arXiv:2411.14151v2 [math.NA] 24 Nov 2024

ERROR ANALYSIS OF THE DEEP MIXED RESIDUAL METHOD FOR HIGH-ORDER ELLIPTIC EQUATIONS

MENGJIA BAI, JINGRUN CHEN, RUI DU, AND ZHIWEI SUN

Abstract

This paper presents an a priori error analysis of the Deep Mixed Residual method (MIM) for solving high-order elliptic equations with non-homogeneous boundary conditions, including Dirichlet, Neumann, and Robin conditions. We examine MIM with two types of loss functions, referred to as first-order and second-order least squares systems. By providing boundedness and coercivity analysis, we leverage Céa's Lemma to decompose the total error into the approximation, generalization, and optimization errors. Utilizing the Barron space theory and Rademacher complexity, an a priori error is derived regarding the training samples and network size that are exempt from the curse of dimensionality. Our results reveal that MIM significantly reduces the regularity requirements for activation functions compared to the deep Ritz method, implying the effectiveness of MIM in solving high-order equations.

Key words. Neural network approximation, deep mixed residual method, highorder Elliptic equation

AMS subject classifications. 65N15, 68Q25

1. INTRODUCTION

Partial differential equations (PDEs) are of fundamental importance in modeling phenomena across various disciplines in natural science and society. Developing reliable and efficient numerical methods has a long history in scientific computing and engineering applications. Traditional numerical methods, such as finite difference and finite element, have been successfully established and widely applied. However, these methods often encounter challenges when applied to high-dimensional problems, primarily due to high computational costs. In fact, approximating PDE solutions using traditional methods incurs a computational cost that grows exponentially with the dimensionality of the problem—a phenomenon commonly referred to as the "curse of dimensionality" (CoD).

In recent years, neural networks have emerged as a promising tool for solving PDEs, demonstrating their potential to address the CoD effectively [3,6,9,17,18,25,31]. Notable approaches include the Deep Galerkin method [28] and Physics-Informed Neural Networks (PINNs) [25], which employ the PDE residual in a least-squares framework as the loss function. Another notable approach, the Deep Ritz Method (DRM) [6], leverages the variational form (when available) of the target PDE to define the loss function. More recently, the Deep Mixed Residual method (MIM) [17, 18] has introduced

auxiliary networks to approximate the solution derivatives, allowing for exact enforcement of boundary and initial conditions. Compared to DRM and PINN, MIM has shown advantages in certain models, producing better approximations and accelerating the training process. Additionally, MIM offers unique benefits for handling high-order PDEs by transforming complex high-order problems into lower-order representations, thereby reducing computational complexity and improving solution stability.

In this work, we present an error analysis of the MIM for solving highorder elliptic equations using two-layer neural networks. High-order elliptic equations have extensive applications in materials science [5,11], image processing [1], and elastic mechanics [12]. To illustrate the MIM framework for high-order equations, consider a 2n-order elliptic equation with general boundary conditions:

(1)
$$\Delta^{n} u = f, \qquad x \in \Omega, \\ B(u, \nabla u, \Delta u, \cdots, \nabla \Delta^{n-1} u) = g, \qquad x \in \partial \Omega.$$

MIM introduces auxiliary networks ϕ_i and vector-valued networks ψ_j to approximate $\Delta^i u$ and $\nabla \Delta^j u$ for $0 \leq i, j \leq n-1$. Combining the squared residual loss with a penalty term yields the mixed residual loss function:

(2)
$$\|\operatorname{div} \boldsymbol{\psi}_{n-1} - f\|_{L^{2}(\Omega)}^{2} + \lambda_{1} \|B(\phi_{0}, \boldsymbol{\psi}_{0}, \cdots, \boldsymbol{\psi}_{n-1}) - \boldsymbol{g}\|_{L^{2}(\partial\Omega)}^{2} \\ + \lambda_{2} \Big(\sum_{i=0}^{n-1} \|\nabla\phi_{i} - \boldsymbol{\psi}_{i}\|_{L^{2}(\Omega)}^{2} + \sum_{i=0}^{n-2} \|\phi_{i+1} - \operatorname{div} \boldsymbol{\psi}_{i}\|_{L^{2}(\partial\Omega)}^{2} \Big).$$

This formulation is also referred to as the first-order least squares system and has been used in the finite element method [4]. Moreover, we also introduce the second-order least squares system, where we use networks φ_i to approximate $\Delta^i u$. Then, the mixed residual loss function is given by:

(3)
$$\begin{aligned} \|\Delta \varphi_{n-1} - f\|_{L^{2}(\Omega)}^{2} + \lambda_{1} \|B(\varphi_{0}, \nabla \varphi_{0}, \cdots, \nabla \varphi_{n-1}) - \boldsymbol{g}\|_{L^{2}(\partial \Omega)}^{2} \\ + \lambda_{2} \sum_{i=0}^{n-2} \|\Delta \varphi_{i} - \varphi_{i+1}\|_{L^{2}(\Omega)}^{2}. \end{aligned}$$

