{B_{e_{kl}}}(u) - \overline{B_{e'_{kl}}}(u)) v_h(x) \frac{|F_k|}{|e_{kl}|} \right| &\lesssim h^2 |u|_{3,\infty,\Omega} \|v_h\|_{\infty,\partial\Omega} \\ &\lesssim h^2 |\log h|^{1/2} |u|_{3,\infty,\Omega} \|v_h\|_{1,\Omega}, \end{aligned}$$

where the following Sobolev inequality has been used,

$$\|v_h\|_{\infty,\Omega} \lesssim |\log h|^{1/2} \|v_h\|_{1,\Omega}.$$

Following a standard argument, here $\|v_h\|_{1,\Omega}$ can be replaced by $|v_h|_{1,\Omega}$. Combining this estimate with (4.10), we have

$$\begin{aligned} |\tilde{I}_2| &\lesssim h^2 (h^{1/2} |u|_{3,\infty,\Omega} + |\log h|^{1/2} |u|_{3,\infty,\Omega}) |v_h|_{1,\Omega} \\ &\lesssim h^2 |\log h|^{1/2} \|u\|_{3,\infty,\Omega} |v_h|_{1,\Omega}. \end{aligned}$$

Thus the final estimate for I_2 is

$$|I_2| \lesssim h^2 |\log h|^{1/2} \|u\|_{3,\infty,\Omega} |v_h|_{1,\Omega}. \quad (4.11)$$

Combining (4.9) and (4.11), we finally obtain the interpolation estimate (4.6). $\square$

For pure Dirichlet boundary conditions, we have the following better estimate.

Lemma 4.10. *For a second order elliptic problem with pure Dirichlet boundary conditions, assume the conditions of Lemma 4.9, then*

$$\left| \sum_{\tau \in \mathcal{T}_h} \int_{\tau} \nabla(u - u_I) \cdot \mathcal{D}_{\tau} \nabla v_h \right| \lesssim h^2 \|u\|_{3,\infty,\Omega} |v_h|_{1,\Omega}, \quad (4.12)$$

where $u \in W^{3,\infty}(\Omega)$ and $v_h \in \mathcal{V}_h$.

Proof. Use $I_2 = 0$ in Lemma 4.9. $\square$

Theorem 4.11. *Assume that the solution of (4.1) satisfies $u \in W^{3,\infty}(\Omega)$. Further, assume the hypotheses of Lemma 4.10. Then*

$$\|u_h - u_I\|_{1,\Omega} \lesssim h^2 \|u\|_{3,\infty,\Omega}.$$

Proof. We begin with the identity

$$\begin{aligned} B(u - u_I, v_h) &= \sum_{\tau \in \mathcal{T}_h} \int_{\tau} \nabla(u - u_I) \cdot \mathcal{D}_{\tau} \nabla v_h \, dx + \sum_{\tau \in \mathcal{T}_h} \int_{\tau} \nabla(u - u_I) \cdot (\mathcal{D} - \mathcal{D}_{\tau}) \nabla v_h \, dx \\ &\quad + \int_{\Omega} (u - u_I)(\mathbf{b} \cdot \nabla v_h + cv_h) \, dx = I_1 + I_2 + I_3. \end{aligned}$$

The first term I_1 is estimated by Lemma 4.10. I_2 and I_3 can be easily estimated by

$$|I_2| + |I_3| \lesssim h^2 \|u\|_{2,\Omega} \|v_h\|_{1,\Omega}.$$

Thus

$$|B(u - u_I, v_h)| \lesssim h^2 \|u\|_{3,\infty,\Omega} \|v_h\|_{1,\Omega}.$$

We complete the proof using the fact that

$$\begin{aligned} \mu \|u_h - u_I\|_{1,\Omega} &\leq \sup_{v_h \in \mathcal{V}_h} \frac{B(u_h - u_I, v_h)}{\|v_h\|_{1,\Omega}} \\ &= \sup_{v_h \in \mathcal{V}_h} \frac{B(u - u_I, v_h)}{\|v_h\|_{1,\Omega}} \\ &\lesssim h^2 \|u\|_{3,\infty,\Omega}. \end{aligned}$$

□

4.4.2 Superconvergence between the gradient recovered by SPR and true gradient

Superconvergence Patch Recovery (SPR) is a gradient recovery method introduced by Zienkiewicz and Zhu in [55]. The SPR-recovery gradient is used to produce the ZZ error estimator in [56], namely ZZ-SPR. This method is widely used in engineering practices for its robustness in a posteriori error estimates and its efficiency in computer implementation.

We define $\mathcal{N}_h$ as the nodal set of a Par6 tessellation $\mathcal{T}_h$. Given $z \in \mathcal{N}_h$, we consider an element patch ω around z and we choose z as the origin of a local coordinates. Under this coordinate system, we let (x_j, y_j, z_j) be the barycenter of a tetrahedron $\tau_j \subset \omega, j = 1, 2, \dots, m$. From further observation on Par6, we will find the following geometric condition is satisfied for any interior vertex z :

$$\frac{1}{m} \sum_{j=1}^m (x_j, y_j, z_j) = 0. \quad (4.13)$$

This geometric condition holds because of the highly symmetric structure of Par6. And for the boundary vertices, the corresponding geometric condition is:

$$\frac{1}{m} \sum_{j=1}^m (x_j, y_j, z_j) = O(h^{1+\alpha})(1, 1, 1),$$

where $\alpha \in [0, 1]$. While the tetrahedrons with boundary vertices only occupy small volume compared with whole domain Ω , that is to say

$$\sum_{\tau \text{ with boundary vertices}} |\tau| \lesssim Nh^3 \lesssim h,$$

where N is the number of tetrahedrons with boundary vertices.

Let $u_I \in \mathcal{V}_h$ be the linear interpolation of a given function u . We shall discuss a gradient recovery operator G_h and prove the superconvergence property between ∇u and $G_h u_I$. The value of $G_h u_I$ is first determined at a vertex, and then linearly interpolated over the whole domain. SPR uses the local discrete least-squares fitting

to seek linear functions $p_l \in P_1(\omega)$ ($l = 1, 2, 3$), such that

$$\sum_{j=1}^m [p_l(x_j, y_j, z_j) - \partial_l u_I(x_j, y_j, z_j)] q(x_j, y_j, z_j) = 0, \quad \forall q \in P_1(\omega), \quad l = 1, 2, 3. \quad (4.14)$$

Then we define $G_h u_I(z) = (p_1(0, 0, 0), p_2(0, 0, 0), p_3(0, 0, 0))$. The existence and uniqueness of the minimizer in (4.14) can be found in [82].

Lemma 4.12. *Let ω be an element patch around a vertex $z \in \mathcal{N}_h$, let $u \in W^{3,\infty}(\omega)$, and let $G_h u_I(z)$ be produced by the local discrete least-squares fitting under condition (4.13). Then*

$$|G_h u_I(z) - \nabla u(z)| \lesssim h^2 \|u\|_{3,\infty,\omega}.$$

Proof. Set $q = 1$ in (4.14) to obtain

$$\sum_{j=1}^m p_l(x_j, y_j, z_j) = \sum_{j=1}^m \partial_l u_I(x_j, y_j, z_j).$$

Therefore,

$$\begin{aligned} p_l(0, 0, 0) - \frac{1}{m} \sum_{j=1}^m \partial_l u_I(x_j, y_j, z_j) &= p_l(0, 0, 0) - \frac{1}{m} \sum_{j=1}^m p_l(x_j, y_j, z_j) \\ &= -\frac{1}{m} \nabla p_l(0, 0, 0) \cdot \sum_{j=1}^m (x_j, y_j, z_j) \\ &= 0, \end{aligned} \quad (4.15)$$

where Taylor expansion and condition (4.13) have been used. Next,

$$\begin{aligned}
& \frac{1}{m} \sum_{j=1}^m \partial_l u_I(x_j, y_j, z_j) - \partial_l u(0, 0, 0) \\
&= \frac{1}{m} \sum_{j=1}^m \partial_l (u_I - u)(x_j, y_j, z_j) + \frac{1}{m} \sum_{j=1}^m [\partial_l u(x_j, y_j, z_j) - \partial_l u(0, 0, 0)] \\
&= \frac{1}{m} \sum_{j=1}^m \partial_l (u_I - u)(x_j, y_j, z_j) + \frac{1}{m} \nabla \partial_l u(0, 0, 0) \cdot \sum_{j=1}^m (x_j, y_j, z_j) + R(u),
\end{aligned}$$

where, by Taylor expansion, the high order term $R(u)$ is estimated by

$$|R(u)| \lesssim h^2 \|u\|_{3,\infty,\omega}.$$

Therefore,

$$\left| \frac{1}{m} \sum_{j=1}^m \partial_l u_I(x_j, y_j, z_j) - \partial_l u(0, 0, 0) \right| \lesssim h^2 \|u\|_{3,\infty,\omega}. \quad (4.16)$$

Combining (4.15) and (4.16), we have proved

$$|p_l(0, 0, 0) - \partial_l u(0, 0, 0)| \lesssim h^2 \|u\|_{3,\infty,\omega}.$$

□

Lemma 4.13. *The recovery operator G_h satisfies*

$$G_h v(z) = \sum_{j=1}^m c_j \nabla v(x_j, y_j, z_j), \quad \sum_{j=1}^m c_j = 1,$$

unconditionally. Furthermore, $c_j > 0$ for the local discrete least-squares fitting under the condition (4.13).

Proof. Let $p_l(x, y, z) = a_0 + a_1 x + a_2 y + a_3 z$. Then for the local discrete least-squares

fitting, a_i 's are given by

$$\begin{pmatrix} m & \sum_j x_j & \sum_j y_j & \sum_j z_j \\ \sum_j x_j & \sum_j x_j^2 & \sum_j x_j y_j & \sum_j x_j z_j \\ \sum_j y_j & \sum_j x_j y_j & \sum_j y_j^2 & \sum_j y_j z_j \\ \sum_j z_j & \sum_j x_j z_j & \sum_j y_j z_j & \sum_j z_j^2 \end{pmatrix} \begin{pmatrix} a_0 \\ a_1 \\ a_2 \\ a_3 \end{pmatrix} = \begin{pmatrix} \sum_j \partial_l u_h(x_j, y_j, z_j) \\ \sum_j x_j \partial_l u_h(x_j, y_j, z_j) \\ \sum_j y_j \partial_l u_h(x_j, y_j, z_j) \\ \sum_j z_j \partial_l u_h(x_j, y_j, z_j) \end{pmatrix}, \quad (4.17)$$

Under condition (4.13),

$$\sum_j x_j = 0, \quad \sum_j y_j = 0 \quad \sum_j z_j = 0.$$

Therefore, from (4.17) we get

$$\begin{aligned} a_0 &= \frac{1}{m} \sum_j \partial_l u_h(x_j, y_j, z_j) - \frac{a_1}{m} \sum_j x_j - \frac{a_2}{m} \sum_j y_j - \frac{a_3}{m} \sum_j z_j \\ &= \sum_j c_j \partial_l u_h(x_j, y_j, z_j) \end{aligned}$$

with

$$c_j = \frac{1}{m} > 0.$$

□

Remark 4.14. Under the given condition, the recovered gradient at a vertex z is a convex combination of gradient values on the element patch surrounding z . Since Par6 is uniform tessellation, SPR has the same performance as simple averaging or weighted averaging theoretically but more robust in practice.

Theorem 4.15. *Let the solution of (4.1) satisfy $u \in W^{3,\infty}(\Omega)$, let u_h be the solution of (4.2), and let G_h be a recovery operator defined by the local discrete least-squares*

fitting. Assume the tessellation is Par6 $\mathcal{T}_h$. Then

$$\|\nabla u - G_h u_h\|_{0,\Omega} \lesssim h^2 \|u\|_{3,\infty,\Omega}. \quad (4.18)$$

Proof. We decompose

$$\nabla u - G_h u_h = (\nabla u - (\nabla u)_I) + ((\nabla u)_I - G_h u_I) + G_h(u_I - u_h), \quad (4.19)$$

where $(\nabla u)_I \in \mathcal{V}_h^3$ is the linear interpolation of ∇u . By the standard approximation theory,

$$\|\nabla u - (\nabla u)_I\|_{0,\Omega} \lesssim h^2 |\nabla u|_{3,\Omega}. \quad (4.20)$$

Using Lemma 4.12, we have

$$\begin{aligned} \|(\nabla u)_I - G_h u_I\|_{0,\Omega} &\leq \left(\sum_{\tau \in \mathcal{T}_h} |\tau| \sum_{z \in \mathcal{N}_h \cap \bar{\tau}} |G_h u_I(z) - \nabla u(z)|^2 \right)^{1/2} \\ &\lesssim h^2 \|u\|_{3,\infty,\Omega} |\Omega|^{1/2} \lesssim h^2 \|u\|_{3,\infty,\Omega}. \end{aligned} \quad (4.21)$$

Similarly, by the fact proved in Lemma 4.13, that $G_h v(z)$ is a convex combination of $\nabla v|_\tau$ in the patch ω ,

$$\begin{aligned} \|G_h(u_I - u_h)\|_{0,\Omega} &\leq \left(\sum_{\tau \in \mathcal{T}_h} |\tau| \sum_{z \in \mathcal{N}_h \cap \bar{\tau}} |G_h(u_I - u_h)(z)|^2 \right)^{1/2} \\ &\lesssim \left(\sum_{\tau \in \mathcal{T}_h} |\tau| |\nabla(u_I - u_h)|_\tau^2 \right)^{1/2} \\ &= \|\nabla(u_I - u_h)\|_{0,\Omega} \\ &\lesssim h^2 \|u\|_{3,\infty,\Omega}, \end{aligned} \quad (4.22)$$

where Theorem 4.11 has been used. Combining (4.19), (4.20), (4.21) and (4.22), we obtain the final estimation (4.18). $\square$

Table 4.2: Error estimation and convergence order of the recovered gradient on Par6.

Mesh size h	SPR $\ \nabla u - G_h u_h\ _{0,\Omega}$
0.100	2.02e-3
0.050	5.18e-4
0.033	2.32e-4
0.025	1.32e-4
Order	1.9779

4.5 Numerical substantiation

In this section, we present a simple numerical example to verify the theoretical results deduced in previous section. The superconvergence order of $\|\nabla u - G_h u_h\|_{0,\Omega}$ for linear finite element solution on Par6 tessellation is close to 2, coinciding with the theoretical results exactly.

The linear finite element solution of the following Poisson equation is considered

$$\begin{aligned} -\Delta u &= f \quad \text{in } \Omega \\ u &= g \quad \text{on } \partial\Omega \end{aligned} \tag{4.23}$$

where Ω is a 3D-bounded Lipschitz domain with boundary $\partial\Omega$, f and g are smooth, and the solution u of equation (4.23) is assumed to be sufficiently smooth. The right hand side f is chosen to be $3\sin(x+y+z)$, thus the exact solution is $u = \sin(x+y+z)$ and the boundary condition is properly imposed.

The experiment is conducted on Par6 tessellation, for which the whole parallelepiped domain Ω is divided into small parallelepiped and then each small parallelepiped is subdivided into six identical tetrahedrons (see Figure 4.2). The SPR method is performed on a sequence of meshes with the sizes being $h = 0.100, 0.050, 0.033, 0.025$. The error estimation and convergence order are shown in table 4.2 and Figure 4.6.

The convergence order corresponds to the absolute value of slope in the figure, which is approximately 2, coinciding with our theoretical results exactly.

Figure 4.6: Error estimation and convergence rate of the recovered gradient on Par6.

Chapter 5

LINEAR FINITE ELEMENT SUPERCONVERGENCE ON UNSTRUCTURED SIMPLICIAL MESHES

5.1 Introduction

The geometric structure of the computational mesh has great influence on the finite element superconvergence property. It is well-known that superconvergence property is preserved for both the function values of finite element solution and its derivatives on equilateral meshes in two dimensional spaces. But in higher dimensional spaces, the regular simplex is not a space-filler. In fact, superconvergence in three dimensional spaces is much more a rarity than in two dimensional spaces and it is difficult to analyze partially due to the loss of symmetry in the meshes in three dimensions. This explains why superconvergence results in three dimensions are relatively rare [48, 75, 74, 83, 84, 85, 86, 87].

In this chapter, we study the gradient superconvergence for a second order elliptic boundary value problem with linear finite elements in three and higher dimensional spaces. The major part of our analysis is a superclose result between the gradient ∇u_h

of the finite element approximation u_h and the gradient ∇u_I of the linear Lagrange interpolant u_I in three dimensional spaces, where $\Omega \subset \mathbb{R}^3$ is a bounded domain with Lipschitz boundary $\partial\Omega$ and u_I is the piecewise linear interpolant for the solution u . In particular, we show in Theorem 5.10 that

$$\|u_h - u_I\|_{1,\Omega} \lesssim h^{1+\rho} \|u\|_{3,\infty,\Omega}, \quad \rho = \min(\alpha, \frac{\sigma}{2}, 1). \quad (5.1)$$

Estimate (5.1) holds on tetrahedralizations where the lengths of each pair of opposite edges in most tetrahedrons inside Ω differ only by $O(h^{1+\alpha})$ except for a region of size $O(h^\sigma)$; see section 4 for details. This interpolantwise gradient superconvergence result is the footstone of theoretical analysis for the superconvergence property of the gradient recovered by some postprocessing techniques, such as the well-known Superconvergence Patch Recovery (SPR) method introduced by Zienkiewicz and Zhu [88, 55, 56] and Polynomial Patch Recovery (PPR) method raised by Zhang and Naga [89].

In [90], it is mentioned that unlike in the two dimensional case, two tetrahedra sharing a face do not form a point-symmetric domain. However, there are simple ways to subdivide parallelepipeds into six tetrahedra giving rise to relatively small point-symmetric patches of tetrahedra. Existing three dimensional superconvergence results are all based on such a point-symmetric patch structure. Instead, we take a different local view on superconvergence analysis. The geometric condition we raised, namely the edge pair condition which means the lengths of each pair of opposite edges in a tetrahedra differ only by $O(h^{1+\alpha})$, is imposed on a single element. It is due to the locality of the error expansion formula, which holds on a single element. Another important contribution of our work is that the geometric condition we need is much more wild than the existing results, for which the uniform structured meshes that satisfy point-symmetric condition are needed. There is a disjunction between the superconvergence analysis and the superconvergence engineering application. The former is usually based on symmetric structured meshes while the latter is done on unstructured meshes in general. Our work tries to fill this gap. The edge pair condition trends to be satisfied by unstructured meshes such as CVDT meshes. In

fact, Par6 meshes that are considered as optimal CVDt meshes satisfy our edge pair condition perfectly; see section 5.2 for details.

Preliminary exploration on superconvergence in four and higher-dimensional space is also included in this chapter. Using the local error expansion formula in n dimensional space and under the generalized edge pair condition, the superconvergent result that is analogous to the three dimensional case (5.1) also can be achieved formally. Going a step further, we find that the 4-simplex mesh satisfying generalized edge pair condition does not exist in four dimensional spaces. This means the geometric properties for different dimensions are distinct so is the geometric condition for superconvergence.

The rest of this chapter is organized as follows: In section 5.2, the supercloseness between the gradient of the finite element approximation and the gradient of the linear Lagrange interpolant in three dimensional spaces is analyzed. In section 5.3, numerical examples are presented to verify the theoretical results. Section 5.4 is the preliminary exploration in high dimensional space.

5.2 Superconvergence between the finite element solution and linear interpolant in three dimensional spaces

A superconvergence result between the linear finite element approximation of a model second order elliptic equation and its linear interpolant in three dimensional space is given in this section.

We consider a tetrahedron τ in three-dimensional unstructured meshes illustrated in Figure 4.4. Let $\{\mathbf{p}_k\}_{k=1}^4$ denote four vertices of τ and the corresponding four barycentric coordinates are denoted as $\{\varphi_k\}_{k=1}^4$. We assume τ follow the orientation given by the right-hand rule and $\triangle_{klm}$ is used to denote the face with vertices $\mathbf{p}_k, \mathbf{p}_l$ and $\mathbf{p}_m$. If the orientation of $\triangle_{klm}$, given by the order k, l, m , coincides with the induced orientation from τ , we say $\triangle_{klm}$ has the consistent orientation with τ . F_k is the surface opposite vertex $\mathbf{p}_k$ with the outer normal vector $\mathbf{n}_k$. Let e_{ij} denote

the oriented edges of element τ from $\mathbf{p}_i$ to $\mathbf{p}_j$ and $\mathbf{t}_{ij}, d_{ij}$ the corresponding unit tangent vectors and edge length, respectively. Let θ_{kl} be the angle between $\mathbf{t}_{kl}$ and the supporting plane of F_l . In general, $\theta_{kl} \neq \theta_{lk}$. $\mathcal{D}_\tau$ is a constant symmetric 3×3 matrix defined on τ . $\xi_{ij} = \mathbf{n}_i \cdot \mathcal{D}_\tau \mathbf{n}_j$ and $\xi_{ij} = \xi_{ji}$.

Definition 5.1. *The quasi-uniform tetrahedralization $\mathcal{T}_h = \mathcal{T}_{1,h} \cup \mathcal{T}_{2,h}$ is said to satisfy condition (α, σ) if there exist positive constant α and σ such that: The lengths of each pair of opposite edges in every tetrahedron inside $\mathcal{T}_{1,h}$ differ only by $O(h^{1+\alpha})$, where h is the mesh size, and*

$$\bar{\Omega}_{1,h} \cup \bar{\Omega}_{2,h} = \bar{\Omega}, \quad |\Omega_{2,h}| = O(h^\sigma), \quad \bar{\Omega}_{i,h} \equiv \cup_{\tau \in \mathcal{T}_{i,h}} \bar{\tau}, \quad i = 1, 2.$$

Let Ω_e denote the patch of edge e , which is the union of tetrahedrons sharing e . Let r be the number of elements contained in the edge patch Ω_e .

For the tetrahedron τ with vertex indices k, l, m, o following the orientation given by the right-hand rule, Denote, with respect to τ ,

$$\zeta_{klm} = d_{km}^2 - d_{lm}^2, \quad \gamma_{klm} = 4 |\triangle_{klm}|.$$

Based on (4.5), we have the following fundamental lemma:

Lemma 5.2. *For $v_h \in P_1(\tau)$ and $\phi \in H^3(\tau)$, we have*

$$\begin{aligned} & \int_\tau \nabla(\phi_I - \phi) \cdot \mathcal{D}_\tau \nabla v_h \\ &= \sum_{k,l=1, k \neq l}^4 \frac{\partial v_h}{\partial \mathbf{t}_{kl}} \frac{\xi_{kl}}{4} ((\zeta_{klm} \chi_{klm} - \zeta_{lko} \chi_{lko}) - (\gamma_{klm} \eta_{klm} - \gamma_{lko} \eta_{lko})) \\ &+ O(h^3) \|\phi\|_{3,\tau} \|v_h\|_{1,\tau}, \end{aligned} \tag{5.2}$$

where

$$\begin{aligned}\chi_{klm} &= \frac{1}{\sin \theta_{kl}} \int_{F_k} \varphi_l \varphi_m \frac{\partial^2 \phi}{\partial \mathbf{t}_{kl}^2}, \\ \eta_{klm} &= \frac{1}{\sin \theta_{kl}} \int_{F_k} \varphi_l \varphi_m \frac{\partial^2 \phi}{\partial \mathbf{t}_{kl} \partial \mathbf{n}_{kl,m}}.\end{aligned}$$

Proof. The low order terms in the right-hand side of (4.5) can be rewritten as

$$\begin{aligned}& \sum_{k,l=1,k \neq l}^4 \frac{\partial v_h}{\partial \mathbf{t}_{kl}} \frac{\xi_{kl}}{2 \sin \theta_{kl}} \left[(d_{km}^2 - d_{lm}^2) \int_{F_k} \varphi_l \varphi_m \frac{\partial^2 \phi}{\partial \mathbf{t}_{kl}^2} - 4 |\Delta_{klm}| \int_{F_k} \varphi_l \varphi_m \frac{\partial^2 \phi}{\partial \mathbf{t}_{kl} \partial \mathbf{n}_{kl,m}} \right] \\&= \frac{1}{2} \sum_{k,l=1,k \neq l}^4 \left\{ \frac{\partial v_h}{\partial \mathbf{t}_{kl}} \frac{\xi_{kl}}{2 \sin \theta_{kl}} \left[(d_{km}^2 - d_{lm}^2) \int_{F_k} \varphi_l \varphi_m \frac{\partial^2 \phi}{\partial \mathbf{t}_{kl}^2} \right. \right. \\&\quad \left. \left. - 4 |\Delta_{klm}| \int_{F_k} \varphi_l \varphi_m \frac{\partial^2 \phi}{\partial \mathbf{t}_{kl} \partial \mathbf{n}_{kl,m}} \right] + \frac{\partial v_h}{\partial \mathbf{t}_{lk}} \frac{\xi_{lk}}{2 \sin \theta_{lk}} \left[(d_{lo}^2 - d_{ko}^2) \int_{F_l} \varphi_k \varphi_o \frac{\partial^2 \phi}{\partial \mathbf{t}_{lk}^2} \right. \right. \\&\quad \left. \left. - 4 |\Delta_{lko}| \int_{F_l} \varphi_k \varphi_o \frac{\partial^2 \phi}{\partial \mathbf{t}_{lk} \partial \mathbf{n}_{lk,o}} \right] \right\} \\&= \sum_{k,l=1,k \neq l}^4 \frac{\partial v_h}{\partial \mathbf{t}_{kl}} \frac{\xi_{kl}}{4} \left\{ \left[\frac{(d_{km}^2 - d_{lm}^2)}{\sin \theta_{kl}} \int_{F_k} \varphi_l \varphi_m \frac{\partial^2 \phi}{\partial \mathbf{t}_{kl}^2} - \frac{(d_{lo}^2 - d_{ko}^2)}{\sin \theta_{lk}} \int_{F_l} \varphi_k \varphi_o \frac{\partial^2 \phi}{\partial \mathbf{t}_{lk}^2} \right] \right. \\&\quad \left. - \left[4 \frac{|\Delta_{klm}|}{\sin \theta_{kl}} \int_{F_k} \varphi_l \varphi_m \frac{\partial^2 \phi}{\partial \mathbf{t}_{kl} \partial \mathbf{n}_{kl,m}} - 4 \frac{|\Delta_{lko}|}{\sin \theta_{lk}} \int_{F_l} \varphi_k \varphi_o \frac{\partial^2 \phi}{\partial \mathbf{t}_{lk} \partial \mathbf{n}_{lk,o}} \right] \right\} \\&= \sum_{k,l=1,k \neq l}^4 \frac{\partial v_h}{\partial \mathbf{t}_{kl}} \frac{\xi_{kl}}{4} \left((\zeta_{klm} \chi_{klm} - \zeta_{lko} \chi_{lko}) - (\gamma_{klm} \eta_{klm} - \gamma_{lko} \eta_{lko}) \right),\end{aligned}$$

thus the desired result follows. $\square$

Remark 5.3. From the fundamental lemma, we can see that the local error is expanded along the tangential direction. The remaining things we want to do are to group the coefficients of $\frac{\partial v_h}{\partial \mathbf{t}_{kl}}$ from a single element or an edge patch together to cancel the lowest order terms.

Starting from the fundamental lemma, we first estimate the first terms $(\zeta_{klm} \chi_{klm} - \zeta_{lko} \chi_{lko})$, which can be achieved on a single element.

Lemma 5.4. *If the lengths of each pair of opposite edges in τ_{klmo} differ only by $O(h^{1+\alpha})$, then,*

$$|\zeta_{klm}\chi_{klm} - \zeta_{lko}\chi_{lko}| \lesssim h^{1+\min(\alpha,1)} \int_{\tau} (|\nabla^2 u| + |\nabla^3 u|), \quad (5.3)$$

where $u \in W^{3,\infty}(\Omega)$.

Proof. Since

$$d_{km} \simeq d_{lo}, \quad d_{lm} \simeq d_{ko},$$

the coefficient $|\zeta_{klm} - \zeta_{lko}|$ is estimated by

$$|\zeta_{klm} - \zeta_{lko}| \lesssim O(h^{2+\alpha}). \quad (5.4)$$

Let

$$c = \frac{1}{|\Omega|} \int_{\Omega} \frac{\partial^2 u}{\partial \mathbf{t}_{kl}^2}.$$

Then using the third equation in Lemma (4.3), the trace inequality and Friedrichs inequality, we have

$$\begin{aligned} & \left| \frac{1}{\sin \theta_{kl}} \int_{F_k} \varphi_l \varphi_m \frac{\partial^2 u}{\partial \mathbf{t}_{kl}^2} - \frac{1}{\sin \theta_{lk}} \int_{F_l} \varphi_k \varphi_o \frac{\partial^2 u}{\partial \mathbf{t}_{lk}^2} \right| \\ &= \left| \frac{1}{\sin \theta_{kl}} \int_{F_k} \varphi_l \varphi_m \left(\frac{\partial^2 u}{\partial \mathbf{t}_{kl}^2} - c \right) - \frac{1}{\sin \theta_{lk}} \int_{F_l} \varphi_k \varphi_o \left(\frac{\partial^2 u}{\partial \mathbf{t}_{lk}^2} - c \right) \right| \\ &\lesssim \left\| \frac{\partial^2 u}{\partial \mathbf{t}_{kl}^2} - c \right\|_{L^1(\partial\tau)} \\ &\lesssim h^{-1} \left\| \frac{\partial^2 u}{\partial \mathbf{t}_{kl}^2} - c \right\|_{L^1(\tau)} + \left\| \nabla \left(\frac{\partial^2 u}{\partial \mathbf{t}_{kl}^2} - c \right) \right\|_{L^1(\tau)} \\ &= h^{-1} \left\| \frac{\partial^2 u}{\partial \mathbf{t}_{kl}^2} - \frac{1}{|\Omega|} \int_{\Omega} \frac{\partial^2 u}{\partial \mathbf{t}_{kl}^2} \right\|_{L^1(\tau)} + \left\| \nabla \frac{\partial^2 u}{\partial \mathbf{t}_{kl}^2} \right\|_{L^1(\tau)} \\ &\lesssim \left\| \nabla \frac{\partial^2 u}{\partial \mathbf{t}_{kl}^2} \right\|_{L^1(\tau)} \lesssim |u|_{3,1,\tau}, \end{aligned} \quad (5.5)$$

which is to say the other coefficient $|\chi_{klm} - \chi_{lko}|$ satisfies

$$|\chi_{klm} - \chi_{lko}| \lesssim \int_{\tau} |\nabla^3 u|. \quad (5.6)$$

Using the elementary identity

$$\left| \int_F f \right| \lesssim h^{-1} \int_{\tau} |f| + \int_{\tau} |\nabla f|,$$

we get

$$|\chi_{klm}| \lesssim h^{-1} \int_{\tau} |\nabla^2 u| + \int_{\tau} |\nabla^3 u|. \quad (5.7)$$

Using (5.4), (5.6), (5.7) and noticing $\zeta_{lkn} \lesssim O(h^2)$, we achieve the estimate

$$\begin{aligned} & |\zeta_{klm}\chi_{klm} - \zeta_{lko}\chi_{lko}| \\ &= |(\zeta_{klm} - \zeta_{lko})\chi_{klm} + (\chi_{klm} - \chi_{lko})\zeta_{lko}| \\ &\lesssim h^{1+\alpha} \int_{\tau} (|\nabla^2 u| + h |\nabla^3 u|) + h^2 \int_{\tau} |\nabla^3 u| \\ &\lesssim h^{1+\min(\alpha,1)} \int_{\tau} (|\nabla^2 u| + |\nabla^3 u|). \end{aligned}$$

□

Then we begin to estimate the second terms $(\gamma_{klm}\eta_{klm} - \gamma_{lko}\eta_{lko})$. Since the integration η_{klm} and η_{lko} involve the directional derivatives on $\mathbf{n}_{kl,m}$ and $\mathbf{n}_{lk,o}$ respectively, the lowest order terms can not be eliminated in a single element. An edge patch structure is introduced to do the cancellation. For our ideal case, say par6 mesh (see section 5 for details), there are only two types of patches: the longer edge with 4 elements in the patch and the shorter edge with 6 elements in the patch (see Figure 5.1). In general unstructured tetrahedralization, r , which is the number of elements contained in the edge patch, usually varies from 4 to 7. We estimate the second terms for two cases: r is even and r is odd.

For ease of exposition, let $\{m_i\}_{i=1}^r$ denote the other vertices in Ω_{ekl} , where the

Figure 5.1: The edge patch $\Omega_{e_{kl}}$.

subscript $i + 1$ permute cyclically, i.e., $m_{r+1} = m_1$. We give the relationship of outer norm vectors $\mathbf{n}_{kl,m_i}$ and $\mathbf{n}_{lk,m_i}$, which is useful in the estimation of the second terms.

Lemma 5.5. *If all the elements in $\Omega_{e_{kl}}$ satisfy edge pair condition, then*

$$\begin{aligned} \left| \mathbf{n}_{kl,m_i} + \mathbf{n}_{kl,m_{\frac{r}{2}+i}} \right| &\lesssim O(h^\alpha), \quad \text{for } r \text{ is even,} \\ \left| \sum_{i=1}^r \mathbf{n}_{kl,m_i} \right| &= \left| \sum_{i=1}^r \mathbf{n}_{lk,m_i} \right| \lesssim O(h^\alpha), \quad \text{for } r \text{ is odd.} \end{aligned}$$

Remark 5.6. Roughly speaking, if the dihedral angles on edge e_{kl} are equally distributed approximately, these estimates will hold for the outer norm vectors $\mathbf{n}_{kl,m_i}$ and $\mathbf{n}_{lk,m_i}$. The latter estimation also holds for the case r is even. The proof of this lemma is presented in the appendix.

Lemma 5.7. *If all the elements in $\Omega_{e_{kl}}$ satisfy edge pair condition, then*

$$\left| \sum_{\tau \in \Omega_{e_{kl}}} (\gamma_{klm} \eta_{klm} - \gamma_{lko} \eta_{lko}) \right| \lesssim h^{1+\min(\alpha,1)} \int_{\Omega_{e_{kl}}} (|\nabla^2 u| + |\nabla^3 u|),$$

where $u \in W^{3,\infty}(\Omega)$.

Proof. First we consider the case r is even (see Figure 5.1 for example). We emphasize that the local error expansion formula (5.2) is deduced on an element τ_{klmo} with vertex

indices k, l, m, o . When we use it on a specific element, the new vertex indices should be substituted into it. All the elements in $\Omega_{e_{kl}}$ satisfy edge pair condition, i.e.,

$$\begin{aligned} d_{kl} &\simeq d_{m_i m_{i+1}}, \\ d_{km_i} &\simeq d_{lm_{i+1}}, \\ d_{lm_i} &\simeq d_{km_{i+1}}, \quad \text{for } i = 1, 2, \dots, r. \end{aligned}$$

Since r is even, we pair element $\tau_{klm_i m_{i+1}}$ and $\tau'_{klm_{\frac{r}{2}+i} m_{\frac{r}{2}+i+1}}$ together to do the cancellation, for $i = 1, 2, \dots, \frac{r}{2}$. The coefficient $\left| \gamma_{klm_i} - \gamma_{klm_{\frac{r}{2}+i}} \right|$ is estimated by

$$\left| \gamma_{klm_i} - \gamma_{klm_{\frac{r}{2}+i}} \right| \lesssim O(h^{2+\alpha}), \quad (5.8)$$

where γ_{klm_i} is from $\tau_{klm_i m_{i+1}}$ and $\gamma_{klm_{\frac{r}{2}+i}}$ is from $\tau'_{klm_{\frac{r}{2}+i} m_{\frac{r}{2}+i+1}}$. We already know

$$|\eta_{klm_i}| \lesssim h^{-1} \int_{\tau} |\nabla^2 u| + \int_{\tau} |\nabla^3 u|. \quad (5.9)$$

Let

$$\mathbf{n} = \frac{\mathbf{n}_{kl, m_i} + \mathbf{n}_{kl, m_{\frac{r}{2}+i}}}{\left| \mathbf{n}_{kl, m_i} + \mathbf{n}_{kl, m_{\frac{r}{2}+i}} \right|},$$

pairing terms from τ and τ' together and applying Lemma 5.5 and (5.9), we get

$$\begin{aligned}
& \left| \eta_{klm_i} + \eta_{klm_{\frac{r}{2}+i}} \right| \\
&= \left| \frac{1}{\sin \theta_{kl}} \int_{F_k} \varphi_l \varphi_{m_i} \frac{\partial^2 u}{\partial \mathbf{t}_{kl} \partial \mathbf{n}_{kl, m_i}} + \frac{1}{\sin \theta'_{kl}} \int_{F'_k} \varphi_l \varphi_{m_{\frac{r}{2}+i}} \frac{\partial^2 u}{\partial \mathbf{t}_{kl} \partial \mathbf{n}_{kl, m_{\frac{r}{2}+i}}} \right| \\
&= \left| \frac{1}{\sin \theta_{kl}} \int_{F_k} \varphi_l \varphi_{m_i} \frac{\partial^2 u}{\partial \mathbf{t}_{kl} \partial \mathbf{n}_{kl, m_i}} - \frac{1}{\sin \theta'_{kl}} \int_{F'_k} \varphi_l \varphi_{m_{\frac{r}{2}+i}} \frac{\partial^2 u}{\partial \mathbf{t}_{kl} \partial \mathbf{n}_{kl, m_i}} \right. \\
&\quad \left. + \frac{1}{\sin \theta'_{kl}} \int_{F'_k} \varphi_l \varphi_{m_{\frac{r}{2}+i}} \frac{\partial^2 u}{\partial \mathbf{t}_{kl} \partial \mathbf{n}_{kl, m_i}} + \frac{1}{\sin \theta'_{kl}} \int_{F'_k} \varphi_l \varphi_{m_{\frac{r}{2}+i}} \frac{\partial^2 u}{\partial \mathbf{t}_{kl} \partial \mathbf{n}_{kl, m_{\frac{r}{2}+i}}} \right| \quad (5.10) \\
&\lesssim |u|_{3,1,\tau \cup \tau'} + \left| \frac{1}{\sin \theta'_{kl}} \int_{F'_k} \varphi_l \varphi_{m_{\frac{r}{2}+i}} \left(\frac{\partial^2 u}{\partial \mathbf{t}_{kl} \partial \mathbf{n}_{kl, m_i}} + \frac{\partial^2 u}{\partial \mathbf{t}_{kl} \partial \mathbf{n}_{kl, m_{\frac{r}{2}+i}}} \right) \right| \\
&\lesssim |u|_{3,1,\tau \cup \tau'} + \left| \frac{1}{\sin \theta'_{kl}} \int_{F'_k} \varphi_l \varphi_{m_{\frac{r}{2}+i}} \frac{\partial^2 u}{\partial \mathbf{t}_{kl} \partial \mathbf{n}} \right| \times \left| \mathbf{n}_{kl, m_i} + \mathbf{n}_{kl, m_{\frac{r}{2}+i}} \right| \\
&\lesssim |u|_{3,1,\tau \cup \tau'} + h^{\alpha-1} |u|_{2,1,\tau'} + h^\alpha |u|_{3,1,\tau'},
\end{aligned}$$

where estimate (5.5) has been used and the term $\frac{1}{\sin \theta_{kl}} \int_{F_k} \varphi_l \varphi_{m_i} \frac{\partial^2 u}{\partial \mathbf{t}_{kl} \partial \mathbf{n}_{kl, m_i}}$ is from tetrahedron τ and $\frac{1}{\sin \theta'_{kl}} \int_{F'_k} \varphi_l \varphi_{m_{\frac{r}{2}+i}} \frac{\partial^2 u}{\partial \mathbf{t}_{kl} \partial \mathbf{n}_{kl, m_{\frac{r}{2}+i}}}$ is from tetrahedron τ' . Without confusion, if the term $\frac{1}{\sin \theta_{kl}} \int_{F_k} \varphi_l \varphi_{m_i} \frac{\partial^2 u}{\partial \mathbf{t}_{kl} \partial \mathbf{n}_{kl, m_i}}$ is from element τ , then φ_l and φ_{m_i} are the barycentric coordinates defined on that element. This is to say the other coefficient $\left| \eta_{klm_i} + \eta_{klm_{\frac{r}{2}+i}} \right|$ satisfies

$$\left| \eta_{klm_i} + \eta_{klm_{\frac{r}{2}+i}} \right| \lesssim \int_{\tau \cup \tau'} |\nabla^3 u| + h^{\alpha-1} \int_{\tau'} |\nabla^2 u| + h^\alpha \int_{\tau'} |\nabla^3 u|. \quad (5.11)$$

Similarly, we have

$$\left| \eta_{klm_{i+1}} + \eta_{klm_{\frac{r}{2}+i+1}} \right| \lesssim \int_{\tau \cup \tau'} |\nabla^3 u| + h^{\alpha-1} \int_{\tau'} |\nabla^2 u| + h^\alpha \int_{\tau'} |\nabla^3 u|. \quad (5.12)$$

Figure 5.2: An edge patch $\Omega_{e_{kl}}$ with 5 elements.