In this paper, we examine the 2n-order elliptic equation (1) under Dirichlet, Neumann, and Robin boundary conditions. Both first-order and secondorder least squares formulations, (2)-(3), are analyzed. To derive the error estimates for MIM, we apply a general approach in the notion of bilinear form introduced in [32], where one can utilize Céa's Lemma by performing boundedness and coercivity analysis. As a result, the total error is decomposed into three components: approximation error, generalization error, and optimization error. We bound the approximation error by applying the density of ReLU^k-activated neural networks in Barron space. Moreover, the generalization error is controlled by utilizing Rademacher complexity, while the optimization error is beyond the scope of this article. A significant challenge in our analysis arises from the coercivity analysis of the low-order least squares systems (Equations (2) and (3)), on how to specifically control the coupling terms. We refer to the work [4] where the second-order elliptic equation without boundary penalty is studied. In the case of high-order elliptic equations, we employ a perturbation technique, in which we select a special sequence of small parameters to effectively bound these cross terms by decoupled terms. In addition, when considering the Dirichlet boundary condition, it is well-documented [23,26] that using an L^2 boundary penalty leads to a loss of regularity of 3/2. This implies that approximations in H^2 yield a posteriori estimates only in $H^{\frac{1}{2}}$. In this work, we utilize the idea in [13] and derive a priori estimates in H^1 under the Dirichlet boundary condition. This is achieved by extending Céa's Lemma and conducting a sup-linear coercivity analysis.

1.1. Related works. Methods including PINN [29], DRM [6], and MIM [18] have been utilized to simulate high-order PDEs using neural networks. Additionally, theoretical error analyses have been derived for DRM [27] and PINN [10] when solving high-order elliptic equations, incorporating arbitrary dictionaries of functions and studying greedy algorithms. Furthermore, the works in [16, 19–21, 32] provide error analyses for PDEs solved via neural networks. In this study, we concentrate on the error analysis of MIM using two-layer neural networks, leveraging Barron space theory [2] to address the curse of dimensionality (CoD). For a deeper understanding of Barron space, we recommend [14, 16, 30].

1.2. Our Contributions. We expand upon the existing literature through the following key contributions:

- We apply a general approach in the bilinear form introduced in [32] to the MIM, where the error estimate is derived by performing boundedness and coercivity analysis. Our analysis covers first-order and second-order system least squares systems for high-order elliptic equations.
- Our analysis encompasses non-homogeneous boundary conditions, including Dirichlet, Neumann, and Robin conditions, whereas previous works on the DRM [27] and PINN [10] are limited to homogeneous boundary conditions.
- Compared to DRM and PINN, our theoretical analysis reveals that MIM significantly reduces the regularity requirements for activation functions. Specifically, for a 2*n*-order elliptic equation, DRM [27] requires ReLU^{*n*+1}, while MIM only requires ReLU² and ReLU³ for first-order and second-order least squares systems, respectively.
- Previous studies [23, 26] have shown that an L^2 Dirichlet boundary penalty results in a regularity loss of 3/2. In this work, we extend Céa's Lemma by establishing a sup-linear coercivity, yielding an H^1 error estimate inspired by the approach in [13].

• A core component of our work is the coercivity analysis of low-order systems. The primary challenge lies in how to control the coupling terms, in which we introduce a special sequence of small parameters to effectively control these terms through a perturbation technique.

This paper is organized as follows. In Section 2, we provide the basic setup and the main results of this work. The proof of our main results is given in Section 3 by using a general framework of bilinear form. In Section 4, we present the proof of the crucial coercivity estimates for the first-order least squares system, which is essential for the error estimates. The coercivity estimates for the second-order least squares system are provided in Section 5.

2. Main results

In this section, we introduce the basic setup and present the main results.

2.1. Model problem. Throughout this paper, we let $\Omega = [0, 1]^d$ with dimension $d \ge 1$. For any integer $n \ge 1$, we consider the following 2*n*-order elliptic equation:

(4)
$$\Delta^n u = f \quad \text{in } \Omega,$$

with certain boundary conditions, including the Dirichlet boundary:

(5)
$$(u, \Delta u, \cdots, \Delta^{n-1}u) = \mathbf{g}_{\mathrm{D}} \quad \text{on } \partial\Omega,$$

the Neumann boundary:

(6)
$$(\partial_{\boldsymbol{n}} u, \partial_{\boldsymbol{n}} \Delta u, \cdots, \partial_{\boldsymbol{n}} \Delta^{n-1} u) = \boldsymbol{g}_{\mathrm{N}} \text{ on } \partial\Omega,$$

and the Robin boundary:

(7)
$$(u + \partial_n u, \Delta u + \partial_n \Delta u, \cdots, \Delta^{n-1} u + \partial_n \Delta^{n-1} u) = \boldsymbol{g}_{\mathrm{R}} \text{ on } \partial\Omega.$$

Here, \boldsymbol{n} denotes the outer normal vector of $\partial \Omega$.

2.2. Neural networks. A neural network is a nonlinear parametric model defined as a concatenation of affine maps and activation functions. Let $\boldsymbol{x} \in \mathbb{R}^d$ be the input element and $\boldsymbol{y} \in \mathbb{R}^m$ be the output vector function. An *L*-layer neural network can be written as:

$$h_0 = \boldsymbol{x},$$

$$h_{\ell} = \sigma(W_{\ell}h_{\ell-1} + b_{\ell}) \text{ for } \ell = 1, \cdots, L-1,$$

$$\boldsymbol{y} = W_L h_{L-1} + b_L.$$

Especially, a neural network is classified as shallow if its depth L = 2, and as deep otherwise. Here, W_{ℓ} denotes the weight matrix of the ℓ -th layer, and b_{ℓ} represents the bias vector. The function σ is referred to as an activation function, which introduces non-linearity to enhance the model's expressive power. In this work, we use the activation function $\sigma = \text{ReLU}^k$ defined as follows:

4

Definition 2.1. Let $k \in \mathbb{N}$, the nonlinear univariate function $\operatorname{ReLU}^k(x)$ is defined by

$$\operatorname{ReLU}^{k}(x) = \begin{cases} x^{k}, & x \ge 0, \\ 0, & x < 0. \end{cases}$$

In particular, we denote $\operatorname{ReQU}(x) = \operatorname{ReLU}^2(x)$ and $\operatorname{ReCU}(x) = \operatorname{ReLU}^3(x)$. Furthermore, ReLU^k is applied component-wise, i.e.

$$\operatorname{ReLU}^{k}(\boldsymbol{x}) = \left(\operatorname{ReLU}^{k}(x_{1}), \cdots, \operatorname{ReLU}^{k}(x_{n})\right),$$

for any vector $\mathbf{x} = (x_1, \cdots, x_n)$.

2.3. Two-layer neural networks and Barron space. In this work, we use the two-layer neural networks to approximate Equation (4)-(7), by applying the loss function in the form of both the first-order least squares system (2) and second-order least squares system (3). A suitable functional space as a closed hull of two-layer neural networks is the Barron space. In the following, we introduce the spectral Barron space via a cosine transformation [16]. Given a set of cosine functions defined by

(8)
$$\Phi_{\boldsymbol{k}} := \prod_{i=1}^{d} \cos(\pi k_i x_i), \quad \boldsymbol{k} = \{k_i\}_{1 \le i \le d}, \quad k_i \in \mathbb{N}_0.$$

Suppose $u \in L^1(\Omega)$, let $\hat{u}(\mathbf{k})$ be the expansion coefficients of u under the basis $\{\Phi_k\}_{k \in \mathbb{N}^d_*}$. We define for $s \ge 0$ the spectral Barron space $\mathcal{B}^s(\Omega)$ as

(9)
$$\mathcal{B}^{s}(\Omega) := \left\{ u \in L^{1}(\Omega) : \sum_{\boldsymbol{k} \in \mathbb{N}_{0}^{d}} (1 + \pi^{s} |\boldsymbol{k}|_{1}^{s}) |\hat{u}(\boldsymbol{k})| < \infty \right\}.$$

The spectral Barron norm of a function $u \in \mathcal{B}^{s}(\Omega)$ is given by

$$\|u\|_{\mathcal{B}^s(\Omega)} = \sum_{\boldsymbol{k} \in \mathbb{N}_0^d} (1 + \pi^s |\boldsymbol{k}|_1^s).$$

An important property of Barron functions is that they can be well approximated by two-layer neural networks without the curse of dimensionality, which will be detailed in Lemma 3.6. To proceed, we assume that the solution of 2n-order elliptic equation (4)-(7) belongs to the Barron space \mathcal{B}^{2n+3} . This can be achieved based on the regularity theory of elliptic equations, assuming that the inhomogeneous term and the boundary term are sufficiently smooth [15]. In the following, we introduce two models of two-layer neural networks, associated with first-order and second-order least squares systems, respectively. Additionally, their parameters are assumed to be a priori bounded by the Barron norm of the solution. 2.3.1. Two-layer neural networks induced by first-order system. Assume $u^* \in \mathcal{B}^{2n+2}(\Omega)$ is a solution to the 2*n*-order elliptic equation (4)-(7). We define a set of ReQU-activated networks associated with function u^* by (10)

$$\mathcal{F}_{\text{ReQU},m} := \Big\{ \boldsymbol{c} + \sum_{i=1}^{m} \boldsymbol{a}_{i} \cdot \text{ReQU}(W_{i}\boldsymbol{x} + \boldsymbol{b}_{i}) \in \mathbb{R}^{n(d+1)} \, \Big| \, \boldsymbol{x} \in \mathbb{R}^{d}, \\ |\boldsymbol{c}| \le 2 \|u^{*}\|_{\mathcal{B}^{2n+2}}, \, |W_{i}|_{2} \le 1, \, |\boldsymbol{b}_{i}| \le 1, \, \sum_{i=1}^{m} |\boldsymbol{a}_{i}| \le 4 \|u^{*}\|_{\mathcal{B}^{2n+2}} \Big\}.$$

Denote all the parameters of the network by θ . For any neural network $u_{\theta} \in \mathcal{F}_{\text{ReQU},m}$, we use the notation $\phi_i \in \mathbb{R}$ and $\psi_i \in \mathbb{R}^d$ for $i = 0, \ldots, n-1$, such that

(11)
$$\boldsymbol{u}_{\theta} = \left(\phi_0, \, \boldsymbol{\psi}_0, \cdots, \, \phi_{n-1}, \, \boldsymbol{\psi}_{n-1}\right)$$

To simplify the first-order least squares system (2), we introduce some notations. Denote $\mathbf{f} = (0, \dots, 0, f)^T \in \mathbb{R}^{n(d+1)}$ and define the matrix operator:

(12)
$$\mathcal{P} := \begin{pmatrix} \nabla & -I_{d \times d} & 0 & \cdots & 0 \\ 0 & \operatorname{div} & -I & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & \operatorname{div} \end{pmatrix}_{n(d+1) \times n(d+1)},$$

where $I_{d\times d}$ represents $d\times d$ identity matrix. In addition, given $u_{\theta} \in \mathcal{F}_{\text{ReQU},m}$, we define the trace operator S_{α} for $\alpha = D$, N and R, representing Dirichlet, Neumann and Robin boundary conditions respectively:

(13)
$$\begin{cases} S_{\mathrm{D}}\boldsymbol{u}_{\theta} = (\phi_{0}, \phi_{1}, \cdots, \phi_{n-1}); \\ S_{\mathrm{N}}\boldsymbol{u}_{\theta} = (\boldsymbol{n} \cdot \boldsymbol{\psi}_{0}, \boldsymbol{n} \cdot \boldsymbol{\psi}_{1}, \cdots, \boldsymbol{n} \cdot \boldsymbol{\psi}_{n-1}); \\ S_{\mathrm{R}}\boldsymbol{u}_{\theta} = (S_{\mathrm{D}} + S_{\mathrm{R}})\boldsymbol{u}_{\theta}. \end{cases}$$

Then, for Dirichlet and Robin boundary conditions, i.e. $\alpha = D, R$, we introduce the expected loss functions regarding the first-order least squares system as below:

(14)
$$\mathcal{L}_{\alpha}(\boldsymbol{u}_{\theta}) = \|\mathcal{P}\boldsymbol{u}_{\theta} - \boldsymbol{f}\|_{L^{2}(\Omega)}^{2} + \lambda \|S_{\alpha}\boldsymbol{u}_{\theta} - \boldsymbol{g}_{\alpha}\|_{L^{2}(\partial\Omega)}^{2},$$

and the corresponding empirical loss function is defined as

(15)
$$\widehat{\mathcal{L}}_{\alpha}(\boldsymbol{u}_{\theta}) = \frac{|\Omega|}{N} \sum_{j=1}^{N} |(\mathcal{P}\boldsymbol{u}_{\theta} - \boldsymbol{f})(X_{j})|^{2} + \frac{|\partial\Omega|}{\widehat{N}} \sum_{j=1}^{N} \lambda |(S_{\alpha}\boldsymbol{u}_{\theta} - \boldsymbol{g}_{\alpha})(\widehat{X}_{j})|^{2}.$$

Here, $\{X_j\}_{j=1}^N$ and $\{\widehat{X}_j\}_{j=1}^{\widehat{N}}$ are randomly sampled from Ω and $\partial\Omega$, respectively. The penalty constant λ_2 in (2) is omitted for simplicity, without affecting our main results. For the Neumann boundary condition, an additional penalty is required in the loss function, since the exact solution of Equation (4) is unique up to a constant. In this case, we approximate the

solution with zero mean, and set the loss function for u_{θ} with the representation in (11):

(16)
$$\mathcal{L}_{\mathrm{N}}(\boldsymbol{u}_{\theta}) = \|\mathcal{P}\boldsymbol{u}_{\theta} - \boldsymbol{f}\|_{L^{2}(\Omega)}^{2} + \lambda \|S_{\mathrm{N}}\boldsymbol{u}_{\theta} - \boldsymbol{g}_{\mathrm{N}}\|_{L^{2}(\partial\Omega)}^{2} + \mu \Big| \int_{\Omega} \phi_{0} \,\mathrm{d}\boldsymbol{x} \Big|^{2},$$

and the empirical loss function is given by:

(17)
$$\widehat{\mathcal{L}}_{N}(\boldsymbol{u}_{\theta}) = \frac{|\Omega|}{N} \sum_{j=1}^{N} \left| (\mathcal{P}\boldsymbol{u}_{\theta} - \boldsymbol{f})(X_{j}) \right|^{2} \\
+ \frac{|\partial\Omega|}{\widehat{N}} \sum_{j=1}^{\widehat{N}} \lambda \left| (S_{N}\boldsymbol{u}_{\theta} - \boldsymbol{g}_{N})(\widehat{X}_{j}) \right|^{2} + \mu \left| \frac{|\Omega|}{N} \sum_{j=1}^{N} \phi_{0}(X_{j}) \right|^{2}.$$

2.3.2. Two-layer neural networks induced by second-order system. We assume the solutions $u^* \in \mathcal{B}^{2n+3}(\Omega)$, and define a set of ReCU-activated networks associated with function u^* as follows: (18)

$$\mathcal{F}_{\operatorname{ReCU},m} := \left\{ oldsymbol{c} + \sum_{i=1}^m oldsymbol{a}_i \cdot \operatorname{ReCU}(W_i oldsymbol{x} + oldsymbol{b}_i) \in \mathbb{R}^n \ \Big| \ oldsymbol{x} \in \mathbb{R}^d, \ |oldsymbol{c}| \le 2 \|u^*\|_{\mathcal{B}^{2n+3}}, \ |W_i|_2 \le 1, \ |oldsymbol{b}_i| \le 1, \ \sum_{i=1}^m |oldsymbol{a}_i| \le 4 \|u^*\|_{\mathcal{B}^{2n+3}}
ight\}.$$

For any neural network $v_{\theta} \in \mathcal{F}_{\text{ReCU},m}$, we define the notation $\varphi_i \in \mathbb{R}$ for $i = 0, \ldots, n-1$, and introduce the following representation:

(19)
$$\boldsymbol{v}_{\theta} = (\varphi_0, \varphi_1, \cdots, \varphi_{n-1}).$$

To express the loss function in the form of second-order least squares system (3), we denote $\mathbf{f} = (0, \dots, 0, f)^T \in \mathbb{R}^n$ and define the matrix operator:

(20)
$$\mathcal{P}^* := \begin{pmatrix} \Delta & -I & 0 & \cdots & 0 \\ 0 & \Delta & -I & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & \Delta \end{pmatrix}_{n \times n}$$