Noticing $\gamma_{klm_{\frac{r}{2}+i}} \lesssim O(h^2)$ and applying (5.8), (5.9), (5.11) and (5.12), we get

$$\begin{aligned}
& \left| \sum_{\tau \in \Omega_{e_{kl}}} (\gamma_{klm} \eta_{klm} - \gamma_{lko} \eta_{lko}) \right| \\
&= \left| \sum_{i=1}^{r/2} [(\gamma_{klm_i} \eta_{klm_i} + \gamma_{klm_{\frac{r}{2}+i}} \eta_{klm_{\frac{r}{2}+i}}) - (\gamma_{lkm_{i+1}} \eta_{lkm_{i+1}} + \gamma_{lkm_{\frac{r}{2}+i+1}} \eta_{lkm_{\frac{r}{2}+i+1}})] \right| \\
&= \left| \sum_{i=1}^{r/2} \left[(\gamma_{klm_i} - \gamma_{klm_{\frac{r}{2}+i}}) \eta_{klm_i} + (\eta_{klm_i} + \eta_{klm_{\frac{r}{2}+i}}) \gamma_{klm_{\frac{r}{2}+i}} \right. \right. \\
&\quad \left. \left. - (\gamma_{lkm_{i+1}} - \gamma_{lkm_{\frac{r}{2}+i+1}}) \eta_{lkm_{i+1}} - (\eta_{lkm_{i+1}} + \eta_{lkm_{\frac{r}{2}+i+1}}) \gamma_{lkm_{\frac{r}{2}+i+1}} \right] \right| \\
&\lesssim \sum_{i=1}^{r/2} \left[h^{1+\alpha} \int_{\tau \cup \tau'} (|\nabla^2 u| + h |\nabla^3 u|) + h^2 \int_{\tau \cup \tau'} |\nabla^3 u| \right] \\
&\lesssim h^{1+\min(\alpha, 1)} \int_{\Omega_{e_{kl}}} (|\nabla^2 u| + |\nabla^3 u|).
\end{aligned}$$

Second we consider the case r is odd (see Figure 5.2 for example). Similarly all

the elements in $\Omega_{e_{kl}}$ satisfy edge pair condition, i.e.,

$$\begin{aligned} d_{kl} &\simeq d_{m_i m_{i+1}} \quad \text{for } i = 1, 2, \dots, r \\ d_{km_i} &\simeq d_{lm_j} \quad \text{for } i = 1, 2, \dots, r, \quad j = 1, 2, \dots, r. \end{aligned}$$

Let

$$\bar{\mathbf{n}} = \frac{\sum_{i=1}^r (\mathbf{n}_{kl, m_i} + \mathbf{n}_{lk, m_i})}{|\sum_{i=1}^r (\mathbf{n}_{kl, m_i} + \mathbf{n}_{lk, m_i})|},$$

Applying Lemma 5.5, we obtain

$$\begin{aligned} &\left| \sum_{i=1}^r \left(\frac{1}{\sin \theta_{kl}} \int_{F_k} \varphi_l \varphi_{m_i} \frac{\partial^2 u}{\partial \mathbf{t}_{kl} \partial \mathbf{n}_{kl, m_i}} - \frac{1}{\sin \theta_{lk}} \int_{F_l} \varphi_k \varphi_{m_{i+1}} \frac{\partial^2 u}{\partial \mathbf{t}_{lk} \partial \mathbf{n}_{lk, m_{i+1}}} \right) \right| \\ &\lesssim (2r-1) |u|_{3,1, \Omega_{e_{kl}}} + \left| \frac{1}{\sin \theta_{lk}} \int_{F_l} \varphi_k \varphi_{m_1} \frac{\partial^2 u}{\partial \mathbf{t}_{kl} \partial \bar{\mathbf{n}}} \right| \cdot \left| \sum_{i=1}^r (\mathbf{n}_{kl, m_i} + \mathbf{n}_{lk, m_i}) \right| \\ &\lesssim |u|_{3,1, \Omega_{e_{kl}}} + h^{\alpha-1} |u|_{2,1, \tau} + h^\alpha |u|_{3,1, \tau}, \end{aligned}$$

where the trick used in (5.10) has been repeated $2r-1$ times. We emphasize again the terms $\frac{1}{\sin \theta_{kl}} \int_{F_k} \varphi_l \varphi_{m_i} \frac{\partial^2 u}{\partial \mathbf{t}_{kl} \partial \mathbf{n}_{kl, m_i}}$ and $\frac{1}{\sin \theta_{lk}} \int_{F_l} \varphi_k \varphi_{m_{i+1}} \frac{\partial^2 u}{\partial \mathbf{t}_{lk} \partial \mathbf{n}_{lk, m_{i+1}}}$ are from element $\tau_{klm_i m_{i+1}}$ and $\varphi_k, \varphi_l, \varphi_{m_i}, \varphi_{m_{i+1}}$ represent the barycentric coordinates defined on that element. This means the coefficient $|\sum_{i=1}^r (\eta_{klm_i} - \eta_{lk m_{i+1}})|$ satisfies

$$\left| \sum_{i=1}^r (\eta_{klm_i} - \eta_{lk m_{i+1}}) \right| \lesssim \int_{\Omega_{e_{kl}}} |\nabla^3 u| + h^{\alpha-1} \int_{\tau} |\nabla^2 u| + h^\alpha \int_{\tau} |\nabla^3 u|. \quad (5.13)$$

Applying (5.8), (5.9) and (5.13), we have

$$\begin{aligned}
& \left| \sum_{\tau \in \Omega_{e_{kl}}} (\gamma_{klm} \eta_{klm} - \gamma_{lkn} \eta_{lkn}) \right| \\
&= \left| \sum_{i=1}^r (\gamma_{klm_i} \eta_{klm_i} - \gamma_{lkm_{i+1}} \eta_{lkm_{i+1}}) \right| \\
&= |(\gamma_{klm_1} - \gamma_{lkm_2}) \eta_{lkm_2} + (\eta_{klm_1} - \eta_{lkm_2}) \gamma_{klm_1} \\
&\quad + \sum_{i=2}^r (\gamma_{klm_i} \eta_{klm_i} - \gamma_{lkm_{i+1}} \eta_{lkm_{i+1}})| \\
&\lesssim h^{1+\alpha} \int_{\tau} (|\nabla^2 u| + h |\nabla^3 u|) \\
&\quad + |(\gamma_{klm_1} - \gamma_{klm_2})(\eta_{klm_1} - \eta_{lkm_2}) + (\eta_{klm_1} - \eta_{lkm_2} + \eta_{klm_2}) \gamma_{klm_2} \\
&\quad - \gamma_{lkm_3} \eta_{lkm_3} + \sum_{i=3}^r (\gamma_{klm_i} \eta_{klm_i} - \gamma_{lkm_{i+1}} \eta_{lkm_{i+1}})| \\
&\lesssim (2r-1) h^{1+\alpha} \int_{\Omega_{e_{kl}}} (|\nabla^2 u| + h |\nabla^3 u|) + \left| \sum_{i=1}^r (\eta_{klm_i} - \eta_{lkm_{i+1}}) \right| \cdot |\gamma_{klm_r}| \\
&\lesssim h^{1+\min(\alpha,1)} \int_{\Omega_{e_{kl}}} (|\nabla^2 u| + |\nabla^3 u|).
\end{aligned}$$

□

Remark 5.8. Here we emphasize that the edge patch where all the elements satisfy edge pair condition is not necessary to be a point symmetric structure (or a perturbation of a point symmetric structure). The edge patches with odd number of elements are not point symmetric. An example of edge patches with even number of elements

Figure 5.3: An edge patch $\Omega_{e_{kl}}$ with equal edge pair elements but not point symmetric.

is shown in Figure 5.3, where

$$\begin{aligned}
 d_{kl} &= d_{m_i m_{i+1}} = 1, \\
 d_{km_1} &= d_{lm_2} = d_{km_3} = d_{lm_4} = \sqrt{\frac{5+2\sqrt{2}}{8}}, \\
 d_{lm_1} &= d_{km_2} = d_{lm_3} = d_{km_4} = \sqrt{\frac{5-2\sqrt{2}}{8}}, \quad \text{for } i = 1, 2, \dots, 4.
 \end{aligned}$$

Since $d_{km_i} = d_{lm_{i+1}} \neq d_{lm_i} = d_{km_{i+1}}$, $\Omega_{e_{kl}}$ is not a point symmetric set with respect to the midpoint of edge e_{kl} .

Theorem 5.9. *Assume that the tetrahedralization $\mathcal{T}_h$ satisfy edge pair condition (α, σ) , which means the lengths of each pair of opposite edges in most tetrahedrons τ differ only by $O(h^{1+\alpha})$, then,*

$$\left| \sum_{\tau \in \mathcal{T}_h} \int_{\tau} \nabla(u - u_I) \cdot \mathcal{D}_{\tau} \nabla v_h \right| \lesssim h^{1+\rho} \|u\|_{3,\infty,\Omega} |v_h|_{1,\Omega}, \quad \rho = \min(\alpha, \frac{\sigma}{2}, 1), \quad (5.14)$$

where $u_I \in \mathcal{V}_h$ is the interpolation of u and $u \in W^{3,\infty}(\Omega)$.

Proof. We apply the fundamental identity to get

$$\begin{aligned}
& \sum_{\tau \in \mathcal{T}_h} \int_{\tau} \nabla(u - u_I) \cdot \mathcal{D}_{\tau} \nabla v_h \\
&= \sum_{\tau \in \mathcal{T}_h} \sum_{k,l=1, k \neq l}^4 \frac{\partial v_h}{\partial \mathbf{t}_{kl}} \frac{\xi_{kl}}{4} ((\zeta_{klm} \chi_{klm} - \zeta_{lko} \chi_{lko}) - (\gamma_{klm} \eta_{klm} - \gamma_{lko} \eta_{lko})) \\
&= I_1 + I_2,
\end{aligned}$$

where

$$I_i = \sum_{e_{kl} \in \mathcal{E}_i} \sum_{\tau \in \Omega_{e_{kl}}} \frac{\partial v_h}{\partial \mathbf{t}_{kl}} \frac{\xi_{kl}}{4} ((\zeta_{klm} \chi_{klm} - \zeta_{lko} \chi_{lko}) - (\gamma_{klm} \eta_{klm} - \gamma_{lko} \eta_{lko})),$$

for $i = 1, 2$. $\mathcal{E}_1$ is the set of edges e such that all the tetrahedrons contained in the edge patch Ω_e satisfy the condition that the lengths of opposite edges differ only by $O(h^{1+\alpha})$ and $\mathcal{E}_2$ is the set of remaining edges.

Applying Lemma 5.4 and 5.7, I_1 is estimated by

$$|I_1| \lesssim h^{1+\min(\alpha,1)} \int_{\Omega} (|\nabla^2 u| + |\nabla^3 u|) |\nabla v_h|. \quad (5.15)$$

Then we turn to estimate I_2 . Since the tetrahedrons in $\Omega_{2,h}$ do not satisfy the condition that the opposite edge lengths differ by $O(h^{1+\alpha})$, we simply estimate

$$\begin{aligned}
|\zeta_{klm} - \zeta_{lko}| &\leq |\zeta_{klm}| + |\zeta_{lko}| \lesssim O(h^2), \\
|\gamma_{klm} - \gamma_{lko}| &\leq |\gamma_{klm}| + |\gamma_{lko}| \lesssim O(h^2).
\end{aligned}$$

For a tetrahedron $\tau \in \mathcal{T}_{2,h}$, we have the following interpolant estimation

$$\begin{aligned}
& \int_{\tau} \nabla(u - u_I) \cdot \mathcal{D}_{\tau} \nabla v_h \\
& \lesssim h \int_{\tau} (|\nabla^2 u| + h |\nabla^3 u|) |\nabla v_h| + h^2 \int_{\tau} |\nabla^3 u| |\nabla v_h|.
\end{aligned}$$

This leads to

$$\begin{aligned}
|I_2| &\lesssim h \sum_{\tau \in \mathcal{T}_{2,h}} \int_{\tau} (|\nabla^2 u| + h |\nabla^3 u|) |\nabla v_h| \\
&\lesssim h \|u\|_{3,\infty,\Omega} \sum_{\tau \in \mathcal{T}_{2,h}} \int_{\tau} |\nabla v_h| \\
&\lesssim h^{1+\frac{\sigma}{2}} \|u\|_{3,\infty,\Omega} \|\nabla v_h\|_{0,\Omega_{2,h}},
\end{aligned} \tag{5.16}$$

where the well-known Cauchy-Schwarz inequality has been used. Finally combining (5.15) and (5.16), we obtain (5.14). $\square$

Theorem 5.10. *Assume that the solution of (4.1) satisfies $u \in W^{3,\infty}(\Omega)$. Further, assume the hypotheses of Theorem 5.9 and let $\mathcal{D}_{\tau}$ be a piecewise constant matrix function defined on $\mathcal{T}_h$, whose elements $\mathcal{D}_{\tau ij}$ satisfy*

$$|\mathcal{D}_{\tau ij}| \lesssim 1, \quad |\mathcal{D}_{\tau ij} - \mathcal{D}_{\tau' ij}| \lesssim h^{\alpha},$$

for $i, j = 1, 2, 3$. Here τ and τ' are tetrahedrons sharing a common edge. Then

$$\|u_h - u_I\|_{1,\Omega} \lesssim h^{1+\rho} \|u\|_{3,\infty,\Omega}, \quad \rho = \min(\alpha, \frac{\sigma}{2}, 1),$$

where $u \in W^{3,\infty}(\Omega)$.

Proof. We begin with the identity

$$\begin{aligned}
B(u - u_I, v_h) &= \sum_{\tau \in \mathcal{T}_h} \int_{\tau} \nabla(u - u_I) \cdot \mathcal{D}_{\tau} \nabla v_h \, dx + \sum_{\tau \in \mathcal{T}_h} \int_{\tau} \nabla(u - u_I) \cdot (\mathcal{D} - \mathcal{D}_{\tau}) \nabla v_h \, dx \\
&\quad + \int_{\Omega} (u - u_I)(\mathbf{b} \cdot \nabla v_h + c v_h) \, dx = I_1 + I_2 + I_3.
\end{aligned}$$

The first term I_1 is estimated by Theorem 5.9. I_2 and I_3 can be easily estimated by

$$|I_2| \lesssim h^{1+\alpha} \|u\|_{2,\Omega} \|v_h\|_{1,\Omega}, \quad |I_3| \lesssim h^2 \|u\|_{2,\Omega} \|v_h\|_{1,\Omega}$$

Thus

$$|B(u - u_I, v_h)| \lesssim h^{1+\rho} \|u\|_{3,\infty,\Omega} \|v_h\|_{1,\Omega}.$$

We complete the proof using the fact that

$$\begin{aligned} \mu \|u_h - u_I\|_{1,\Omega} &\leq \sup_{v_h \in \mathcal{V}_h} \frac{B(u_h - u_I, v_h)}{\|v_h\|_{1,\Omega}} \\ &= \sup_{v_h \in \mathcal{V}_h} \frac{B(u - u_I, v_h)}{\|v_h\|_{1,\Omega}} \\ &\lesssim h^{1+\rho} \|u\|_{3,\infty,\Omega}. \end{aligned}$$

□

5.3 Numerical substantiation

In this section, we present a few numerical examples to verify the theoretical results deduced in previous sections.

The linear finite element solution of the following Poisson equation is considered

$$\begin{aligned} -\Delta u &= f \quad \text{in } \Omega \\ u &= g \quad \text{on } \partial\Omega \end{aligned} \tag{5.17}$$

where Ω is a 3D-bounded Lipschitz domain with boundary $\partial\Omega$, f and g are smooth, and the solution u of equation (5.17) is assumed to be sufficiently smooth. The right hand side f is chosen to be $3\sin(x+y+z)$, thus the exact solution is $u = \sin(x+y+z)$ and the boundary condition is properly imposed.

The first experiment is conducted on Par6 tessellation which is an assembly that can be repeated indefinitely to fill space [76]. Par6 assembly is obtained by distorting a cube into a parallelepiped involving a 35.3° rotation of the edges about the y- and z-axis. And then each parallelepiped is divided into six identical tetrahedrons. Furthermore, the four faces of these tetrahedrons are all the same—an isosceles triangle with one edge of length p and the other two of length $\sqrt{3}p/2$. Repeating this assembly

to get Par6 tessellation (see Figure 4.2). Par6 tessellation is predicted as the optimal CVDT meshes in three dimensional space by Gersho's conjecture [78], which states that: *asymptotically speaking, all cells of the optimal CVT, while forming a tessellation, are congruent to a basic cell which depends on the dimension.* This claim is trivially true in one dimension. It has been proved for the two-dimensional case [79] with the basic cell being the two-dimensional regular hexagon. Gersho's conjecture remains open for three and higher dimensions [80].

Par6 meshes satisfy our edge pair condition perfectly. The mesh is composed of the unique element, in which the opposite edge lengths are exactly the same. Thus α and σ in our geometric condition approach to ∞ . From Theorem 5.10, we can see that the superconvergence order of interpolant estimate $\|\nabla(u_h - u_I)\|_{0,\Omega}$ should be 2. The numerical experiments are conducted on a sequence of meshes with the sizes being $h = 0.100, 0.050, 0.033, 0.025$. The error estimation and convergence order are shown in Table 4.2 and Figure 4.6. The convergence order corresponds to the absolute value of slope in the figure, which is approximately 2, coinciding with our theoretical results exactly.

The second experiment is conducted on a consequence of perturbational Par6 tessellations. We keep the connection unchanged and give a small perturbation to the vertices position so that the perturbational Par6 tessellation does not satisfy the edge pair condition perfectly. The perturbation quantity is chosen to be $0.025 \times h_0, 0.05 \times h_0, 0.1 \times h_0$, where h_0 is the original mesh size, respectively. To check the edge pair condition (α, σ) , we evaluate an α_0 value on each element in following way: the length difference of opposite edges in this element is controlled by $c \times h^{1+\alpha_0}$, where c is a constant with a value 1 approximately. Recalling Definition 5.1, the whole computational domain is divided into a "good" region $\mathcal{T}_{1,h}$ and a "bad" region $\mathcal{T}_{2,h}$ by a threshold α . If $\alpha_0 \geq \alpha$, that element belongs to $\mathcal{T}_{1,h}$. Otherwise, it belongs to $\mathcal{T}_{2,h}$. For the Par6 mesh with perturbation size $0.025 \times h_0$, the threshold is chosen to 0.80 and condition $(0.80, \infty)$ is satisfied. For the Par6 mesh with perturbation size $0.050 \times h_0$, condition $(0.70, \infty)$ is satisfied and for the Par6 mesh with perturbation size $0.100 \times h_0$, condition $(0.50, \infty)$ is satisfied. We can see that the superconvergence order on perturbational Par6 meshes decays as long as the perturbation size increases.

Table 5.1: Error estimation and convergence order of the recovered gradient on perturbational Par6.

Mesh size h	Perturbation size $0.025 \times h_0$	Error estimate $\ \nabla(u_h - u_I)\ _{0,\Omega}$
1.26e-1	2.50e-3	2.41e-3
6.36e-2	1.25e-3	6.45e-4
4.25e-2	8.35e-4	3.05e-4
3.19e-2	6.25e-4	1.69e-4
Order	—	1.91
Mesh size h	Perturbation size $0.050 \times h_0$	Error estimate $\ \nabla(u_h - u_I)\ _{0,\Omega}$
1.26e-1	5.00e-3	2.46e-3
6.37e-2	2.50e-3	6.96e-4
4.26e-2	1.67e-3	3.63e-4
3.20e-2	1.25e-3	1.92e-4
Order	—	1.78
Mesh size h	Perturbation size $0.100 \times h_0$	Error estimate $\ \nabla(u_h - u_I)\ _{0,\Omega}$
1.27e-1	1.00e-2	2.68e-3
6.38e-2	5.00e-3	8.67e-4
4.27e-2	3.33e-3	5.17e-4
3.21e-2	2.50e-3	2.65e-4
Order	—	1.55

The error estimation and convergence order are shown in Figure 5.4 and Table 5.1.

To illustrate the fact that edge patches where all the elements satisfy edge pair condition are not necessary to be point symmetric, we give the following definition of the point symmetry set. An edge patch $\Omega_{e_{kl}}$ is called point symmetric if

$$\mathbf{p}_0 - (\mathbf{p}_{m_i} - \mathbf{p}_0) \in \mathcal{B}(\mathbf{p}_{m_j}), \quad \text{for } i = 1, \dots, r,$$

where $\mathbf{p}_0$ is the midpoint of edge e_{kl} and $\mathcal{B}(\mathbf{p}_{m_j}) = \{\mathbf{x} : |\mathbf{x} - \mathbf{p}_{m_j}| < c \times h^{1+\alpha}\}$ is the neighborhood of some point $\mathbf{p}_{m_j}$ in edge patch $\Omega_{e_{kl}}$. See [48, 86] for details.

The following two experiments are preliminary explorations on unstructured meshes. For the third experiment, the Poisson equation (5.17) is solved on a sequence of unstructured CVDT meshes on a cubic domain $[0, 1]^3$ (see Figure 5.5). For this example,

Figure 5.4: Error estimation and convergence rate of the recovered gradient on perturbational Par6.

Table 5.2: The volume of elements that do not satisfy edge pair condition (upper) and the volume of edge patches that are not symmetric (lower) on the cubic CVDT mesh under different threshold α and constant c . The size of the domain is 1.

The volume of elements that do not satisfy edge pair condition				
$\alpha, c \backslash h$	0.10	7.56e-2	5.00e-2	3.48e-2
$\alpha = 0.40, c = 1$	4.03e-3	3.42e-3	3.06e-3	6.26e-3
$\alpha = 0.45, c = 1$	6.04e-3	6.15e-3	9.35e-3	2.37e-2
The volume of edge patches that are not symmetric				
$\alpha, c \backslash h$	0.10	7.56e-2	5.00e-2	3.48e-2
$\alpha = 0.40, c = 1$	4.80e-2	0.11	0.29	0.45
$\alpha = 0.45, c = 1$	0.13	0.24	0.46	0.62

the threshold α is chosen to be 0.45 and c is 1 so that condition (0.45, 1.56) is satisfied. With the same threshold α and constant c , the edge patches which are not point symmetric occupy a volume of size 0.80 compared to the total volume 1.00. The size of $\mathcal{T}_{2,h}$ and the size of edge patches that are not point symmetric on the cubic CVDT mesh are given in Table 5.2. We can see that our edge pair condition trends to be satisfied by unstructured meshes while the point symmetry condition does not. The error estimation and convergence order are shown in Figure 5.6 and Table 5.4.

The fourth experiment is conducted on a spherical domain $\{\mathbf{x} : |\mathbf{x}| \leq 1\}$ (see Figure 5.5). For this example, the threshold is chosen to be 0.50 and c is 1 so that condition (0.50, 1.75) is satisfied. The edge patches with edge pair condition satisfied but not point symmetric occupy a volume of size 1.14 compared to the total volume $\frac{4}{3}\pi$. The size of $\mathcal{T}_{2,h}$ and the size of edge patches that are not point symmetric on the spherical CVDT mesh are given in Table 5.3. The error estimation and convergence order are also shown in Figure 5.6 and Table 5.4.

(a) CVDT mesh on a cubic domain

(b) CVDT mesh on a spherical domain

Figure 5.5: CVDT meshes

Table 5.3: The volume of elements that do not satisfy edge pair condition (upper) and the volume of edge patches that are not symmetric (lower) on the spherical CVDT mesh under different threshold α and constant c . The size of the domain is $\frac{4}{3}\pi$.

The volume of elements that do not satisfy edge pair condition				
$\alpha, c \backslash h$	0.14	9.55e-2	8.61e-2	5.92e-2
$\alpha = 0.40, c = 1$	0	1.40e-3	2.27e-3	2.82e-3
$\alpha = 0.50, c = 1$	1.09e-3	1.65e-2	3.52e-2	5.81e-2
The volume of edge patches that are not symmetric				
$\alpha, c \backslash h$	0.14	9.55e-2	8.61e-2	5.92e-2
$\alpha = 0.40, c = 1$	0.15	0.21	0.33	0.81
$\alpha = 0.50, c = 1$	0.76	1.14	1.47	2.82

Table 5.4: Error estimation and convergence order of the recovered gradient on CVDT meshes. The upper table is for the cubic domain and the lower one is for the spherical domain.

Mesh size h	Error estimate $\ \nabla(u_h - u_I)\ _{0,\Omega}$
0.101	6.02e-3
7.56e-2	4.11e-3
5.00e-2	2.16e-3
3.48e-2	1.33e-3
Order	1.47

Mesh size h	Error estimate $\ \nabla(u_h - u_I)\ _{0,\Omega}$
0.224	2.42e-2
0.140	1.08e-2
9.55e-2	5.56e-3
5.92e-2	2.77e-3
Order	1.58

Figure 5.6: Error estimation and convergence rate of the recovered gradient on CVDT meshes. The left graph is for the cubic domain and the right one is for the spherical domain.

5.4 Preliminary exploration on superconvergence in high dimensional space

In this section, we extend the theoretical analysis in section 5.2 to n ($n > 3$) dimensional spaces briefly and show that the 4-simplex mesh satisfying edge pair condition does not exist in four dimensional space.

The following lemma is analogous to the fundamental lemma (Lemma 5.2) in three dimensions.

Lemma 5.11. *Assume τ is a n -simplex in n dimensional spaces. For $v_h \in P_1(\tau)$ and $\phi \in H^3(\tau)$, we have*

$$\begin{aligned} & \int_{\tau} \nabla(\phi_I - \phi) \cdot \mathcal{D}_{\tau} \nabla v_h \\ &= \sum_{k,l=1,k < l}^{n+1} \frac{\partial v_h}{\partial \mathbf{t}_{kl}} \frac{\xi_{kl}}{4} \left\{ \sum_{m=1,m \neq k,l}^{n+1} ((\zeta_{klm} \chi_{klm} - \zeta_{lko} \chi_{lko}) + \right. \\ & \quad \left. (\gamma_{klm} \eta_{klm} - \gamma_{lko} \eta_{lko})) \right\} + O(h^3) \|\phi\|_{3,\tau} \|v_h\|_{1,\tau}, \end{aligned} \quad (5.18)$$

where

$$\begin{aligned} \zeta_{klm} &= d_{lm}^2 - d_{km}^2, \\ \gamma_{klm} &= 4 |\triangle_{klm}|, \\ \chi_{klm} &= \frac{1}{\mathbf{n}_l \cdot \mathbf{t}_{kl}} \int_{\mathbf{F}_k} \varphi_l \varphi_m \frac{\partial^2 \phi}{\partial \mathbf{t}_{kl}^2}, \\ \eta_{klm} &= \frac{1}{\mathbf{n}_l \cdot \mathbf{t}_{kl}} \int_{\mathbf{F}_k} \varphi_l \varphi_m \frac{\partial^2 \phi}{\partial \mathbf{t}_{kl} \partial \mathbf{n}_{kl,m}}. \end{aligned}$$

o is chosen to be different from m and o traverse all the other vertices except k, l . Thus $\triangle_{klmo}^3$ is a 3-face in τ .

Proof. From Lemma 4.6 we have

$$\begin{aligned}
& \int_{\tau} \nabla(\phi_I - \phi) \cdot \mathcal{D}_{\tau} \nabla v_h \\
&= \sum_{k,l=1,k \neq l}^{n+1} \frac{\partial v_h}{\partial \mathbf{t}_{kl}} \frac{\xi_{kl}}{4 \mathbf{n}_l \cdot \mathbf{t}_{kl}} \left(\sum_{m=1,m \neq k,l}^{n+1} \int_{\mathbf{F}_k} \varphi_l \varphi_m [(d_{lm}^2 - d_{km}^2) \frac{\partial^2 \phi}{\partial \mathbf{t}_{kl}^2} \right. \\
&\quad \left. + 4 |\Delta_{klm}| \frac{\partial^2 \phi}{\partial \mathbf{t}_{kl} \partial \mathbf{n}_{kl,m}}] \right) \\
&= \sum_{k,l=1,k < l}^{n+1} \frac{\partial v_h}{\partial \mathbf{t}_{kl}} \frac{\xi_{kl}}{4 \mathbf{n}_l \cdot \mathbf{t}_{kl}} \left(\sum_{m=1,m \neq k,l}^{n+1} \int_{\mathbf{F}_k} \varphi_l \varphi_m [(d_{lm}^2 - d_{km}^2) \frac{\partial^2 \phi}{\partial \mathbf{t}_{kl}^2} \right. \\
&\quad \left. + 4 |\Delta_{klm}| \frac{\partial^2 \phi}{\partial \mathbf{t}_{kl} \partial \mathbf{n}_{kl,m}}] \right) + \sum_{k,l=1,k > l}^{n+1} \frac{\partial v_h}{\partial \mathbf{t}_{kl}} \frac{\xi_{kl}}{4 \mathbf{n}_l \cdot \mathbf{t}_{kl}} \left(\sum_{o=1,o \neq k,l}^{n+1} \right. \\
&\quad \left. \int_{\mathbf{F}_k} \varphi_l \varphi_o [(d_{lo}^2 - d_{ko}^2) \frac{\partial^2 \phi}{\partial \mathbf{t}_{kl}^2} + 4 |\Delta_{klo}| \frac{\partial^2 \phi}{\partial \mathbf{t}_{kl} \partial \mathbf{n}_{kl,o}}] \right) \\
&= \sum_{k,l=1,k < l}^{n+1} \frac{\partial v_h}{\partial \mathbf{t}_{kl}} \frac{\xi_{kl}}{4 \mathbf{n}_l \cdot \mathbf{t}_{kl}} \left(\sum_{m=1,m \neq k,l}^{n+1} \int_{\mathbf{F}_k} \varphi_l \varphi_m [(d_{lm}^2 - d_{km}^2) \frac{\partial^2 \phi}{\partial \mathbf{t}_{kl}^2} \right. \\
&\quad \left. + 4 |\Delta_{klm}| \frac{\partial^2 \phi}{\partial \mathbf{t}_{kl} \partial \mathbf{n}_{kl,m}}] \right) + \sum_{k,l=1,k < l}^{n+1} \frac{\partial v_h}{\partial \mathbf{t}_{lk}} \frac{\xi_{kl}}{4 \mathbf{n}_k \cdot \mathbf{t}_{lk}} \left(\sum_{o=1,o \neq k,l}^{n+1} \right. \\
&\quad \left. \int_{\mathbf{F}_l} \varphi_k \varphi_o [(d_{ko}^2 - d_{lo}^2) \frac{\partial^2 \phi}{\partial \mathbf{t}_{lk}^2} + 4 |\Delta_{lko}| \frac{\partial^2 \phi}{\partial \mathbf{t}_{lk} \partial \mathbf{n}_{lk,o}}] \right) \\
&= \sum_{k,l=1,k < l}^{n+1} \frac{\partial v_h}{\partial \mathbf{t}_{kl}} \frac{\xi_{kl}}{4} \left\{ \sum_{m=1,m \neq k,l}^{n+1} \left(\left[\frac{(d_{lm}^2 - d_{km}^2)}{\mathbf{n}_l \cdot \mathbf{t}_{kl}} \int_{\mathbf{F}_k} \varphi_l \varphi_m \frac{\partial^2 \phi}{\partial \mathbf{t}_{kl}^2} \right. \right. \right. \\
&\quad \left. \left. - \frac{(d_{ko}^2 - d_{lo}^2)}{\mathbf{n}_k \cdot \mathbf{t}_{lk}} \int_{\mathbf{F}_l} \varphi_k \varphi_o \frac{\partial^2 \phi}{\partial \mathbf{t}_{lk}^2} \right] + \left[4 \frac{|\Delta_{klm}|}{\mathbf{n}_l \cdot \mathbf{t}_{kl}} \int_{\mathbf{F}_k} \varphi_l \varphi_m \frac{\partial^2 \phi}{\partial \mathbf{t}_{kl} \partial \mathbf{n}_{kl,m}} \right. \right. \\
&\quad \left. \left. - 4 \frac{|\Delta_{lko}|}{\mathbf{n}_k \cdot \mathbf{t}_{lk}} \int_{\mathbf{F}_l} \varphi_k \varphi_o \frac{\partial^2 \phi}{\partial \mathbf{t}_{lk} \partial \mathbf{n}_{lk,o}} \right] \right) \right\} \\
&= \sum_{k,l=1,k < l}^{n+1} \frac{\partial v_h}{\partial \mathbf{t}_{kl}} \frac{\xi_{kl}}{4} \left\{ \sum_{m=1,m \neq k,l}^{n+1} \left((\zeta_{klm} \chi_{klm} - \zeta_{lko} \chi_{lko}) + \right. \right. \\
&\quad \left. \left. (\gamma_{klm} \eta_{klm} - \gamma_{lko} \eta_{lko}) \right) \right\}.
\end{aligned}$$

□

Remark 5.12. Observing this n dimensional fundamental lemma, we find that it is quite similar to the three dimensional version except the coefficients of $\frac{v_h}{t_{kl}}$ are on 3-faces instead of the whole tetrahedron.

Based on Remark 5.12, we raise the following edge pair condition in n dimensional space.

Definition 5.13. *In n dimensional spaces ($n > 3$), The mesh $\mathcal{T}_h = \mathcal{T}_{1,h} \cup \mathcal{T}_{2,h}$ is said to satisfy condition (α, σ) if there exist positive constant α and σ such that: The lengths of each pair of opposite edges in each 3-face of every n -simplex inside $\mathcal{T}_{1,h}$ differ only by $O(h^{1+\alpha})$ and*

$$\bar{\Omega}_{1,h} \cup \bar{\Omega}_{2,h} = \bar{\Omega}, \quad |\Omega_{2,h}| = O(h^\sigma), \quad \bar{\Omega}_{i,h} \equiv \cup_{\tau \in \mathcal{T}_{i,h}} \bar{\tau}, \quad i = 1, 2.$$

With the n dimensional edge pair condition holds and using the same technic in Lemma 5.4 and Lemma 5.7, we can analogously obtain the superconvergent interpolant estimate in n dimensional space. Here we emphasize that this procedure needs the lengths of each pair of opposite edges in all the 3-faces in every n -simplex inside $\mathcal{T}_{1,h}$ diff only by a high order term. However, we do not want to present these formal results here, since the following theorem is found.

Theorem 5.14. *The 4-simplex mesh satisfying edge pair condition does not exist in four dimensional spaces.*

Proof. The dihedral angle of the regular 4-simplex is $\alpha = \arccos \frac{1}{4} \approx 76^\circ$. Consequently, $k\alpha \neq 360^\circ$ for any integer k . This means that the regular 4-simplex is not a space-filler.

In a pentatope, there are 5 vertices, 10 edges, 10 faces and 5 cells (3-face) which are tetrahedrons in three dimensions. The following two facts are used in our arguments:

- each edge is surrounded by three cells.
- every two cells meet only at a common face.

There are three position relationships between two edges:

- belong to the same face.
- belong to the same cell, but not on the same face. That is to say they are opposite edges in a cell.
- not belong to the same cell.

Without losing generality, we consider the extreme situation of edge pair condition, i.e., the lengths of each pair of opposite edges in each 3-face of every n -simplex are equal. Assuming τ is a space filling pentatope, there must be edges of at least 2 lengths. For the case there are two types of edges, say a, b , let k be the number of edges of length a , then there are $10 - k$ edges of length b .

$k = 1$ the 4-simplex does not satisfy edge pair condition.

$k = 2$ if these two edges belong to the same face, then the pentatope does not satisfy edge pair condition. If they belong to the same cell and not on the same face, that cell satisfies edge pair condition. But since every two cells meet only at a common face, they belong to the other two different cells, respectively. Thus the 4-simplex does not satisfy edge pair condition.

$k = 3$ since one edge is surrounded by three cells, one edge appear three times when we check the edge pair condition, thus 3 edges appear 9 times totally. So the 4-simplex does not satisfy edge pair condition.

$k = 4$ since one edge is surrounded by three cells, if we want the pentatope to satisfy the edge pair condition, we need to put the other three edges on its opposite position in these three cells respectively. But there must be a cell that constructed all by other type of edges to be the neighbor of one of these three cells. Thus the 4-simplex does not satisfy edge pair condition.

$k = 5$ same as the case $k = 3$, the 4-simplex does not satisfy edge pair condition.

The cases that there are more than 2 types of edge lengths are even worse. So the 4-simplex mesh satisfying edge pair condition does not exist in four dimensional spaces. $\square$

5.5 Appendix

This appendix is devoted to proof Lemma 5.5 with the help of *Cayley-Menger bideterminant*.

The *Cayley-Menger bideterminant* of two sequences of n points, $[\mathbf{p}_1, \dots, \mathbf{p}_n]$ and $[\mathbf{q}_1, \dots, \mathbf{q}_n]$ is defined as

$$D(\mathbf{p}_1, \dots, \mathbf{p}_n; \mathbf{q}_1, \dots, \mathbf{q}_n) = 2\left(\frac{-1}{2}\right)^n \begin{vmatrix} 0 & 1 & 1 & 1 & 1 \\ 1 & D(\mathbf{p}_1, \mathbf{q}_1) & D(\mathbf{p}_1, \mathbf{q}_2) & \cdots & D(\mathbf{p}_1, \mathbf{q}_n) \\ 1 & D(\mathbf{p}_2, \mathbf{q}_1) & D(\mathbf{p}_2, \mathbf{q}_2) & \cdots & D(\mathbf{p}_2, \mathbf{q}_n) \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & D(\mathbf{p}_n, \mathbf{q}_1) & D(\mathbf{p}_n, \mathbf{q}_2) & \cdots & D(\mathbf{p}_n, \mathbf{q}_n) \end{vmatrix},$$

where $D(\mathbf{p}_i, \mathbf{q}_j)$ denotes the squared distance between the points $\mathbf{p}_i$ and $\mathbf{q}_j$. This determinant plays a fundamental role in the so-called "distance geometry", a term coined by Blumenthal in [91] which refers to the analytical study of Euclidean geometry in terms of invariants, without resorting to artificial coordinate systems. Since in many cases of interest the two sequences of points are the same, it will be convenient to abbreviate $D(\mathbf{p}_1, \dots, \mathbf{p}_n; \mathbf{p}_1, \dots, \mathbf{p}_n)$ by $D(\mathbf{p}_1, \dots, \mathbf{p}_n)$, which is simply called a *Cayley-Menger determinant*. We will use the geometric interpretation of these determinants for $n = 3$ in the proof of Lemma 5.5. For further details, the reader is referred to [92, pp. 126–129] and [93].

Proof. Let S_i denote the area of triangle $\triangle_{klm_i}$ and β_i is the dihedral angle between face $\triangle_{klm_i}$ and $\triangle_{klm_{i+1}}$. We assume all the elements in $\Omega_{e_{kl}}$ satisfy edge pair condition.

Specifically, for element $\tau_{klm_i m_{i+1}}$ and $\tau'_{klm_{i+1} m_{i+2}}$, $i = 1, \dots, r-1$,

$$\begin{aligned}
d_{kl} &= d_{kl}, \\
d_{km_i} &\simeq d_{lm_{i+1}}, \\
d_{km_{i+1}} &\simeq d_{lm_{i+2}}, \\
d_{lm_i} &\simeq d_{km_{i+1}}, \\
d_{lm_{i+1}} &\simeq d_{km_{i+2}}, \\
d_{m_i m_{i+1}} &\simeq d_{m_{i+1} m_{i+2}},
\end{aligned}$$

which means the corresponding edge lengths in $\tau_{klm_i m_{i+1}}$ and $\tau'_{klm_{i+1} m_{i+2}}$ are same or nearly same. As a consequence, $\tau_{klm_i m_{i+1}}$ and $\tau'_{klm_{i+1} m_{i+2}}$ are of the same shape approximately. Thus dihedral angles β_i and β_{i+1} , which are corresponding angles, are roughly the same. More precisely, we will give a quantitative analysis for this statement.

Using the *Cayley-Menger determinant*, we obtain Herron's formula relating S_i with the side lengths

$$D(\mathbf{p}_k, \mathbf{p}_l, \mathbf{p}_{m_i}) = \|(\mathbf{p}_l - \mathbf{p}_k) \times (\mathbf{p}_{m_i} - \mathbf{p}_k)\|^2 = 4S_i^2. \quad (5.19)$$

It can be shown that

$$\begin{aligned}
&D(\mathbf{p}_k, \mathbf{p}_{m_{i+1}}, \mathbf{p}_l; \mathbf{p}_k, \mathbf{p}_l, \mathbf{p}_{m_i}) \\
&= ((\mathbf{p}_k - \mathbf{p}_l) \times (\mathbf{p}_{m_{i+1}} - \mathbf{p}_l)) \cdot ((\mathbf{p}_k - \mathbf{p}_{m_i}) \times (\mathbf{p}_l - \mathbf{p}_{m_i})) \\
&= 4S_i S_{i+1} \cdot \cos \beta_i.
\end{aligned}$$

Using Herron's formula (5.19), we have

$$\begin{aligned}
\cos \beta_i &= \frac{D(\mathbf{p}_k, \mathbf{p}_{m_{i+1}}, \mathbf{p}_l; \mathbf{p}_k, \mathbf{p}_l, \mathbf{p}_{m_i})}{D^{\frac{1}{2}}(\mathbf{p}_k, \mathbf{p}_{m_{i+1}}, \mathbf{p}_l) D^{\frac{1}{2}}(\mathbf{p}_k, \mathbf{p}_l, \mathbf{p}_{m_i})} \\
&= \frac{D(\mathbf{p}_k, \mathbf{p}_{m_{i+1}}, \mathbf{p}_l; \mathbf{p}_k, \mathbf{p}_l, \mathbf{p}_{m_i})}{4S_i S_{i+1}},
\end{aligned} \quad (5.20)$$

which is the formula for the cosine of β_i in terms of edge lengths. The area difference between face $\triangle_{klm_i}$ and $\triangle_{klm_{i+1}}$ is estimated by

$$|S_i - S_{i+1}| \lesssim O(h^{2+\alpha}).$$

Applying (5.20), a direct calculation shows that

$$|\cos \beta_i - \cos \beta_{i+1}| \lesssim O(h^\alpha).$$

Following the mean value property, we get

$$\frac{\cos \beta_i - \cos \beta_{i+1}}{\beta_{i+1} - \beta_i} = \sin \theta,$$

where θ is a value between β_i and β_{i+1} . The regularity of tetrahedralization $\mathcal{T}_h$ requires $\beta_i, \beta_{i+1} > \theta_0 > 0$, where θ_0 is the lower bound of the dihedral angle in $\mathcal{T}_h$. Therefore $\frac{1}{\sin \theta}$ is a constant related to the minimum dihedral angle in $\mathcal{T}_h$. Thus

$$|\beta_{i+1} - \beta_i| \lesssim O(h^\alpha).$$

Going a step further, we have

$$|\beta_i - \beta_j| \lesssim O(h^\alpha), \quad i \neq j, \quad i, j = 1, \dots, r.$$

Since $\sum_{i=1}^r \beta_i = 2\pi$, we obtain

$$\left| \beta_i - \frac{2\pi}{r} \right| \lesssim O(h^\alpha), \quad i = 1, \dots, r.$$

Noticing $\mathbf{n}_{kl,m_i}$ and $\mathbf{n}_{lk,m_i}$ are unit outer norm vectors, at last we achieve

$$\begin{aligned} \left| \mathbf{n}_{kl,m_i} + \mathbf{n}_{kl,m_{\frac{r}{2}+i}} \right| &\lesssim O(h^\alpha), \quad \text{for } r \text{ is even,} \\ \left| \sum_{i=1}^r \mathbf{n}_{kl,m_i} \right| &= \left| \sum_{i=1}^r \mathbf{n}_{lk,m_i} \right| \lesssim O(h^\alpha), \quad \text{for } r \text{ is odd.} \end{aligned}$$

Chapter 6

ADAPTIVE TETRAHEDRAL MESH GENERATION BY CONFORMING CENTROIDAL VORONOI-DELAUNAY TESSELLATIONS FOR FINITE ELEMENT METHODS

6.1 Introduction

It is well recognized that the application of adaptive mesh refinements based on a posteriori error estimators is an effective means to ensure the accuracy and efficiency of a finite element solution process. The main issues in designing reliable and efficient adaptive finite element methods are the mesh size and mesh quality, which can be addressed by a posteriori error estimators and mesh adaptivity techniques, respectively. Both mesh adaptivity and a posteriori error estimators have been extensively studied, beginning in the late 1970s [94, 95, 96, 97] and followed by a vast literature,

the key objectives of which are that an existing mesh is refined in such a way that the errors in the approximate solution of the PDE on the new mesh are distributed as uniformly as possible, that those approximate solutions converge, as the mesh size decreases, to the exact solution as well as can be expected, and that the first two objectives are met with a relatively simple complexity.