Furthermore, given $\boldsymbol{v}_{\theta} \in \mathcal{F}_{\text{ReCU},m}$, the trace operator S_{α} for $\alpha = D$, N, R, can be defined as follow:

(21)
$$\begin{cases} S_{\mathrm{D}}^{*}\boldsymbol{v}_{\theta} = (\varphi_{0}, \varphi_{1}, \cdots, \varphi_{n-1}); \\ S_{\mathrm{N}}^{*}\boldsymbol{v}_{\theta} = (\partial_{n}\varphi_{0}, \partial_{n}\varphi_{1}, \cdots, \partial_{n}\varphi_{n-1}); \\ S_{\mathrm{R}}^{*}\boldsymbol{v}_{\theta} = (S_{\mathrm{D}}^{*} + S_{\mathrm{R}}^{*})\boldsymbol{v}_{\theta}. \end{cases}$$

Then, for the case $\alpha = D, R$, we define the expected loss functions regarding the second-order least squares system (3) as

(22)
$$\mathcal{L}^*_{\alpha}(\boldsymbol{v}_{\theta}) = \|\mathcal{P}^*\boldsymbol{v}_{\theta} - \boldsymbol{f}\|^2_{L^2(\Omega)} + \lambda \|S^*_{\alpha}\boldsymbol{v}_{\theta} - \boldsymbol{g}_{\alpha}\|^2_{L^2(\partial\Omega)},$$

and the corresponding empirical loss function is given by

(23)
$$\widehat{\mathcal{L}}_{\alpha}^{*}(\boldsymbol{v}_{\theta}) = \frac{|\Omega|}{N} \sum_{j=1}^{N} \left| (\mathcal{P}^{*}\boldsymbol{v}_{\theta} - \boldsymbol{f})(X_{j}) \right|^{2} + \frac{|\partial\Omega|}{\widehat{N}} \sum_{j=1}^{\widehat{N}} \lambda \left| (S_{\alpha}^{*}\boldsymbol{v}_{\theta} - \boldsymbol{g}_{\alpha})(\widehat{X}_{j}) \right|^{2}.$$

For the Neumann boundary condition, we add a zero-mean penalty and define

(24)
$$\mathcal{L}_{\mathrm{N}}^{*}(\boldsymbol{v}_{\theta}) = \|\mathcal{P}^{*}\boldsymbol{v}_{\theta} - \boldsymbol{f}\|_{L^{2}(\Omega)}^{2} + \lambda \|S_{\mathrm{N}}^{*}\boldsymbol{v}_{\theta} - \boldsymbol{g}_{\alpha}\|_{L^{2}(\partial\Omega)}^{2} + \mu \Big| \int_{\Omega} \varphi_{0,\theta} \,\mathrm{d}\boldsymbol{x} \Big|^{2},$$

together with the empirical loss function:

(25)
$$\begin{aligned} \widehat{\mathcal{L}}_{\mathrm{N}}^{*}(\boldsymbol{v}_{\theta}) =& \frac{|\Omega|}{N} \sum_{j=1}^{N} \left| (\mathcal{P}^{*}\boldsymbol{v}_{\theta} - \boldsymbol{f})(X_{j}) \right|^{2} \\ &+ \frac{|\partial\Omega|}{\widehat{N}} \sum_{j=1}^{\widehat{N}} \lambda \left| (S_{\mathrm{N}}^{*}\boldsymbol{v}_{\theta} - \boldsymbol{g}_{\mathrm{N}})(\widehat{X}_{j}) \right|^{2} + \mu \left| \frac{|\Omega|}{N} \sum_{j=1}^{N} \varphi_{0}(X_{j}) \right|^{2}. \end{aligned}$$

2.4. **Main results.** Now, we present the quantitative estimates for the error between exact solutions and MIM neural networks with Monte Carlo sampling. Define the norm

$$\|\boldsymbol{v}\|_{H(\operatorname{div};\Omega)} = \left(\|\boldsymbol{v}\|_{L^2(\Omega)}^2 + \|\operatorname{div}\,\boldsymbol{v}\|_{L^2(\Omega)}^2\right)^{\frac{1}{2}}.$$

Moreover, given N and \widehat{N} in (17) and (25), which represent the number of sample points in Ω and on $\partial\Omega$ respectively, we make the assumption that $\widehat{N} = O(\frac{N}{d^2}).$

Theorem 2.1 (First-order least squares system). Suppose $u_{\alpha}^* \in \mathcal{B}^{2n+2}(\Omega)$ with $\alpha = D, N, R$ is a solution of problem (4) satisfying boundary conditions (5), (6) or (7). Let

$$\hat{\boldsymbol{u}}_{\theta} = \left(\hat{\phi}_{0}, \, \hat{\boldsymbol{\psi}}_{0}, \cdots, \hat{\phi}_{n-1}, \, \hat{\boldsymbol{\psi}}_{n-1}\right) = \arg\min_{\boldsymbol{u}_{\theta} \in \mathcal{F}_{\operatorname{ReQU},m}} \widehat{\mathcal{L}}_{\alpha}(\boldsymbol{u}_{\theta}).$$