The term *a posteriori* means that the estimate is built upon the computed approximation. There are several types of *a posteriori* error estimators used in finite element methods, e.g., explicit estimator, hierarchical method, residual-type and recovery-type methods, among which the residual-type and recovery-type methods have been widely accepted. The residual based error estimators were first introduced by Babuška-Rheinboldt in 1978 [10] and have been studied by many others. Zienkiewicz-Zhu (Z-Z) introduced first, in 1987, the recovery based error estimators, then in 1992, the Superconvergent Patch Recovery (SPR) using local discrete least-squares fitting [88, 55, 56]. Recently, Zhang and Naga raised another recovery based method, the Polynomial-Preserving Recovery (PPR) method [89]. In this chapter, we implement both the residual-type and recovery-type *a posteriori* error estimators for adding vertices and modifying the mesh density in our algorithm.

The performance of adaptive methods for PDEs depends not only on the error estimators, but also on the techniques used for adaptively refining and generating meshes. The current mesh adaptivity techniques can be decomposed into three categories: adaptive re-meshing methods [98, 99], element subdivision methods [100, 101, 102, 103], and fixed order mesh modification procedures [104, 105, 106]. Adaptive re-meshing methods construct an adaptive mesh by regenerating the entire mesh through the application of automatic mesh generation algorithms governed by desired element size and shape information. Element subdivision methods can control element shape by specific split orders, for example, the regular refinement algorithm by Bank [101], the longest edge refinement based algorithm by Rivara [102]. The third mesh adaptation techniques apply local mesh modifications in a fixed order. For example, Briere *et al.* [104], de Cougny *et al.* [105] and Joe *et al.* [106] have improved the quality of an existing mesh using procedures consisting of four local mesh modification operations: swap, collapse, split and relocation. In this chapter, we adopt

adaptive re-meshing based on centroidal Voronoi Delaunay tessellations [112] which offer many superior properties compared to ordinary Delaunay triangulation. It may be expected that the centroidal Voronoi Delaunay tessellation (CVDT) might provide better alternatives to existing methodologies for generating high quality meshes.

It is well known that the accuracy and convergence of numerical methods depend on shape and size of the mesh elements. A notable problem in generating a well-shaped tetrahedral mesh is that such a mesh may contain some types of badly shaped tetrahedra, so-called slivers, which are very flat, with volumes being close to zero. Slivers can have both very large (near 180°) and very small (close to 0°) dihedral angles that cause arbitrarily big interpolation errors. Since CVTs offer an optimal distribution of generators so that they are uniformly or locally uniformly distributed for a constant or nonconstant density function, no relatively short edge will be contained in CVDTs. Therefore, among all kinds of badly shaped tetrahedra, only two specific types may appear in CVDTs, which are called cap and sliver, respectively. See subsection 6.3.4 for details. Techniques of mesh optimization and mesh smoothing provide an effective way to remove slivers and to improve the overall mesh quality, see e.g. [120, 121, 122, 123]. In this chapter, we adopt a relatively simple way to remove the slivers to some extent by using a projection method to distinguish the types of slivers contained in the mesh.

The rest of this chapter is organized as follows. In section 6.2, we introduce the a posteriori error estimators based on the residual error and on superconvergent gradient recovery. In section 6.3, the mesh generation and optimization methods used in our adaptivity algorithm are discussed in detail. An adaptive finite element method based on CCVDT is given in section 6.4. In section 6.5, we use several numerical examples to illustrate the effectiveness and efficiency of our mesh adaptation approach.

6.2 A posterior error estimator for linear finite element methods

Let Ω be a three dimensional bounded domain, we consider the following boundary value problem

$$\begin{cases} -\nabla \cdot (a \nabla u) &= f, & \text{in } \Omega, \\ u &= g, & \text{on } \partial\Omega, \end{cases} \quad (6.1)$$

where a, f and g are functions defined on $\bar{\Omega}$.

Let $V := \{v \in H^1(\Omega) : v|_{\partial\Omega} = g\}$. The weak form of problem (6.1) is to find $u \in V$ such that

$$B(u, v) = L(v) \quad \forall v \in H_0^1(\Omega),$$

where B is the bilinear form and L is the linear functional respectively defined by

$$B(u, v) = \int_{\Omega} a \nabla u \cdot \nabla v \, dx \quad \text{and} \quad L(v) = \int_{\Omega} f v \, dx.$$

Let $\mathcal{T}$ be a conforming tetrahedral mesh of Ω and denote the diameter of the tetrahedron $T \in \mathcal{T}$ by h_T . Let p denote a nonnegative integer and $\mathbb{P}_p$ the space of polynomials of degree less than or equal to p . The finite element space of degree p associated with the tetrahedral mesh $\mathcal{T}$ is defined by $V_h = \{v \in C(\bar{\Omega}) \mid v|_T \in \mathbb{P}_p(T) \ \forall T \in \mathcal{T}\}$. In this chapter, for simplicity, we consider the case $p = 1$; i.e., V_h is the continuous piecewise linear finite element space with respect to $\mathcal{T}$. But the techniques described in the remaining sections can be easily extended to other higher-order approximations.

Define $V_h^g := \{v \in V_h : v|_{\partial\Omega} = I_h g\}$ where $I_h g \in V_h$ denotes a interpolation or projection of g . It is clear that $V_h^g \subset V$. Then, the finite element approximation $u_h \in V_h^g$ of the problem (6.1) is determined from the discrete problem

$$B(u_h, v_h) = L(v_h) \quad \forall v_h \in V_h^0,$$

where $V_h^0 := \{v \in V_h : v|_{\partial\Omega} = 0\}$.

6.2.1 A posteriori error estimator based on the residual error

The theory of residual a posteriori error estimator is well-established. The analysis procedure is based on clément interpolation. Here we simply present the main results we are using. For details, see [41] and the references cited therein.

For any $u \in V$, we define its energy norm $\|\cdot\|_E$ by $\|u\|_E = (B(u, u))^{1/2}$ and let $e_h = u - u_h$ be the error of the approximate solution u_h . Let $\mathcal{F}_I$ denote the set of interior faces of $\mathcal{T}$. If T and T' share the common face $\gamma \in \mathcal{F}_I$, define the jump in the normal flux across the face γ by

$$[(a\nabla u_h) \cdot \mathbf{n}_\gamma] = (a\nabla u_h)|_T \cdot \mathbf{n}_T + (a\nabla u_h)|_{T'} \cdot \mathbf{n}_{T'},$$

where $\mathbf{n}_T$ is the unit outward normal vector to ∂T .

Let $r = f + \nabla \cdot (a\nabla u_h)$ and $R = -[(a\nabla u_h) \cdot \mathbf{n}_\gamma]$. Then an H^1 -type local error estimator η_{T,H^1} associated with the element $T \in \mathcal{T}$ is given by

$$\eta_{T,H^1}^2 = h_T^2 \|r\|_{L^2(T)}^2 + \frac{1}{2} h_T \|R\|_{L^2(\partial T)}^2. \quad (6.2)$$

Theorem 6.1. *Let η_{T,H^1} be defined in (6.2) and let $\eta_{H^1}^2 = \sum_{T \in \mathcal{T}} \eta_{T,H^1}^2$. Then, there exist constant C_1 and C_2 depending only on the domain Ω , the coefficient function a and the regularity of $\mathcal{T}$ such that*

$$\|e_h\|_E^2 \leq C_1 \eta_{H^1}^2. \quad (6.3)$$

Moreover, let T_γ denote the union of the tetrahedrons having γ as one of their faces; then, the lower bound

$$\eta_{T,H^1}^2 \leq C_2 \{ \|e_h\|_{E,T_\gamma}^2 + h_T^2 \|f - \bar{f}\|_{L^2(T_\gamma)}^2 \} \quad (6.4)$$

also holds, where $\bar{f}$ denotes the mean value of f over T .

The inequality (6.3) is the upper bound of the true error e_h and the inequality

(6.4) is referred to as *reliability* and *efficiency*, respectively. These two properties show that the a posteriori error estimator η_{T,H^1} is sharp.

The L^2 -type local error estimator η_{T,L^2} is given by

$$\eta_{T,L^2}^2 = h_T^4 \|r\|_{L^2(T)}^2 + h_T^3 \|R\|_{L^2(\partial T)}^2. \quad (6.5)$$

Theorem 6.2. *Suppose that the domain Ω is convex. Let η_{T,L^2} be defined in (6.5) and let $\eta_{L^2}^2 = \sum_{T \in \mathcal{T}} \eta_{T,L^2}^2$. Then, there exists a constant C depending only on the domain Ω , the coefficient function a and the regularity of $\mathcal{T}$ such that*

$$\|e_h\|_E^2 \leq C \eta_{L^2}^2. \quad (6.6)$$

6.2.2 A posterior error estimator based on superconvergent patch recovery

SPR method is widely used in engineering practices for its robustness in a posteriori error estimates and its efficiency in computer implementation. Due to the nice quality of CVDT mesh, the gradient recovered by SPR enjoys superconvergent property on a general two dimensional domain [107]. Different from the two dimensional case, although the nodes of three dimensional CVDT mesh are quasi-distributed, there may be some badly shaped tetrahedrons which are called slivers in the mesh. Slivers are characterized by small volume while not being bounded by any relatively short edge. See subsection 6.3.4 for details. Slivers have great influence on both the accuracy of finite element solutions and the convergence rate of the recovered gradient. We raise a modified SPR (MSPR) recovery method to overcome the influence of slivers in this subsection.

Let $G_h : V_h \rightarrow \prod_{i=1}^n V_h$ denote the MSPR operator, where $n = 3$ is the space dimension and $\prod_{i=1}^n V_h$ is a vector space. Let $\mathcal{N}_h$ be the set of mesh nodes and the basis of V_h is the standard 1-order Lagrange basis $\{\phi_z | z \in \mathcal{N}_h\}$. As in MSPR, the MSPR recovery gradient of u_h , relies on the fact that every function in V_h is uniquely defined by its values at the mesh nodes. If the values $\{G_h u_h(z) : z \in \mathcal{N}_h\}$

are well-defined, then

$$\mathbf{G}_h u_h \triangleq \sum_{z \in \mathcal{N}_h} (\mathbf{G}_h u_h)(z) \phi_z.$$

The remaining thing is to define $\mathbf{G}_h u_h$ at mesh nodes. Let $z \in \mathcal{N}_h$ be a mesh vertex and $\mathcal{K}_z$ denotes a patch of elements around z , i.e.,

$$\mathcal{K}_z = \cup \{T : T \in \mathcal{T}, z \in \bar{T}\}$$

Since the linear finite element approximation is used here, in each element the finite element solution $u_h \in \mathbb{P}_1$, i.e.

$$u_h|_T = \sum_{z \in T} u_h(z) \phi_z, \quad \forall T \in \mathcal{T}$$

is a linear polynomial. Thus $u_h|_T$ determines a gradient in element T , which is a constant vector, namely $\mathbf{p}_T = [p_{1,T} \ p_{2,T} \ p_{3,T}]$. As slivers have great influence on the accuracy of u_h , $\mathbf{p}_T$ is inaccurate approximation of ∇u in a sliver tetrahedron. Motivated by the idea of weighted averaging, which is also a typical recovery approach, we introduce the averaged gradient $\tilde{\mathbf{p}}_T = [\tilde{p}_{1,T} \ \tilde{p}_{2,T} \ \tilde{p}_{3,T}]$ in MSPR method.

For each element $T \in \mathcal{T}$, $\mathcal{L}_T$ is the patch of elements that share a common face with T , i.e.,

$$\mathcal{L}_T = \cup_i \{T_i : T \cap T_i = \gamma, T_i \in \mathcal{T}\} \cup T,$$

where γ is a face of T . Then the averaged gradient $\tilde{\mathbf{p}}_T$ is defined as following:

$$\tilde{\mathbf{p}}_T = \frac{\sum_{T_i \in \mathcal{L}_T} \mathbf{p}_{T_i} * |T_i|}{|\mathcal{L}_T|},$$

where $|T_i|$ and $|\mathcal{L}_T|$ are the volumes of element T_i and patch $\mathcal{L}_T$, respectively.

Then each component of $\mathbf{G}_h u_h$ is assumed to be the linear polynomial that best

fits the corresponding component of $\tilde{\mathbf{p}}_T$ at the sampling nodes in $\mathcal{K}_z$ in discrete least-square sense, i.e.,

$$\sum_{T \in \mathcal{K}_z} |((G_h u_h)_i(\tilde{z}) - (\tilde{\mathbf{p}}_T)_i)|^2 = \min_{(G_h u_h)_i \in \mathbb{P}_1(\mathcal{K}_z)} \sum_{T \in \mathcal{K}_z} |((G_h u_h)_i(\tilde{z}) - (\tilde{\mathbf{p}}_T)_i)|^2 \quad (6.7)$$

for $i = 1, \dots, n$, where i means the i th component of the recovered gradient $G_h u_h$ and sampling nodes $\tilde{z}$ are chosen to the barycenter of each element T in $\mathcal{K}_z$.

We outline the details of solving the above least-square problem (6.7). Let $\{z_1, z_2, \dots, z_{N(\mathcal{K}_z)}\}$ denotes the sampling nodes of element $\{T_1, T_2, \dots, T_{N(\mathcal{K}_z)}\}$ in $\mathcal{K}_z$. To overcome the computational instability resulting from small mesh size, the relative coordinates are used here. The computations will be carried out on the reference patch $\hat{\mathcal{K}}_z$ associated with z where

$$\hat{\mathcal{K}}_z \triangleq F_z(\mathcal{K}_z) \quad \text{and} \quad F_z : z_j \rightarrow \hat{z}_j = z_j - z, \quad j = 1, 2, \dots, N(\mathcal{K}_z).$$

Thus $(G_h u_h)_i(\hat{z}_j)$ can be expressed as

$$(G_h u_h)_i(\hat{z}_j) = c_{i,1}\xi_j + c_{i,2}\eta_j + c_{i,3}\sigma_j + c_{i,4} = [\xi_j \ \eta_j \ \sigma_j \ 1] \mathbf{c}_i(z)$$

for $i = 1, \dots, n$, where $(\xi_j, \eta_j, \sigma_j)$ is the coordinate of $\hat{z}_j$ and $\mathbf{c}_i(z) = [c_{i,1} \ c_{i,2} \ c_{i,3} \ c_{i,4}]^T$ is the solution of the least-square problem (6.7). Then solving the this least-square problem is equivalent to solve the following linear system:

$$\mathbf{A}_z^T \mathbf{A}_z \mathbf{c}_i(z) = \mathbf{A}_z^T v_{\mathcal{K}_z}, \quad (6.8)$$

where

$$\mathbf{A}_z \triangleq \begin{bmatrix} \xi_1 & \eta_1 & \sigma_1 & 1 \\ \xi_2 & \eta_2 & \sigma_2 & 1 \\ \vdots & \vdots & \vdots & \vdots \\ \xi_{N(\mathcal{K}_z)} & \eta_{N(\mathcal{K}_z)} & \sigma_{N(\mathcal{K}_z)} & 1 \end{bmatrix}$$

and

$$v_{\mathcal{K}_z} \triangleq \begin{bmatrix} \tilde{p}_{i,1} \\ \tilde{p}_{i,2} \\ \vdots \\ \tilde{p}_{i,N(\mathcal{K}_z)} \end{bmatrix}.$$

If $\mathbf{A}_z$ has full column rank, the linear system (6.8) has unique solution. Remember $N_{\mathcal{K}}$ denotes the number of elements contained in the patch $\mathcal{K}_z$. It is usually much bigger than 4 in three dimensions. Thus it is always the situation that $\mathbf{A}_z$ has full column rank.

The recovery-type local error estimator η_T associated with the element $T \in \mathcal{T}$ is given by

$$\eta_T = \|\nabla u_h - G_h u_h\|_{L^2(T)}.$$

Thus the a posteriori error estimate can be conducted as

$$\eta_{\Omega}^2 = \sum_{T \in \mathcal{T}} \eta_T^2 = \|\nabla u_h - G_h u_h\|_{L^2(\Omega)}^2. \quad (6.9)$$

Abundant numerical examples show that the gradient $G_h u_h$ recovered by MSPR shares the superconvergent property on CVDT meshes in three dimensions [108]. As a consequence, the asymptotical exactness of the a posteriori error estimate can be guaranteed.

6.3 Mesh generation and optimization

6.3.1 Centroidal Voionoi tessellations and Delaunay tetrahedrization

A very popular method for unstructured mesh generation is the Voronoi-Delaunay triangulation. Let $\{z_i\}_{i=1}^k$ be a finite set of points belonging to a domain $\Omega \in \mathbb{R}^n$ and

for each i , the point set V_i is defined as: $V_i = \{p \in \Omega : \|p - z_i\| \leq \|p - z_j\|, \forall j \neq i\}$, where $\|\cdot\|$ are metrics associated with the spaces and the Euclidean L^2 norm is frequently used in the area of mesh generation. Thus V_i is called the Voronoi region corresponding to the point z_i . The collection of all the Voronoi regions $\{V_i\}_{i=1}^k$ forms a partition of Ω and is known as the Voronoi tessellation of Ω with respect to the generating points $\{z_i\}_{i=1}^k$. The Delaunay triangulation of $\{z_i\}_{i=1}^k$ is defined as the dual of the Voronoi tessellation [109, 110, 111]. Delaunay triangulation is optimal in many ways due to the fact that the circum-ball associated with each element does not contain any other point of the triangulation except for the degenerate cases.

Recently, the centroidal Voronoi tessellation (CVT) and its wide range of applications have been studied in [112, 113, 114, 115, 116, 117, 118]. Often, CVT provides optimal points placement with respect to a given density function. Its dual structure, the so-called centroidal Voronoi Delaunay triangulation (CVDT), results in a high quality Delaunay mesh.

Given a density function $\rho(x)$ defined on a region V_i , the mass centroid z^* of V_i is defined by

$$z^* = \frac{\int_{V_i} x \rho(x) dx}{\int_{V_i} \rho(x) dx}$$

Thus, given k points $z_i, i = 1, \dots, k$, in the domain Ω , we can define their associated Voronoi regions $V_i, i = 1, \dots, k$, which forms a tessellation of Ω . On the other hand, given the regions $V_i, i = 1, \dots, k$, we can define their mass centroids $z_i^*, i = 1, \dots, k$.

Definition 6.3 (CVT and CVDT). *Given the set of points $\{z_i\}_{i=1}^k$ in the domain and a positive density function $\rho(x)$ defined on Ω , a Voronoi tessellation is called a centroidal Voronoi tessellation (CVT) if*

$$z_i = z_i^*, \quad i = 1, \dots, k,$$

i.e., the generators of the Voronoi regions V_i, z_i , are themselves the mass centroids of those regions. The dual Delaunay triangulation is referred to as the Centroidal Voronoi-Delaunay triangulation (CVDT).

For any tessellation $\{V_i\}_{i=1}^k$ of the domain Ω and a set of points $\{z_i\}_{i=1}^k$ in Ω , we can define the following *cost* (or *error* or *energy*) functional:

$$\mathcal{F}(\{V_i\}_{i=1}^k, \{z_i\}_{i=1}^k) = \sum_{i=1}^k \int_{V_i} \rho(x) \|x - z_i\|^2 dx. \quad (6.10)$$

The standard CVTs along with their generators are critical points of this functional. Using the concept of cost functional, we have

Definition 6.4 (CCVDT). *Given the set of points $\{z_i\}_{i=1}^k$ in Ω , a density function $\rho(x)$, and a constraint set P , a Voronoi tessellation is called a constrained centroidal Voronoi tessellation (CCVT) if $\{\{V_i\}_{i=1}^k, \{z_i\}_{i=1}^k\}$ is a solution of the problem*

$$\min_{\{z_i\}_{i=1}^k \in P, \{V_i\}_{i=1}^k} \mathcal{F}(\{V_i\}_{i=1}^k, \{z_i\}_{i=1}^k).$$

The dual Delaunay triangulation is referred to as the constrained centroidal Voronoi-Delaunay tessellation (CCVDT).

6.3.2 Algorithms for CCVDTs

One useful application of CVDT (CCVDT) is in mesh generation, including unconstrained and constrained mesh generation. For constrained mesh generation, the construction of CVDT deals mainly with the distribution of the generators according to some given density function $\rho(x)$. Such a function $\rho(x)$ is used to reflect the properties of the underlying solution to be calculated on the mesh. The selection of density function will be discussed in detail in subsection 4.1. In [113], several different approaches were proposed to handle the geometrical boundary constraints of the given domain in construction of CCVDT:

1. From the boundary to the interior: a subset of generating points on the boundary is predetermined.
2. From the interior to the boundary: construct the CVT and CVDT without applying any constraints using a standard algorithm such as the Lloyd method

and during the construction process, for those Voronoi regions that extend to the exterior of the domain, their corresponding generators are projected to the boundary.

3. Variational formulation: to formulate a general variational approach which covers both of the above. For details, please refer to Reference [113].

We combine the first and second approaches together in our modified CCVDT algorithm. First we use the algorithm for constrained CVTs on general surfaces in [116] to predetermine a subset of generators on the boundary. And then we carry out Lloyd iteration [113] to construct CVT for interior points. If the mass center of a Voronoi region moves very close to the boundary, or even outside the domain, it will be projected to the boundary or deleted.

We present the computational aspects of mass centers in three dimensional spaces. Let V_i be the Voronoi region of the interior unconstrained point z_i . In the 3D case, V_i is a polyhedron containing the point z_i . One possible way to compute the mass center of V_i with the density function being ρ is as follows:

First, V_i is decomposed into N tetrahedra. The decomposition approach is very simple: let $\{e_j, j = 1, \dots, n(V_i)\}$ be the set of edges (of the mesh) connecting z_i . From the construction of V_i , we know V_i is composed of $n(V_i)$ simpler polyhedra. Each simpler polyhedron is formed by a 3D planar polygon S and the point z_i , as illustrated in Figure 6.1. We then find the intersection point Q of the edge e_j with S . z_i, Q , and an edge of S forms a tetrahedron. This gives a complete decomposition of V_i into $N = \sum_{j=1}^{n(V_i)} m_j$ tetrahedra where m_j are the number of edges of S .

We next compute the mass center of each tetrahedron using numerical integration together with linear interpolation for the density function values of quadrature points. If any vertex of some tetrahedron is outside the given domain, the contribution of this vertex is deleted in the mass center's computation. We denote the mass center and the mass of each tetrahedron by X_j and M_j . The mass center Y_i of V_i can be

then computed by:

$$Y_i = \frac{\int_{V_i} Y \rho(Y) dY}{\int_{V_i} \rho(Y) dY} = \frac{\sum_{j=1}^N X_j M_j}{\sum_{j=1}^N M_j}.$$

Then we illustrate the details of projection and merging technique. When the domain has a complicated geometry or the density function varies substantially, the computed mass centers of some Voronoi regions may move very close to the boundary, or even outside the domain. If we directly insert these generators into the boundary tetrahedronization, some highly-distorted elements would be generated in the mesh or the insertion procedure may fail. In these cases, we have the following remedies: if the mass center moves outside the domain, we just delete this candidate generator; if the mass center moves close to the boundary and the distance is less than some given criterion, we apply the following projection and merging technique (for simplicity, the 2D case is illustrated in Figure 6.2):

Let P_m be the mass center. P_m is first projected to the boundary surface in the normal direction via the surface parameterization (see related discussion in Reference [116]). Denote the projection point by P_N . Let B be the nearest boundary point to P_N . If B is not allowed to move on the boundary due to the domain's geometric requirement (for example, the eight vertices of a cube domain are not allowed to move on the boundary), the generator P_m is deleted. Otherwise, the midpoint P_l of the line segment BP_N is projected onto the boundary surface similarly as P_m ; then the mass center P_m is deleted and B is moved to P_l 's projection point P_w . This is to say, the possibly problematic mass centers are not inserted into the existing mesh; instead, their nearest boundary points are changed to appropriate new positions on the boundary surface if these boundary points are allowed to move without violating any boundary geometric constraints. Such measures keep a more reasonable points placement near the boundary and enhances the quality of the nearby elements. A direct consequence is the removal of slivers or badly shaped elements near the boundary. This technique has been used by many other researchers for element quality improvement [119].

Figure 6.1: Tetrahedra division with respect to a connecting edge.

Figure 6.2: Projection and merging.

Algorithm 6.3.1 (modified CCVDT). *Given a three dimensional domain Ω , a density function $\rho(x)$ defined on Ω and an initial constrained Delaunay tetrahedral mesh,*

1. *predetermine a subset of generating points on the boundary via a lower dimensional CVT construction based on the pre-defined density function $\rho(x)$;*
2. *construct the Voronoi regions for all interior points that are allowed to change their positions and compute the mass centers of the Voronoi regions based on the given density function $\rho(x)$ and use the computed mass centers as generating points;*
3. *retetrahedronlization the domain Ω using CDT with generating points; the resulting tetrahedronlization is the new $\mathcal{T}$;*
4. *if the tetrahedronlization $\mathcal{T}$ meets some convergence criterion, return $\mathcal{T}$ and terminate; otherwise, go to step 1.*

6.3.3 Equidistribution of energy

An important and very useful property of CVTs is that the energy is equally distributed over the Voronoi regions V_i 's asymptotically. For example, it was shown in [112] that, in one-dimensional case,

$$\int_{V_i} \rho(x)(x - z_i)^2 dx \approx c \quad \forall i$$

for some constant c when the number of generators is large. This means, asymptotically speaking, the energy or cost is equally distributed in the Voronoi intervals.

For the multidimensional CVT, a conjecture has been made [78] which states that asymptotically, as the number of generators becomes large, all Voronoi regions are approximately congruent to the same basic cell that only depends on the dimension. The basic cell was shown to be the regular hexagon in two dimensions and Par6 assembly (Figure 4.5) in three dimensions, which tells us that the CVDT provides a high quality mesh. The Par6 assembly is obtained by distorting the cube into a parallelepiped with a 35.3° rotation of the edges about the y- and z-axis. Each

parallelepiped is divided into six tetrahedrons and all the tetrahedrons in Par6 are the same. Furthermore, the four faces of these tetrahedrons are all the same—an isosceles triangle with one edge of length p and the other two of length $\sqrt{3}p/2 \approx 0.866p$ (see Figure 4.5). The conjecture remains open for three and higher dimensions, but its validity has been verified through extensive numerical studies and it is widely used in practical applications such as in the area of vector quantizations [80].

This equipartition property plays an important role in the definition of the density function. For a constant density function, the generators $\{z_i\}_{i=1}^k$ are uniformly distributed and the Voronoi regions $\{V_i\}_{i=1}^k$ are all almost the same size. For a non-constant density function, the generators $\{z_i\}_{i=1}^k$ are still locally uniformly distributed [112]. Let h_{V_i} be the radius of a three-dimensional Voronoi region V_i and the number of generators n goes to infinity. Then there is a point z_i^* in V_i such that

$$\int_{V_i} \rho(z)(z - z_i)^2 dz \approx \rho(z_i^*) h_{V_i}^2 |V_i| \quad \forall i$$

where $|V_i|$ denotes the volume of V_i . The right side roughly equals $\alpha h_{V_i} \rho(z_i^*)$ for some constant α . Hence, combining with the equidistribution principle, we have:

$$\rho(z_i^*) h_{V_i}^5 = C (= c/\alpha) \quad (6.11)$$

or in another form

$$\left(\frac{h_{V_i}}{h_{V_j}} \right)^5 \approx \frac{\rho(z_j^*)}{\rho(z_i^*)}$$

From the second formula, we can see that the density is a relative quantity and the choice of C is not important, hence we take $C = 1$.

Thus, in principle, one could control the distribution of generators to obtain an equal distribution of the error by connecting the density function $\rho(x)$ to an a posteriori error estimator.

Figure 6.3: Badly shaped tetrahedra with four vertices close to a line

6.3.4 Sliver elimination and local optimization

The mesh literature is rich in measures of simplex quality. The following measure is used in this chapter:

$$Q_T = 2\sqrt{6}r/h \quad (6.12)$$

where r is the radius of the largest contained sphere and h is the length of the longest edge in a tetrahedron T . For a regular tetrahedron, Q_T equals 1 and for a tetrahedron in Par6, Q_T equals 0.866. In [120], the badly shaped tetrahedrons are divided into two categories. A tetrahedra of type I has four vertices close to a line and has at least three badly shaped triangles, see Figure 6.3. A tetrahedra of type II has four vertices close to a plane. This type of tetrahedrons are distinguished in detail where two points are close to each other (wedge), where three points are close to a line (spade), where the orthogonal projection to the plane is a triangle with a point inside (cap), and where the projection is a quadrilateral (sliver), see Figure 6.4.

The quality of the Voronoi Delaunay tetrahedronlization is often associated with the distribution of the generating points. CVTs offer an optimal distribution of generators so that they are uniformly or locally uniformly distributed for a constant or a nonconstant density function. Therefore no relatively short edge will be contained in CVDTs. Thus, among the tetrahedra of poor quality, only cap and sliver may

Figure 6.4: Badly shaped tetrahedra with four vertices close to a plane

appear in CVDTs.

Many algorithms have been proposed that take as input a tetrahedral mesh and refine it into a sliver-free, high quality mesh [120, 121, 122, 123]. Only the *Sliver Exudation* algorithm of Cheng *et al.* [120] is implemented and experimental results are reported. In this chapter, we use a relatively simple method to eliminate slivers. In particular, for sliver, the reason is the small distance between a pair of opposite edges of the tetrahedron, so one (or both) of the edges must be eliminated (the key entities are the two edges). For cap, the reason is that a vertex is too close to its opposite face, so either the vertex or the face must be eliminated (key entities are the vertex and its opposite face). The qualification of the two sliver types is determined based on projection method. The first step of projection method is the selection of a base triangle, which can be any mesh face of the tetrahedron. Then the vertex of the tetrahedron opposite to the base face is projected onto the base face plane. The type and key mesh entities of the tetrahedron are then determined in terms of the relative location of this projected point. Figure 6.5 shows the top view of the base triangle plane ($\triangle ABC$) for tetrahedra T_{ABCD} , which is subdivided into seven subareas (R1 to R7) defined by extending the mesh edges of the base triangle. There is one subarea associated with each edge, one associated with each vertex, and one with the base triangle itself. Table 6.1 indicates the tetrahedron type and key mesh entities in terms of which the projection is in. The projection will not be close to any of the mesh vertices of the base triangle since this would correspond to the existence of a short edge.

Figure 6.5: Top view of the base triangle

Table 6.1: Type and key mesh entities in terms of projection location		
Projection location	Type	Key mesh entities
R1	cap	D and its opposite face
R2		A and its opposite face
R3		B and its opposite face
R4		D and its opposite face
R5	sliver	AB and CD
R6		BC and AD
R7		AC and BD

6.4 Adaptive finite element algorithm based on CCVDT

In our adaptive method, we use CCVDTs to refine and optimize the mesh at each level, but first we need to determine, from the error estimators, the density function used in the CCVDT algorithm.

6.4.1 Modification of density function

Density function based on the residual error

Let $\mathcal{T}^{(\ell)}$ denote the tetrahedronization of Ω with vertices $\{z_i^\ell\}_{i=1}^{n^\ell}$ at the refinement level ℓ . Let $\eta_{T,H^1}^{(\ell)}$ and $\eta_{T,L^2}^{(\ell)}$ represent the corresponding local H^1 -type and L^2 -type error estimators on $\mathcal{T}^{(\ell)}$ defined by (6.2) and (6.5), respectively. In order to reflect the local variations of true error more accurately, both $\eta_{T,H^1}^{(\ell)}$ and $\eta_{T,L^2}^{(\ell)}$ are divided by $\sqrt{a}$. Thus, we define

$$(\xi_{T,H^1}^{(\ell)})^2 = \frac{(\eta_{T,H^1}^{(\ell)})^2}{a_T} \quad \text{and} \quad (\xi_{T,L^2}^{(\ell)})^2 = \frac{(\eta_{T,L^2}^{(\ell)})^2}{a_T}, \quad (6.13)$$

where a_T is the mean value of $a(x)$ on the tetrahedra T , i.e., $a_T = \int_T a(x) \, dx / |T|$. In order to minimize

$$(\xi_{H^1}^{(\ell)})^2 = \sum_{T \in \mathcal{T}^{(\ell)}} (\xi_{T,H^1}^{(\ell)})^2 \quad \text{or} \quad (\xi_{L^2}^{(\ell)})^2 = \sum_{T \in \mathcal{T}^{(\ell)}} (\xi_{T,L^2}^{(\ell)})^2,$$

we need to distribute $(\xi_{T,H^1}^{(\ell)})^2$ or $(\xi_{T,L^2}^{(\ell)})^2$ equally over all tetrahedrons of $\mathcal{T}^{(\ell)}$.

Set

$$\tilde{\rho}_{T,H^1}^{(\ell)} = \frac{(\xi_{T,H^1}^{(\ell)})^2}{h_T^5} \quad \text{and} \quad \tilde{\rho}_{T,L^2}^{(\ell)} = \frac{(\xi_{T,L^2}^{(\ell)})^{\frac{4}{3}}}{h_T^5}. \quad (6.14)$$

We then uniquely determine two piecewise linear functions (with respect to $\mathcal{T}^{(\ell)}$)

$\rho_{H^1}^{(\ell+1)}$ and $\rho_{L^2}^{(\ell+1)}$ on Ω such that for any vertex $z_i^{(\ell)}$ of $\mathcal{T}^{(\ell)}$,

$$\rho_{H^1}^{(\ell+1)}(z_i^{(\ell)}) = \frac{\sum_{T \in \mathcal{K}_i} \tilde{\rho}_{T,H^1}^{(\ell)}}{N(\mathcal{K}_i)} \quad \text{and} \quad \rho_{L^2}^{(\ell+1)}(z_i^{(\ell)}) = \frac{\sum_{T \in \mathcal{K}_i} \tilde{\rho}_{T,L^2}^{(\ell)}}{N(\mathcal{K}_i)}, \quad (6.15)$$

where $\mathcal{K}_i = \{T \in \mathcal{T}^{(\ell)} | z_i^{(\ell)} \in \bar{T}\}$ and $N(\mathcal{K}_i)$ is number of tetrahedrons contained in the node patch $\mathcal{K}_i$.

We will refer to the density function $\rho_{H^1}^{(\ell+1)}$ and $\rho_{L^2}^{(\ell+1)}$ as the H^1 -based and L^2 -based density functions, respectively. Note that, in some sense, if the solution $u \in H^2(\Omega)$, we have

$$(\xi_{T,H^1}^{(\ell)})^2 \approx a_T |\Delta u|^2 h_T^5 \quad \text{and} \quad (\xi_{T,L^2}^{(\ell)})^2 \approx a_T |\Delta u|^2 h_T^7. \quad (6.16)$$

Combining (6.16) with the CVDT property (6.11), i.e.,

$$\left(\frac{h_{V_i}}{h_{V_j}}\right)^5 \approx \frac{\rho(z_j^*)}{\rho(z_i^*)}$$

for a CVT $\{z_i, V_i\}_{i=1}^n$ of Ω with respect to the density function ρ , it is then not difficult to verify that the CCVDT mesh $\mathcal{T}^{(\ell+1)}$ generated by the density function $\rho_{H^1}^{(\ell+1)}$ and $\rho_{L^2}^{(\ell+1)}$ will approximately have the property that

$$(\xi_{T_i,H^1}^{(\ell+1)})^2 \approx (\xi_{T_j,H^1}^{(\ell+1)})^2 \quad \text{or} \quad (\xi_{T_i,L^2}^{(\ell+1)})^2 \approx (\xi_{T_j,L^2}^{(\ell+1)})^2,$$

respectively, for any tetrahedra $T_i, T_j \in \mathcal{T}^{(\ell+1)}$.

Density function based on superconvergent gradient recovery

Since the a posteriori error estimator based on superconvergent gradient recovery η_T approaches to the true error $|e_h|_{H^1(T)}$ asymptotically, we first use η_T to modify the sizing field on vertices $\{z_i^\ell\}_{i=1}^{n^\ell}$ at the refinement level ℓ . And then with the help of equidistribution principle, density function $\rho^{(\ell+1)}$ will be defined based on the modified sizing field.

We define the permissable error $\mathcal{E}_P$ by

$$\mathcal{E}_p = \delta \sqrt{\frac{\|u_h\|_E^2 + \eta_\Omega^2}{N^{(\ell)}}},$$

where $N^{(\ell)}$ is the number of elements in $\mathcal{T}^{(\ell)}$ and δ is a pre-assigned positive constant usually with a value less than 1. In order to minimize $\eta_\Omega^2 = \sum_{T \in \mathcal{T}} \eta_T^2 = \|\nabla u_h - G_h u_h\|_{L^2(\Omega)}^2$, we need to distribute $\eta_T^2 = \|\nabla u_h - G_h u_h\|_{L^2(T)}^2$ equally over all tetrahedrons of $\mathcal{T}^{(\ell)}$. Thus we modify the size of a element by

$$\tilde{h}_T^{(\ell)} = \frac{h_T^{(\ell)}}{\eta_T / \mathcal{E}_p}.$$

We then uniquely determine a piecewise linear function $h^{(\ell+1)}$ on Ω such that for any vertex $z_i^{(\ell)}$ of $\mathcal{T}^{(\ell)}$,

$$h^{(\ell+1)}(z_i^{(\ell)}) = \frac{\sum_{T \in \mathcal{K}_i} \tilde{h}_T^{(\ell)}}{N(\mathcal{K}_i)},$$

where $\mathcal{K}_i = \{T \in \mathcal{T}^{(\ell)} | z_i^{(\ell)} \in \bar{T}\}$ and $N(\mathcal{K}_i)$ is number of tetrahedrons contained in the node patch $\mathcal{K}_i$. Using (6.11), the density function for $\mathcal{T}^{(\ell+1)}$ is finally defined by

$$\rho^{(\ell+1)}(z_i^{(\ell)}) = \frac{1}{(h^{(\ell+1)}(z_i^{(\ell)}))^5}.$$

6.4.2 Adaptive algorithm based on CCVDT

The following adaptation loop is typical and well-known

$$\text{Solve} \longrightarrow \text{Estimate} \longrightarrow \text{Mark} \longrightarrow \text{Refine}.$$

For the traditional bisection refinement strategy, the marked elements are treated equally no matter how big the error estimator is in a specific element. For example, in the regular refinement algorithm proposed by Bank [101], all marked triangles are divided into four triangles of the same shape. The longest edge refinement proposed

by Rivara [102], only bisects along the longest edge of a specified triangle by connecting the vertex to the midpoint of the opposite side. The error estimator brings us abundant information that can be used not only at the **mark** step but also at the **refine** step. A simple idea is that the bigger the error estimator is, the more mesh nodes should be added to that element. But this simple idea is not easy to realize. Direct questions are how to determine the positions of these added nodes and how to change the local topology to guarantee the mesh quality. As we mentioned in the previous section, CCVDT has the ability to relocate the positions of mesh nodes and reconnect the mesh nodes to generate a mesh with relatively high mesh quality as long as the proper density is assigned to each node. With the help of CCVDT, we use error estimator to determine the number of added nodes for each marked element and give the following adaptive algorithm based on CCVDT.

Algorithm 6.4.1 (CCVDT-based adaptive finite element mothod). *Given a tolerance $\text{TOL} > 0$.*

- *Generate an initial CVT mesh $\mathcal{T}$ over domain Ω .*
- *Solve the PDE using finite element method on $\mathcal{T}$.*
- *Compute the error estimators η_T on $\mathcal{T}$.*
- *While $\eta_\Omega > \text{TOL}$ do*
 - *Using the error estimator η_T to update the density function ρ .*
 - *Choose a set of elements $\hat{\mathcal{T}}_h \subset \mathcal{T}$ such that*

$$\left(\sum_{T \in \hat{\mathcal{T}}_h} \eta_T^2\right)^{1/2} > \theta \left(\sum_{T \in \mathcal{T}} \eta_T^2\right)^{1/2}.$$
 - *Set $\tilde{\eta}_T = \inf_{T \in \hat{\mathcal{T}}_h} \eta_T$ as a threshold.*
 - *For a element $T \in \hat{\mathcal{T}}_h$, insert $r = \text{int}(\log_2(\eta_T/\tilde{\eta}_T)) + 1$ nodes to $\bar{T}$ and the densities of added nodes are interpolant of four vertices of T .*
 - *Using CCVDT to optimize the mesh and update $\mathcal{T}$.*

- Solve the PDE using finite element method on $\mathcal{T}$.
- Compute the error estimators η_T on $\mathcal{T}$.

end while.