Then for the cases of Neumann and Robin boundary, i.e. $\alpha = N, R$, we have

$$\sum_{k=0}^{n-1} \left(\mathbb{E} \| \hat{\phi}_k - \Delta^k u_\alpha^* \|_{H^1(\Omega)}^2 + \mathbb{E} \| \hat{\psi}_k - \nabla(\Delta)^k u_\alpha^* \|_{H(\operatorname{div};\Omega)}^2 \right)$$
$$\lesssim \frac{\| u_\alpha^* \|_{\mathcal{B}^{2n+2}(\Omega)}^2}{m} + \frac{\| u_\alpha^* \|_{\mathcal{B}^{2n+2}(\Omega)}^2}{\sqrt{N}};$$

In the case of the Dirichlet boundary, we have

$$\sum_{k=0}^{n-1} \left(\mathbb{E} \| \hat{\phi}_k - \Delta^k u_{\mathrm{D}}^* \|_{H^1(\Omega)}^2 + \mathbb{E} \| \hat{\psi}_k - \nabla(\Delta)^k u_{\mathrm{D}}^* \|_{H(\mathrm{div};\Omega)}^2 \right) \\ \asymp \frac{\| u_{\mathrm{D}}^* \|_{\mathcal{B}^{2n+2}(\Omega)}^2}{\sqrt{m}} + \frac{\| u_{\mathrm{D}}^* \|_{\mathcal{B}^{2n+2}(\Omega)}^2}{\sqrt[4]{N}},$$

where the expectation is taken on the random sampling of training data in Ω and $\partial \Omega$.

Theorem 2.2 (Second-order least square system). Suppose $u_{\alpha}^* \in \mathcal{B}^{2n+3}(\Omega)$ with $\alpha = D, N, R$ is a solution of problem (4) satisfying boundary conditions (5), (6) or (7). Let

$$\hat{\boldsymbol{v}}_{\theta} = \left(\hat{\phi}_{0}, \cdots, \hat{\phi}_{n-1}\right) = \arg\min_{\boldsymbol{v}_{\theta} \in \mathcal{F}_{\operatorname{ReCU},m}} \widehat{\mathcal{L}}^{*}_{\alpha}(\boldsymbol{v}_{\theta}).$$

Then for the cases of Neumann and Robin boundary, i.e. $\alpha = N, R$, we have

$$\sum_{k=0}^{n-1} \left(\mathbb{E} \| \hat{\phi}_k - \Delta^k u_\alpha^* \|_{H^1(\Omega)}^2 + \mathbb{E} \| \nabla \hat{\phi}_k - \nabla \Delta^k u_\alpha^* \|_{H(\operatorname{div};\Omega)}^2 \right)$$
$$\lesssim \frac{\| \phi_\alpha^* \|_{\mathcal{B}^{2n+3}(\Omega)}^2}{m} + \frac{\| \phi_\alpha^* \|_{\mathcal{B}^{2n+3}(\Omega)}^2}{\sqrt{N}};$$

In the case of the Dirichlet boundary, we have

$$\sum_{k=0}^{n-1} \left(\mathbb{E} \| \hat{\phi}_k - \Delta^k u_{\mathrm{D}}^* \|_{H^1(\Omega)}^2 + \mathbb{E} \| \nabla \hat{\phi}_k - \nabla \Delta^k u_{\mathrm{D}}^* \|_{H(\mathrm{div};\Omega)}^2 \right)$$
$$\lesssim \frac{\| u_{\mathrm{D}}^* \|_{\mathcal{B}^{2n+3}(\Omega)}^2}{\sqrt{m}} + \frac{\| u_{\mathrm{D}}^* \|_{\mathcal{B}^{2n+3}(\Omega)}^2}{\sqrt[4]{N}}$$

where the expectation is taken on the random sampling of training data over Ω and $\partial\Omega$.

3. Proof of main results

In this section, we give the detailed proof of Theorem 2.1 and Theorem 2.2. The central idea is to use the general approach from [32], where one can apply Céa's Lemma by performing boundedness and coercivity analysis of the bilinear form induced form (2) and (3).

3.1. Coercivity and boundedness. To apply Céa's Lemma, we first introduce the results of coercivity and boundedness.

3.1.1. Case I: First-order system. Given functions $\boldsymbol{u}, \boldsymbol{w} \in \left(H^1(\Omega) \times H^1(\Omega)^d\right)^n$

(26)
$$\boldsymbol{u} = (\phi_0, \, \boldsymbol{\psi}_0, \cdots, \, \phi_{n-1}, \, \boldsymbol{\psi}_{n-1}), \\ \boldsymbol{w} = (\theta_0, \, \boldsymbol{\xi}_0, \cdots, \, \theta_{n-1}, \, \boldsymbol{\xi}_{n-1}),$$

where $\phi_i, \theta_i \in \mathbb{R}$ and $\psi_i, \xi_i \in \mathbb{R}^d$. Moreover, we introduce the following bilinear form, induced from (14) and (16): for $\alpha = D, R$, we define

(27)
$$\mathcal{B}_{\alpha}(\boldsymbol{u},\boldsymbol{w}) = (\mathcal{P}\boldsymbol{u},\mathcal{P}\boldsymbol{w}) + \lambda(S_{\alpha}\boldsymbol{u},S_{\alpha}\boldsymbol{w}),$$

and for the Neumann boundary condition, we define

(28)
$$\mathcal{B}_{N}(\boldsymbol{u},\boldsymbol{w}) = (\mathcal{P}\boldsymbol{u},\mathcal{P}\boldsymbol{w}) + \lambda(S_{N}\boldsymbol{u},S_{N}\boldsymbol{w}) + \mu \int_{\Omega} \phi_{0} d\boldsymbol{x} \int_{\Omega} \theta_{0} d\boldsymbol{x}.$$

Here, the matrix operator \mathcal{P} and trace operator \mathcal{S}_{α} are defined in (12)-(13).