The parameter θ in Algorithm 6.4.1 is used here to control the refinement process, usually taking a value of 0.7.

Remark 6.5. The quantity information of error estimator is used in the step of **refine**. r nodes will be added to $\bar{T}$ if $\eta_T \in [2^{r-1}\tilde{\eta}_T, 2^r\tilde{\eta}_T)$. And the CCVDT will automatically adjust the positions of these added nodes and regenerate a new mesh of relatively high quality. This makes our algorithm more effective especially in the first several refinement levels.

6.5 Numerical examples

In this section, we use numerical experiments to illustrate the effectiveness of the CCVDT-based adaptive finite element method. For our adaptive methods, the convergence rate CR with respect to the norm $\|\cdot\|$ at the refinement level ℓ is roughly computed as

$$\text{CR} = \frac{3 \log(\|e_{h,\ell}\| / \|e_{h,\ell-1}\|)}{\log(n_{\ell-1}/n_\ell)}, \quad (6.17)$$

where n_ℓ denotes the number of nodes and $e_{h,\ell}$ denotes the error $u - u_h$ at the refinement level ℓ .

6.5.1 Experiment 1

Let $\Omega = [0, 1] \times [0, 1] \times [0, 1]$, $a = 1$. The exact solution u of equation (6.1) is chosen to be

$$u(x, y) = \frac{1.0}{(x - 0.5)^2 + (y - 0.5)^2 + (z - 0.5)^2 + 0.01} \quad (6.18)$$

and f and g are determined from u so that (6.1) is satisfied.

The exact solution u given in (6.18) is a smooth function that achieves its maximum value 100 at the point $(0.5, 0.5, 0.5)$ but decays very quickly away from its extremum and thus has large gradients near this point.

The initial coarse mesh used for experiment 1 is a uniform CVDT mesh with 1976 nodes. Figure 6.7, Figure 6.8, and Figure 6.9 present repeatedly refined meshes at some levels generated by Algorithm 6.4.1 using H^1 -type, L^2 -type, and MSPR a posteriori error estimator, respectively. An important optimal property of CCVDT-based adaptive methods is the equidistribution of the errors over Ω . In order to verify this, we illustrate the quantity of the semi- H^1 norm $|e_h|_{H^1(T)}$ in Figure 6.7 and Figure 6.9, and the L^2 norm $\|e_h\|_{L^2(T)}$ in Figure 6.8 on the cross section $x = 0.5$ by color. It is obvious that the local errors are nearly equidistributed by the adaptive methods.

Table 6.2 and Table 6.3 contain information about mesh quality, solution errors, and convergence rates at all refinement levels for different refinement strategies for Example 1; the corresponding plots of the error norms ($\|e_h\|_{L^2(\Omega)}$ and $|e_h|_{H^1(\Omega)}$) versus the number of nodes are given in Figure 6.6. The values of q_{avg} given in Table 6.2 and Table 6.3 demonstrate that the shape quality of the meshes resulting from the CCVDT-based adaptive strategy is always very good at all levels for density functions ρ_{L^2} , ρ_{H^1} , and ρ , although the mesh sizes vary a lot over Ω . Also from Table 6.2 and Table 6.3, one can observe that the CCVDT-based adaptive method is much more efficient relative to the uniform refinement strategy.

6.5.2 Experiment 2

Let $\Omega = [0, 1] \times [0, 1] \times [0, 1]$, $a = 1$. The exact solution u is chosen to be

$$u(x, y, z) = \begin{cases} 1 & r \leq 0.25 - \epsilon/2 \\ g(r) & 0.25 - \epsilon/2 < r \leq 0.25 + \epsilon/2 \\ 0 & r > 0.25 + \epsilon/2 \end{cases} \quad (6.19)$$

where

$$r = \sqrt{(x - 0.5)^2 + (y - 0.5)^2 + (z - 0.5)^2}$$

Table 6.2: Data statistics of the mesh, solution errors and convergence rates for residual error based refinement strategies for experiment 1

l	n_l	q_{avg}	$\ e_h\ _{L^2(\Omega)}$	CR	$ e_h _{H^1(\Omega)}$	CR
Uniform refinement						
0	1976	0.766	6.2192e-1		2.7845e+1	
1	4506	0.779	3.4738e-1	2.1195	2.0293e+1	1.1514
2	14607	0.792	1.6055e-1	1.9688	1.4233e+1	0.9048
3	41660	0.798	8.0057e-2	1.9919	1.0169e+1	0.9624
4	112087	0.802	4.0717e-2	2.0493	7.3246e+0	0.9945
Adaptive refinement using H^1 -type a posteriori error estimator						
0	1976	0.766	6.2192e-1		2.7845e+1	
1	2489	0.739	1.1933e-1	21.458	1.6179e+1	7.0571
2	3437	0.757	7.7575e-2	4.0033	1.2218e+1	2.6104
3	5003	0.754	5.1426e-2	3.2850	1.0193e+1	1.4480
4	9634	0.758	3.4928e-2	1.7712	7.9973e+0	1.1107
5	29757	0.773	1.9198e-2	1.5920	5.2778e+0	1.1055
Adaptive refinement using L^2 -type a posteriori error estimator						
0	1976	0.766	6.2192e-1		2.7845e+1	
1	2484	0.750	1.5773e-1	17.989	1.7025e+1	6.4508
2	3498	0.753	8.6397e-2	5.2751	1.2951e+1	2.3970
3	4834	0.748	6.0213e-2	3.3485	1.0907e+1	1.5930
4	10104	0.751	3.2664e-2	2.4887	7.8109e+0	1.3586
5	23640	0.754	1.9523e-2	1.8165	5.9618e+0	0.9535
6	29832	0.755	1.6787e-2	1.9471	5.4687e+0	1.1133

Figure 6.6: Error norms versus number of nodes for different refinement strategies for experiment 1. Top: $\|e_h\|_{L^2(\Omega)}$. Bottom: $|e_h|_{H^1(\Omega)}$.

Figure 6.7: Refinement meshes and $|e_h|_{H^1(T)}$ distributions on the cross section $x = 0.5$ for H^1 -type a posteriori error estimator at different refinement level for experiment 1. Top left: refinement level 0. Top right: refinement level 2. Bottom left: refinement level 4. Bottom right: refinement level 5.

Figure 6.8: Refinement meshes and $\|e_h\|_{L^2(T)}$ distributions on the cross section $x = 0.5$ for L^2 -type a posteriori error estimator at different refinement level for experiment 1. Top left: refinement level 0. Top right: refinement level 2. Bottom left: refinement level 4. Bottom right: refinement level 6.

Figure 6.9: Refinement meshes and $|e_h|_{H^1(T)}$ distributions on the cross section $x = 0.5$ for MSPR a posteriori error estimator at different refinement level for experiment 1. Top left: refinement level 0. Top right: refinement level 2. Bottom left: refinement level 4. Bottom right: refinement level 5.

Table 6.3: Data statistics of the mesh, solution errors and convergence rates for superconvergent gradient recovery based refinement strategy for experiment 1

l	n_l	q_{avg}	$\ e_h\ _{L^2(\Omega)}$	CR	$ e_h _{H^1(\Omega)}$	CR
Uniform refinement						
0	1976	0.766	6.2192e-1		2.7845e+1	
1	4506	0.779	3.4738e-1	2.1195	2.0293e+1	1.1514
2	14607	0.792	1.6055e-1	1.9688	1.4233e+1	0.9048
3	41660	0.798	8.0057e-2	1.9919	1.0169e+1	0.9624
4	112087	0.802	4.0717e-2	2.0493	7.3246e+0	0.9945
Superconvergent Gradient Recovery Based Adaptive refinement						
0	1976	0.766	6.2192e-1		2.7845e+1	
1	2533	0.755	2.3702e-1	11.654	1.9125e+1	4.5382
2	3748	0.742	1.0446e-1	6.2734	1.3951e+1	2.4152
3	6826	0.747	4.4682e-2	4.2496	9.7041e+0	1.8165
4	14696	0.759	2.5678e-2	2.1671	6.7561e+0	1.4166
5	33989	0.772	1.5272e-2	1.8592	5.0086e+0	1.0709

is the distance to the point $(0.5, 0.5, 0.5)$ and

$$g(\tau) = -6\tau^5 + 15\tau^4 - 10\tau^3 + 1, \quad \tau = \frac{1}{\epsilon}(r - 0.25 + \epsilon/2)$$

ϵ is a constant chosen to be 0.1, and f and g are determined from u so that (6.1) is satisfied.

It is easy to see that $\Omega = \Omega_1 \cup \Omega_2 \cup \Omega_3$, where $\Omega_1 = \{(x, y, z) | (x, y, z) \in \Omega, r \leq 0.25 - \epsilon/2\}$, $\Omega_2 = \{(x, y, z) | (x, y, z) \in \Omega, 0.25 - \epsilon/2 < r \leq 0.25 + \epsilon/2\}$, and $\Omega_3 = \{(x, y, z) | (x, y, z) \in \Omega, r > 0.25 + \epsilon/2\}$. The exact solution is a constant 1 in Ω_1 and 0 in Ω_3 . Ω_2 is a interface where the exact solution jumps from 0 to 1 and ϵ is the thickness of the interface. Function g is chosen that the exact solution u is a smooth function.

The initial coarse mesh used for experiment 2 is a uniform CVDT mesh with 1976 nodes. Figure 6.11, Figure 6.12, and Figure 6.13 present repeatedly refined meshes at some levels generated by Algorithm 6.4.1 using H^1 -type, L^2 -type, and MSPR a posterior error estimator, respectively. It is obvious that our adaptive algorithm has the ability to capture the interface.

Table 6.4: Data statistics of the mesh, solution errors and convergence rates for residual error based refinement strategies for experiment 2

l	n_l	q_{avg}	$\ e_h\ _{L^2(\Omega)}$	CR	$ e_h _{H^1(\Omega)}$	CR
Uniform refinement						
0	1976	0.766	1.7346e-1		4.2693e+0	
1	4506	0.779	0.9604e-1	2.1515	3.2067e+0	1.0416
2	14607	0.792	0.4302e-1	2.0486	2.1027e+0	1.0765
3	41660	0.798	0.2160e-1	1.9722	1.4843e+0	0.9969
4	112087	0.802	0.1103e-1	2.0371	1.0652e+0	1.0057
Adaptive refinement using H^1 -type a posteriori error estimator						
0	1976	0.766	1.7346e-1		4.2693e+0	
1	2677	0.746	4.5349e-2	13.256	2.3754e+0	5.7929
2	3575	0.746	2.8248e-2	4.9093	1.9694e+0	1.9439
3	5411	0.748	1.6321e-2	3.9706	1.5558e+0	1.7063
4	8348	0.745	1.0453e-2	3.0829	1.2159e+0	1.7056
5	11453	0.744	6.0469e-3	5.1925	9.9293e-1	1.9218
6	15766	0.744	5.1311e-3	1.5415	8.5782e-1	1.3729
7	24306	0.745	4.0197e-3	1.6918	7.1507e-1	1.2615
Adaptive refinement using L^2 -type a posteriori error estimator						
0	1976	0.766	1.7346e-1		4.2693e+0	
1	2677	0.750	4.7505e-2	12.797	2.5413e+0	5.1259
2	4320	0.748	2.4506e-2	4.1494	1.9043e+0	1.8089
3	6481	0.745	1.5261e-2	3.5029	1.5161e+0	1.6861
4	9760	0.747	8.3090e-3	4.4548	1.2035e+0	1.6920
5	13748	0.748	6.5073e-3	2.1402	1.0313e+0	1.3521
6	22951	0.750	4.4126e-3	2.2741	8.2948e-1	1.2749

Table 6.4 and Table 6.5 contain information about mesh quality, solution errors, and convergence rates at all refinement levels for different refinement strategies for Example 2; the corresponding plots of the error norms ($\|e_h\|_{L^2(\Omega)}$ and $|e_h|_{H^1(\Omega)}$) versus the number of nodes are given in Figure 6.10. The values of q_{avg} given in Table 6.4 and Table 6.5 demonstrate that the shape quality of the meshes resulting from the CCVDT-based adaptive strategy is always very good at all levels for density functions ρ_{L^2} , ρ_{H^1} , and ρ , although the mesh sizes vary a lot over Ω . Also from Table 6.4 and Table 6.5, one can observe that the CCVDT-based adaptive method is much more efficient relative to the uniform refinement strategy.

Figure 6.10: Error norms versus number of nodes for different refinement strategies for experiment 2. Top: $\|e_h\|_{L^2(\Omega)}$. Bottom: $|e_h|_{H^1(\Omega)}$.

Figure 6.11: Refinement meshes on the cross section $x = 0.5$ for H^1 -type a posteriori error estimator at different refinement level for experiment 2. Top left: refinement level 0. Top right: refinement level 3. Bottom left: refinement level 5. Bottom right: refinement level 7.

Figure 6.12: Refinement meshes on the cross section $x = 0.5$ for L^2 -type a posteriori error estimator at different refinement level for experiment 2. Top left: refinement level 0. Top right: refinement level 3. Bottom left: refinement level 5. Bottom right: refinement level 6.

Figure 6.13: Refinement meshes on the cross section $x = 0.5$ for MSPR a posteriori error estimator at different refinement level for experiment 2. Top left: refinement level 0. Top right: refinement level 3. Bottom left: refinement level 5. Bottom right: refinement level 6.

Table 6.5: Data statistics of the mesh, solution errors and convergence rates for superconvergent gradient recovery based refinement strategy for experiment 2

l	n_l	q_{avg}	$\ e_h\ _{L^2(\Omega)}$	CR	$ e_h _{H^1(\Omega)}$	CR
Uniform refinement						
0	1976	0.766	1.7346e-1		4.2693e+0	
1	4506	0.779	0.9604e-1	2.1515	3.2067e+0	1.0416
2	14607	0.792	0.4302e-1	2.0486	2.1027e+0	1.0765
3	41660	0.798	0.2160e-1	1.9722	1.4843e+0	0.9969
4	112087	0.802	0.1103e-1	2.0371	1.0652e+0	1.0057
Superconvergent Gradient Recovery Based Adaptive refinement						
0	1976	0.766	1.7346e-1		4.2693e+0	
1	3062	0.735	4.2329e-2	9.6609	2.2913e+0	4.2626
2	4812	0.738	2.8079e-2	2.7240	1.7252e+0	1.8833
3	7462	0.735	1.8773e-2	2.7531	1.3321e+0	1.7683
4	11390	0.739	8.7813e-3	5.3897	1.0556e+0	1.6503
5	17216	0.740	6.0260e-3	2.7345	8.6603e-1	1.4375
6	25862	0.742	4.3047e-3	2.4798	7.1790e-1	1.3829

6.5.3 Comparison among different refinement strategies

From (6.2) and (6.5), we can see that the only difference between L^2 and H^1 error estimator is that the former is a higher order scaling in the mesh size of the latter. This makes ρ_{H^1} vary more rapidly than ρ_{L^2} . As a consequence, the adaptive method, using ρ_{L^2} as the density function, generated approximate solutions u_h having smaller $\|e_h\|_{L^2(\Omega)}$ and higher L^2 convergent rate relative to those obtained using ρ_{H^1} ; on the other hand, the latter generated approximate solutions with smaller $|e_h|_{H^1(\Omega)}$ and higher H^1 convergent rate; see Table 6.2 and Table 6.4.

MSPR a posteriori error estimate η_Ω , which convergent to the true error $|e_h|_{H^1(\Omega)}$ in a asymptotical way, has a competitive performance relative to the L^2 and H^1 a posteriori error estimate. Since MSPR a posteriori error estimator gives the local information of gradients, the adaptive method, using MSPR density function ρ , generated approximate solutions u_h having smaller $|e_h|_{H^1(\Omega)}$ to those obtained using ρ_{H^1} and ρ_{L^2} . Another advantage of MSPR a posteriori error estimator is that it has higher efficiency respect to the residual type a posteriori error estimator. It needs less refinement levels to achieve the relative error quantities to the L^2 and H^1 a posteriori

error estimator, so that it saves computational time. Also it illustrates the exactness of the MSPR a posteriori error estimator in another aspect; see Table 6.2, Table 6.3, Table 6.4 and Table 6.5.

Bibliography

- [1] R. A. ADAMS. *Sobolev spaces*, volume 65 of Pure and Applied Mathematics. Academic Press, New York, 1975.
- [2] L. C. EVANS. *Partial differential equations*, volume 19 of Graduate Studies in Mathematics. American Mathematical Society, Providence, RI, 1998.
- [3] P. GRISVARD. *Elliptic problems in nonsmooth domains*, volume 24 of Monographs and Studies in Mathematics. Pitman, Boston, MA, 1985.
- [4] S. C. BRENNER AND L. R. SCOTT. *The mathematical theory of finite element methods*, volume 15 of Texts in Applied Mathematics. Springer-Verlag, New York, 1994.
- [5] J. H. BRAMBLE AND S. R. HILBERT. *Estimation of linear functionals on Sobolev spaces with application to Fourier transforms and spline interpolation*, SIAM J. Numer. Anal., 7 (1970), pp. 112–124.
- [6] P. J. DAVIS. *Interpolation and approximation*. Blaisdell Publishing Co. Ginn and Co., New York-Toronto-London, 1963.
- [7] K. ATKINSON AND W. HAN. *Theoretical numerical analysis. A functional analysis framework*, volume 39 of Texts in Applied Mathematics. Springer-Verlag, New York, 2001.
- [8] R. COURANT. *Variational methods for the solution of problems of equilibrium and vibrations*. Bull. Amer. Math. Soc., 49 (1943), pp. 1–23.

- [9] J. T. ODEN. *Finite elements: an introduction*. In Philippe G. Ciarlet and Jacques-Louis Lions, editors, Handbook of Numerical Analysis. II, pages 3–15. North-Holland, Amsterdam, 1991.
- [10] I. BABUŠKA AND T. STROUBOULIS. *The finite element method and its reliability*. Numerical Mathematics and Scientific Computation. The Clarendon Press, Oxford University Press, New York, 2001.
- [11] D. BRAESS. *Finite elements. Theory, fast solvers, and applications in solid mechanics*. Cambridge University Press, Cambridge, 1997.
- [12] P. G. CIARLET. *The finite element method for elliptic problems*, volume 4 of Studies in Mathematics and its Applications. North-Holland Publishing Co., Amsterdam-New York-Oxford, 1978.
- [13] C. JOHNSON. *Numerical solution of partial differential equations by the finite element method*. Cambridge University Press, Cambridge, 1987.
- [14] B. SZABÓ AND I. BABUŠKA. *Finite element analysis*. John Wiley & Sons, Inc., New York, 1991.
- [15] R. L. TAYLOR. *On completeness of shape functions for finite element analysis*. Internat. J. Numer. Methods Engrg., 4(1) (1972), pp. 17–22.
- [16] B. LI. *Lagrange interpolation and finite element superconvergence*. Numer. Methods Partial Differential Equations, 20(1) (2004), pp. 33–59.
- [17] J. A. STRICKLIN. *Computation of stress resultants from the element stiffness matrices*. AIAA Journal, 4 (1966), pp. 1095–1096.
- [18] J. H. BRAMBLE AND A. H. SCHATZ. *Higher order local accuracy by averaging in the finite element method*. Math. Comp., 31(137) (1977), pp. 94–111.
- [19] C. CHEN. *The good points of the approximate solution of a two-point boundary value problem by the Galerkin method*. Numerical Mathematics. A Journal of Chinese Universities (Chinese), 1(1) (1979), pp. 73–79.