Regarding the coercivity of the bilinear form (27), the case of the secondorder elliptic equation with lower-order terms was studied in [13]. It proved that, for the Neumann boundary, i.e. $\alpha = N$, the bilinear form (27) yields the estimates

$$\mathcal{B}_{\alpha}(\boldsymbol{u},\boldsymbol{u}) \geq a \|\boldsymbol{u}\|_{H^1}^2,$$

for any function $u \in H^1$. As for the Dirichlet boundary, it follows that

$$\mathcal{B}_{\mathrm{D}}(\boldsymbol{u},\boldsymbol{u}) \geq a \|\boldsymbol{u}\|_{H^{\frac{1}{2}}}^{2}.$$

Moreover, the $H^{\frac{1}{2}}$ norm on the right-hand side is optimal. In fact, it was shown in [26,32] that it is impossible to replace the $H^{\frac{1}{2}}$ by H^{α} for any $\alpha > \frac{1}{2}$. This implies that the standard analysis cannot provide the coercivity result to derive an H^1 error estimate for the Dirichlet boundary. To address this challenge, we follow the idea in [13], where a sup-linear coercivity is derived, in the sense that:

$$\mathcal{B}_{\mathrm{D}}(\boldsymbol{u},\boldsymbol{u}) \geq a_E \|\boldsymbol{u}\|_{H^1}^4$$

for any function \boldsymbol{u} satisfying $\|\boldsymbol{u}\|_{H^1(\Omega)} \leq E$, here E > 0 is to be determined by the exact solution u^* , which leads to a priori error estimate. More precisely, we introduce the following result:

Lemma 3.1. For any function $\boldsymbol{u}, \boldsymbol{w} \in (H^1(\Omega) \times H^1(\Omega)^d)^n$, the bilinear form (27), (28) are bounded for $\alpha = D$, N, R, *i.e.*

$$\mathcal{B}_{lpha}(oldsymbol{u},oldsymbol{w}) \leq C_B \|oldsymbol{u}\|_{H^1(\Omega)} \|oldsymbol{w}\|_{H^1(\Omega)}.$$

Furthermore, the bilinear form (27), (28) have coercivity for the Neumann and Robin boundary regarding to $(H^1(\Omega) \times H(\operatorname{div}; \Omega))^n$, i.e. for $\alpha = N$, R, suppose **u** satisfies the representation (26), we have

$$\mathcal{B}_{\alpha}(\boldsymbol{u},\boldsymbol{u}) \geq C \sum_{k=0}^{n-1} \left(\|\phi_k\|_{H^1(\Omega)}^2 + \|\boldsymbol{\psi}_k\|_{H(\operatorname{div};\Omega)}^2 \right).$$

In addition, if we further assume that $\|\boldsymbol{u}\|_{H^1(\Omega)} \leq E$, then it holds the suplinear coercivity for the Dirichlet boundary, i.e.

$$\sqrt{\mathcal{B}_{\mathrm{D}}(\boldsymbol{u},\boldsymbol{u})} \geq C_E \sum_{k=0}^{n-1} \left(\|\phi_k\|_{H^1(\Omega)}^2 + \|\boldsymbol{\psi}_k\|_{H(\mathrm{div};\Omega)}^2 \right).$$

Here, we use the notation $\|\boldsymbol{u}\|_{H^1(\Omega)}$ to denote the sum of $\|\phi_k\|_{H^1(\Omega)}$ and $\|\psi_k\|_{H^1(\Omega)}$.

By repeatedly applying the Cauchy-Schwarz and trace inequalities, one can obtain the boundedness of bilinear operator \mathcal{B}_{α} . In addition, the coercivity can be deduced directly by applying Lemma 4.1 together with the boundness results. Lemma 4.1 and Lemma 5.1 are the main ingredients of the analytical part of this work.

3.1.2. Case II: Second-order system. For any functions $\boldsymbol{v}, \boldsymbol{w} \in (H^2(\Omega))^n$, we denote

(29)
$$\boldsymbol{v} = (\varphi_0, \varphi_1, \cdots, \varphi_{n-1}), \\ \boldsymbol{w} = (\rho_0, \rho_1, \cdots, \rho_{n-1}).$$

Define the following bilinear form induced from loss functions (22) and (24): for $\alpha = D, R$,

(30)
$$\mathcal{B}_{\alpha}(\boldsymbol{v};\boldsymbol{w}) = (\mathcal{P}^*\boldsymbol{v},\mathcal{P}^*\boldsymbol{w}) + \lambda(S^*_{\alpha}\boldsymbol{v},S^*_{\alpha}\boldsymbol{w}),$$

and for Neumann boundary condition,

(31)
$$\mathcal{B}_{N}(\boldsymbol{v};\boldsymbol{w}) = (\mathcal{P}^{*}\boldsymbol{v},\mathcal{P}^{*}\boldsymbol{w}) + \lambda(S_{N}^{*}\boldsymbol{v},S_{N}^{*}\boldsymbol{w}) + \mu \int_{\Omega} \varphi_{0} \,\mathrm{d}\boldsymbol{x} \int_{\Omega} \rho_{0} \,\mathrm{d}\boldsymbol{x}.$$

Here, the matrix operator \mathcal{P}^* and trace operator \mathcal{S}^*_{α} are defined in (20)-(21). With the above definitions, we can further obtain results analogous to those for the first-order system.