- [20] J. J. DOUGLAS AND T. DUPONT. *Superconvergence for Galerkin methods for the two point boundary problem via local projections*. Numer. Math., 21 (1973), pp. 270–278.
- [21] J. J. DOUGLAS, T. DUPONT AND M. F. WHEELER. *An L^∞ estimate and a superconvergence result for a Galerkin method for elliptic equations based on tensor products of piecewise polynomials*. RAIRO Analyse Numérique, 8 (1974), pp. 61–66.
- [22] A. LOUIS. *Acceleration of convergence for finite element solutions of the poisson equation*. Numer. Math., 33(1) (1979), pp. 43–53.
- [23] J. A. NITSCHKE AND A. H. SCHATZ. *Interior estimates for Ritz-Galerkin methods*. Math. Comp., 28 (1974), pp. 937–958.
- [24] V. THOMÉE. *Spline approximation and difference schemes for the heat equation*. In The mathematical foundations of the finite element method with applications to partial differential equations (Proc. Sympos., Univ. Maryland, Baltimore, Md., 1972), pages 711–746, New York, 1972. Academic Press.
- [25] M. ZLÁMAL. *Some superconvergence results in the finite element method*. In Mathematical aspects of finite element methods, (Proc. Conf., Consiglio Naz. delle Ricerche (C.N.R.), Rome, 1975), Lecture Notes in Mathematics, volume 606, pages 353–362, Berlin, 1977. Springer.
- [26] R. E. BANK AND J. XU. *Asymptotically exact a posteriori error estimators, Part I: Grid with superconvergence*. SIAM Journal of Numerical Analysis, 41 (2003), pp. 2294–2312.
- [27] R. E. BANK AND J. XU. *Asymptotically exact a posteriori error estimators, Part II: General unstructured grids*. SIAM J. Numer. Anal., 41(6) (2003), pp. 2313–2332.
- [28] P. BASTIAN AND B. RIVIÈRE. *Superconvergence and $H(\text{div})$ projection for discontinuous Galerkin methods*. Internat. J. Numer. Methods Fluids, 42(10) (2003), pp. 1043–1057.

- [29] C. CARSTENSEN. *Some remarks on the history and future of averaging techniques in a posteriori finite element error analysis.* ZAMM Z. Angew. Math. Mech., 84(1) (2004), pp. 3–21.
- [30] P. CASTILLO. *A superconvergence result for discontinuous Galerkin methods applied to elliptic problems.* Comput. Methods Appl. Mech. Engrg., 192(41–42) (2003), pp. 4675–4685.
- [31] R. E. EWING, M. LIU AND J. WANG. *A new superconvergence for mixed finite element approximations.* SIAM J. Numer. Anal., 40(6) (2002), pp. 2133–2150.
- [32] W. HOFFMANN, A. H. SCHATZ, L. B. WAHLBIN AND G. WITTUM. *Asymptotically exact a posteriori estimators for the pointwise gradient error on each element in irregular meshes. Part I: A smooth problem and globally quasi-uniform meshes.* Math. Comp., 70(235) (2001), pp. 897–909.
- [33] A. M. LAKHANY, I. MAREK AND J. R. WHITEMAN. *Superconvergence results on mildly structured triangulations.* Comput. Methods Appl. Mech. Engrg., 189(1) (2000), pp. 1–75.
- [34] L. LIU, T. LIU, M. KŘÍŽEK, T. LIN AND S. ZHANG. *Global superconvergence and a posteriori error estimators of the finite element method for a quasi-linear elliptic boundary value problem of nonmonotone type.* SIAM J. Numer. Anal., 42(4) (2004), pp. 1729–1744.
- [35] C. MAKRIDAKIS AND R. H. NOCHETTO. *Elliptic reconstruction and a posteriori error estimates for parabolic problems.* SIAM J. Numer. Anal., 41(4) (2003), pp. 1585–1594.
- [36] H. G. ROOS AND T. LINSS. *Gradient recovery for singularly perturbed boundary value problems I: Onedimensional convection-diffusion.* Computing, 66(2) (2001), pp. 163–178.
- [37] A. H. SCHATZ AND L. B. WAHLBIN. *Asymptotically exact a posteriori estimators for the pointwise gradient error on each element in irregular meshes. Part II: The piecewise linear case.* Math. Comp., 73(246) (2004), pp. 517–523.

- [38] J. WANG AND X. YE. *Superconvergence of finite element approximations for the Stokes problem by projection methods*. SIAM J. Numer. Anal., 39(3) (2001), pp. 1001–1013.
- [39] J. XU AND Z. ZHANG. *Analysis of recovery type a posteriori error estimators for mildly structured grids*. Math. Comp., 73(247) (2004), pp. 1139–1152.
- [40] Z. ZHANG. *Finite element superconvergence on Shishkin mesh for 2-D convection-diffusion problems*. Math. Comp., 72(243) (2003), pp. 1147–1177.
- [41] M. AINSWORTH AND J. T. ODEN. *A posteriori error estimation in finite element analysis*. Pure and Applied Mathematics. Wiley-Interscience [John Wiley & Sons], New York, 2000.
- [42] C. CHEN. *Structure theory of superconvergence of finite elements (in Chinese)*. Hunan Science Press, Hunan, China, 2001.
- [43] M. KŘÍŽEK, P. NEITTAANMÄKI AND R. STENBERG, EDITORS. *Finite element methods. Superconvergence, post-processing, and a posteriori estimates*, volume 196 of Lecture Notes in Pure and Applied Mathematics. Marcel Dekker, Inc., New York, 1998.
- [44] Q. LIN AND N. YAN. *Construction and analysis of high efficient finite elements (in Chinese)*. Hebei University Press, Hebei, China, 1996.
- [45] L. B. WAHLBIN. *Superconvergence in Galerkin finite element methods*, volume 1605 of Lecture Notes in Mathematics. Springer-Verlag, Berlin, 1995.
- [46] Q. ZHU AND Q. LIN. *Superconvergence theory of the finite element method (in Chinese)*. Hunan Science Press, Hunan, China, 1989.
- [47] M. KŘÍŽEK AND P. NEITTAANMÄKI. *Bibliography on superconvergence*. In Finite element methods. Superconvergence, post-processing, and a posteriori estimates, pages 315–348. Marcel Dekker, Inc., New York, 1998.

- [48] A. H. SCHATZ, I. H. SLOAN AND L. B. WAHLBIN. *Superconvergence in finite element methods and meshes that are locally symmetric with respect to a point*. SIAM J. Numer. Anal., 33 (1996), pp. 505–521.
- [49] A. H. SCHATZ AND L. B. WAHLBIN. *Interior maximum norm estimates for finite element methods*. Math. Comp., 31(138) (1977), pp. 414–442.
- [50] A. H. SCHATZ AND L. B. WAHLBIN. *Interior maximum-norm estimates for finite element methods. Part II*. Math. Comp., 64(211) (1995), pp. 907–928.
- [51] I. BABUŠKA, T. STROUBOULIS, C. S. UPADHYAY AND S. K. GANGARAJ. *Computer-based proof of the existence of superconvergence points in the finite element method; superconvergence of the derivatives in finite element solutions of Laplace’s, Poisson’s, and the elasticity equations*. Numer. Methods Partial Differential Equations, 12(3) (1996), pp. 347–392.
- [52] R. LIN AND Z. ZHANG. *Natural superconvergent points of triangular finite elements*. Numer. Methods Partial Differential Equations, 20(6) (2004), pp. 864–906.
- [53] M. KRÍŽEK. *Superconvergence phenomena in the finite element method*. Comput. Methods Appl. Mech. Engrg., 116(1-4) (1994), pp. 157–163.
- [54] M. KRÍŽEK AND P. NEITTAANMÄKI. *On superconvergence techniques*. Acta Appl. Math., 9(3) (1987), pp. 175–198.
- [55] O. C. ZIENKIEWICZ AND J. ZHU. *The superconvergent patch recovery and a posteriori error estimates. Part I: the recovery technique*. Internat. J. Numer. Methods Engrg., 33(7) (1992), pp. 1331–1364.
- [56] O. C. ZIENKIEWICZ AND J. ZHU. *The superconvergent patch recovery and a posteriori error estimates. Part II: error estimates and adaptivity*. Internat. J. Numer. Methods Engrg., 33(7) (1992), pp. 1365–1382.

- [57] O. C. ZIENKIEWICZ AND J. ZHU. *The superconvergent patch recovery (SPR) and adaptive finite element refinement*. Comput. Methods Appl. Mech. Engrg., 101(1-3) (1992), pp. 207–224.
- [58] O. C. ZIENKIEWICZ AND R. L. TAYLOR. *The finite element method*. Vol. 1. The basis. Butterworth-Heinemann, Oxford, fifth edition, 2000.
- [59] B. LI AND Z. ZHANG. *Analysis of a class of superconvergence patch recovery techniques for linear and bilinear finite elements*. Numer. Methods Partial Differential Equations, 15(2) (1999), pp. 151–167.
- [60] Z. ZHANG AND H. D. VICTORY JR. *Mathematical analysis of Zienkiewicz-Zhu's derivative patch recovery technique*. Numer. Methods Partial Differential Equations, 12(4) (1996), pp. 507–524.
- [61] Z. ZHANG AND J. ZHU. *Analysis of the superconvergent patch recovery technique and a posteriori error estimator in the finite element method. Part I*. Comput. Methods Appl. Mech. Engrg., 123(1-4) (1995), pp. 173–187.
- [62] Z. ZHANG AND J. ZHU. *Analysis of the superconvergent patch recovery technique and a posteriori error estimator in the finite element method. Part II*. Comput. Methods Appl. Mech. Engrg., 163(1-4) (1998), pp. 159–170.
- [63] Z. ZHANG. *Ultraconvergence of the patch recovery technique*. Math. Comp., 65(216) (1996), pp. 1431–1437.
- [64] Z. ZHANG. *Ultraconvergence of the patch recovery technique. Part II*. Math. Comp., 69(229) (2000), pp. 141–158.
- [65] Z. ZHANG AND R. LIN. *Ultraconvergence of ZZ patch recovery at mesh symmetry points*. Numer. Math., 95(4) (2003), pp. 781–801.
- [66] T. D. BLACKER AND T. BELYTSCHKO. *Superconvergent patch recovery with equilibrium and conjoint interpolant enhancements*. Internat. J. Numer. Methods Engrg., 37(3) (1994), pp. 517–536.

- [67] N. E. WIBERG, F. ABDULWAHAB AND S. ZIUKAS. *Enhanced superconvergent patch recovery incorporating equilibrium and boundary conditions*. Internat. J. Numer. Methods Engrg., 37(20) (1994), pp. 3417–3440.
- [68] B. BOROOMAND AND O. C. ZIENKIEWICZ. *An improved REP recovery and the effectivity robustness test*. Internat. J. Numer. Methods Engrg., 40(17) (1997), pp. 3247–3277.
- [69] B. BOROOMAND AND O. C. ZIENKIEWICZ. *Recovery by equilibrium in patches (REP)*. Internat. J. Numer. Methods Engrg., 40(1) (1997), pp. 137–164.
- [70] A. NAGA AND Z. ZHANG. *A posteriori error estimates based on the polynomial preserving recovery*. SIAM J. Numer. Anal., 42(4) (2004), pp. 1780–1800.
- [71] Z. ZHANG. *Polynomial preserving gradient recovery and a posteriori estimate for bilinear element on irregular quadrilaterals*. Int. J. Numer. Anal. Model., 11(1) (2004), pp. 1–24.
- [72] Z. ZHANG. *Polynomial preserving recovery for anisotropic and irregular grids*. J. Comput. Math., 22(2) (2004), pp. 331–340.
- [73] Z. ZHANG AND A. NAGA. *Validation of the a posteriori error estimator based on polynomial preserving recovery for linear elements*. Internat. J. Numer. Methods Engrg., 61(11) (2004), pp. 1860–1893.
- [74] J. BRANDTS AND M. KŘÍŽEK, *Gradient superconvergence on uniform simplicial partition of polytopes*, IMA Journal of Numerical Analysis, 23 (2003), pp. 489–505.
- [75] L. CHEN, *Superconvergence of Tetrahedral Linear Finite Elements*, International Journal of Numerical Analysis and Modeling, 3 (2004), pp. 273–282.
- [76] D. J. NAYLOR, *Filling space with tetrahedra*, International Journal for Numerical Methods in Engineering, 44 (1999), pp. 1383–1395.

- [77] Q. DU AND D. WANG, *The Optimal Centroidal Voronoi Tessellations and the Gersho's Conjecture in the Three-Dimensional Space*, Computers and Mathematics with Applications, 49 (2005), pp. 1355–1373.
- [78] A. GERSHO, *Asymptotically optimal block quantization*, IEEE Transactions on Information Theory, 25 (1979), pp. 373–380.
- [79] D. NEWMAN, *The Hexagon theorem*, IEEE Transactions on Information Theory, 28 (1982), pp. 137–139.
- [80] R. M. GRAY AND D. L. NEUHOFF, *Quantization*, IEEE Transactions on Information Theory, 44 (1998), pp. 2325–2383.
- [81] E. S. BARNES AND N. J. A. SLOANE, *The optimal lattice quantizer in three dimensions*, SIAM Journal on Algebraic and Discrete Methods, 4 (1983), pp. 30–41.
- [82] B. LI AND Z. ZHANG, *Analysis of a class of superconvergence patch recovery techniques for linear and bilinear finite elements*, Numerical Methods for Partial Differential Equations, 15 (1999), pp. 151–167.
- [83] C. CHEN. *optimal points of stresses for tetrahedron linear element (in Chinese)*, Natur. Sci. J. Xiangtan Univ., 3 (1980), pp. 16–24.
- [84] G. GOODSELL. *Pointwise superconvergence of the gradient for the linear tetrahedral element*, Numer. Methods Partial Differential Equations, 10 (1994), pp. 651–666.
- [85] V. K. KANTCHEV AND R. D. LAZAROV. *Superconvergence of the gradient of linear finite elements for 3-d Poisson equation*, Proceeding of the Conference on Optimal Algorithms, 1986, pp. 172–182.
- [86] M. KŘÍŽEK, *Superconvergence phenomena on three-dimensional meshes*, International Journal of Numerical Analysis and Modeling, 2 (2005), pp. 43–56.

- [87] J. CHEN AND D. WANG. *Three-dimensional finite element superconvergent Gradient recovery on Par6 patterns*, Numer. Math. Theor. Meth. Appl., 3 (2010), pp. 178–194.
- [88] O. C. ZIENKIEWICZ AND J. ZHU. *A simple error estimator and adaptive procedure for practical engineering analysis*, International Journal for Numerical Methods in Engineering, 24 (1987), pp. 337–357.
- [89] Z. ZHANG AND A. NAGA. *A new finite element gradient recovery method: superconvergence property*, SIAM Journal on Scientific Computing, 26 (2005), pp. 1192–1213.
- [90] J. BRANDTS AND M. KŘÍŽEK. *History and future of superconvergence in three-dimensional finite elements methods*, Proc. Conf. Finite Element Methods: Three-dimensional Problems GAKUTO Internat. Series Math. Sci. Appl., Vol.15. Tokyo: Gakkotosho, pp. 22–33.
- [91] L. M. BLUMENTHAL. *Theory and Applications of Distance Geometry*, Oxford, U.K.: Oxford Univ. Press, 1953.
- [92] G. M. CRIPPEN AND T. HAVEL. *Distance Geometry and Molecular Conformation*, New York: Wiley, 1988.
- [93] T. HAVEL. *Some examples of the use of distances as coordinates in Euclidean geometry*, J. Symbolic Computat., no. 11 (1991), pp. 579–593.
- [94] I. BABUŠKA AND A. MILLER. *A feedback finite element method with a posteriori error estimation Part I*, Computer Methods in Applied Mechanics and Engineering, 61 (1987), pp. 1–40.
- [95] I. BABUŠKA AND W. C. RHEINBOLDT. *Error estimates for adaptive finite element computations*, SIAM Journal on Numerical Analysis, 15 (1978), pp. 736–754.

- [96] I. BABUŠKA AND W. C. RHEINBOLDT. *A posteriori error estimates for the finite element method*, International Journal for Numerical Methods in Engineering, 12 (1978), pp. 1597–1615.
- [97] I. BABUŠKA AND W. C. RHEINBOLDT. *A posteriori error analysis of finite element solutions for one-dimensional problems*, SIAM Journal on Numerical Analysis, 18 (1981), pp. 565–589.
- [98] D. J. MAVRIPLIS. *Adaptive mesh generation for viscous flows using Delaunay triangulation*, Journal of Computational Physics, 90 (1990), pp. 271–291.
- [99] J. PERAIRE, J. PEIRO AND K. MORGAN. *Adaptive remeshing for three dimensional compressible flow computation*, Journal of Computational Physics, 103 (1992), pp. 269–285.
- [100] W. DÖRFLER. *A convergent adaptive algorithm for Poisson’s equation*, SIAM Journal on Numerical Analysis, 33 (1996), pp. 1106–1124.
- [101] R. BANK. *PLTMG: A Software Package for Solving elliptic Partial Differential Equations, User Guide 8.0*, SIAM, 1997.
- [102] M. C. RIVARA. *Mesh refinement process based on the generalized bisection of simplices*, SIAM Journal on Numerical Analysis, 21 (1984), pp. 604–613.
- [103] D. N. ARNOLD, A. MUKHERJEE AND L. POULY. *Locally adapted tetrahedral meshes using bisection*, SIAM Journal on Scientific Computing, 22 (2000), pp. 431–448.
- [104] E. BRIERE AND P. L. GEORGE. *Optimization of tetrahedral meshes*, in: I. Babuska, J.E. Flaherty, W.D. Henshaw, J.E. Hopcroft, J.E. Oliger, T. Tezduyar (Eds.), Modeling, Mesh Generation, and Adaptive Numerical Methods for Partial Differential Equations, Springer-Verlag, (1993), pp. 97–128.
- [105] H. L. COUGNY AND M. S. SHEPHARD. *Parallel refinement and coarsening of tetrahedral meshes*, International Journal for Numerical Methods in Engineering, 46 (1999), pp. 1101–1125.

- [106] B. JOE. *Three-dimensional triangulations from local transformations*, SIAM Journal on Scientific Computing, 10 (1989), pp. 718–741.
- [107] Y. Q. HUANG, H. F. QIN AND D. S. WANG. *Centroidal Voronoi tessellation-based Finite Element Superconvergence*, International Journal for Numerical Methods in Engineering, 12 (2008), pp. 1819–1839.
- [108] J. CHEN, Y. Q. HUANG AND D. S. WANG. *Three Dimensional Superconvergent Gradient Recovery On tetrahedral meshes*, Preprint.
- [109] P. L. GEORGE AND H. BOROUCHAKI. *Delaunay Triangulation and meshing: Application to Finite Elements Methods*, Hermès: Paris, 1998.
- [110] D. WATSON. *Computing the n -dimensional Delaunay tessellation with applications to Voronoi polytopes*, The Computer Journal, 24 (1981), pp. 167–172.
- [111] A. BOWYER. *Computing Dirichlet tessellations*, The Computer Journal, 24(2) (1981), pp. :162–166.
- [112] Q. DU, V. FABER AND M. GUNZBURGER. *Centroidal Voronoi tessellations, Applications and algorithms*, SIAM Review, 41 (1999), pp. 637–676.
- [113] Q. DU AND M. GUNZBURGER. *Grid Generation and Optimization Based on Centroidal Voronoi Tessellations*, Applied and Computational Mathematics, 133 (2002), pp. 591–607.
- [114] Q. DU, M. GUNZBURGER AND L. L. JU. *Meshfree, probabilistic determination of point sets and support regions for meshless computing*, Computer Methods in Applied Mechanics and Engineering, 191 (2002), pp. 1349–1366.
- [115] Q. DU, M. GUNZBURGER, L. L. JU AND X. Q. WANG. *Centroidal Voronoi tessellation algorithms for image compression, segmentation, and Multichannel Restoration*, Journal of Mathematical Imaging and Vision, 24(2) (2006), pp. 177–194.

- [116] Q. DU, M. GUNZBURGER AND L. L. JU. *Constrained Centroidal Voronoi Tessellations on General Surfaces*, SIAM Journal on Scientific Computing, 24 (2003), pp. 1499–1506.
- [117] Q. DU, M. GUNZBURGER AND L. L. JU. *Probablistic methods for centroidal Voronoi tessellations and their parallel implementations*, Journal of Parallel Computing, 28 (2002), pp. 1477–1500.
- [118] Q. DU AND D. S. WANG. *Tetrahedral mesh generation and optimization based on Centroidal Voronoi Tessellations*, International Journal for Numerical Methods in Engineering, 56 (2002), pp. 1355–1373.
- [119] P. D. ZAVATTIERI, E. A. DARI AND G. C. BUSCAGLIA. *Optimization strategies in unstructured mesh generation*, International Journal for Numerical Methods in Engineering, 39 (1996), pp. 2055–2071.
- [120] S.W. CHENG, T. DEY, H. EDELSBRUNNER, M. A. FACELLO AND S. H. TENG. *Sliver exudation*. Journal of Association for Computing Machinery, 47 (2000), pp. 883–904.
- [121] X. Y. LI AND S. H. TENG. *Generating well-shaped Delaunay meshes in 3D*, Proceedings of the 12th Annual ACM-SIAM Symposium on Discrete Algorithms, Washington, DC, U.S.A., (2001), pp. 28–37.
- [122] P. L. CHEW. *Guaranteed-quality Delaunay meshing in 3D*, Proceedings of the 13th Annual ACM Symposium on Computational Geometry, Nice, France, (1997), pp. 391–393.
- [123] H. EDELSBRUNNER, X. Y. LI, G. L. MILLER, A. STATHOPOULOS, D. TALMOR, S. H. TENG, A. ÜNGÖR AND N. WALKINGTON. *Smoothing and cleaning up slivers*, Proceedings of the 32nd ACM Symposium on Theory of Computing, Portland, Oregon, U.S.A., (2000), pp. 273–277.