Lemma 3.2. For any function $\boldsymbol{v}, \boldsymbol{w} \in (H^2(\Omega))^n$, the bilinear form (30), (31) are bounded for $\alpha = D$, N, R, *i.e.*

$$\mathcal{B}_{\alpha}(\boldsymbol{v}, \boldsymbol{w}) \leq C_B \|\boldsymbol{v}\|_{H^2(\Omega)} \|\boldsymbol{w}\|_{H^2(\Omega)}.$$

Moreover, the bilinear form (30), (31) have coercivity for the Neumann and Robin boundary, i.e. for $\alpha = N$, R, suppose v satisfies representation (29), we have

$$\mathcal{B}_{\alpha}(\boldsymbol{v},\boldsymbol{v}) \geq C \sum_{k=0}^{n-1} \left(\|\varphi_k\|_{H^1(\Omega)}^2 + \|\nabla\varphi_k\|_{H(\operatorname{div};\Omega)}^2 \right)$$

In addition, if we further assume that $\|v\|_{H^2(\Omega)} \leq E$, then we have sup-linear coercivity for the Dirichlet boundary, i.e.

$$\sqrt{\mathcal{B}_{\mathrm{D}}(\boldsymbol{v},\boldsymbol{v})} \geq C_E \sum_{k=0}^{n-1} \left(\|\varphi_k\|_{H^1(\Omega)}^2 + \|\nabla\varphi_k\|_{H(\mathrm{div};\Omega)}^2 \right).$$

Here, we use the notation $\|v\|_{H^2(\Omega)}$ to denote the sum of $\|\varphi_k\|_{H^2(\Omega)}$.

The boundedness of bilinear operator \mathcal{B}^*_{α} can be derived directly by using the Cauchy-Schwarz and trace inequalities. The coercivity follows from Lemma 5.1, together with the boundedness result.

3.2. Error decomposition. For simplicity, we first introduce an abstract framework proposed in [32]: Given two Hilbert spaces X, Y, and denote a linear map

$$T: X \to Y, \quad u \mapsto Tu$$

Define the corresponding bilinear form for any $u, v \in X$:

$$(32) \qquad \qquad \mathcal{B}(\boldsymbol{u},\boldsymbol{v}) = (T\boldsymbol{u},T\boldsymbol{v})_Y.$$

Furthermore, denote by \mathcal{F}_{Θ} the collection of all neural network functions with a certain parameter space Θ . Then we have the following lemma:

Lemma 3.3 (Céa's Lemma). For any function $\mathbf{f} \in Y$, define the expected loss function $\mathcal{L}(\mathbf{u}) = ||T\mathbf{u} - \mathbf{f}||_Y^2$, whose unique minimizer is denoted by \mathbf{u}^* . Assume that the bilinear form \mathcal{B} defined in (32) is bounded, i.e.

$$\mathcal{B}(\boldsymbol{u},\boldsymbol{v})\precsim \|\boldsymbol{u}\|_X \|\boldsymbol{v}\|_X.$$

Moreover, there exists a Hilbert space $X \subseteq Z$:

• if \mathcal{B} is coercive with respect to Z, i.e. $\mathcal{B}(\boldsymbol{u}, \boldsymbol{u}) \geq a \|\boldsymbol{u}\|_{Z}^{2}$, then for every $\boldsymbol{u}_{\theta} \in \mathcal{F}_{\Theta}$, it holds that

(33)
$$\|\boldsymbol{u}_{\theta} - \boldsymbol{u}^*\|_Z^2 \precsim \delta(\boldsymbol{u}_{\theta}) + \inf_{\hat{\boldsymbol{u}}_{\theta} \in \mathcal{F}_{\Theta}} \|\hat{\boldsymbol{u}}_{\theta} - \boldsymbol{u}^*\|_X^2.$$

• if \mathcal{B} is sup-linear coercive with respect to Z, i.e. $\mathcal{B}(\boldsymbol{u}, \boldsymbol{u}) \geq a \|\boldsymbol{u}\|_{Z}^{4}$, then we have

(34)
$$\|\boldsymbol{u}_{\theta} - \boldsymbol{u}^*\|_Z^2 \precsim \sqrt{\delta(\boldsymbol{u}_{\theta})} + \sqrt{\inf_{\hat{\boldsymbol{u}}_{\theta} \in \mathcal{F}_{\Theta}} \|\hat{\boldsymbol{u}}_{\theta} - \boldsymbol{u}^*\|_X^2}.$$

Here, $\delta(\boldsymbol{u}_{\theta}) = \mathcal{L}(\boldsymbol{u}_{\theta}) - \inf_{\hat{\boldsymbol{u}}_{\theta} \in \mathcal{F}_{\Theta}} \mathcal{L}(\hat{\boldsymbol{u}}_{\theta}).$

Proof. The proof is essentially the same as that in [22, 32], which is included here for completeness. By the definition (32) of \mathcal{B} , we have

$$\mathcal{L}(\boldsymbol{u}_{\theta}) - \mathcal{L}(\boldsymbol{u}^*) = \mathcal{B}(\boldsymbol{u}_{\theta} - \boldsymbol{u}^*, \boldsymbol{u}_{\theta} - \boldsymbol{u}^*).$$

Because of the coercivity assumptions of \mathcal{B} , there exists a constant $\beta > 0$ such that

$$\mathcal{B}(oldsymbol{u}_{ heta}-oldsymbol{u}^*,oldsymbol{u}_{ heta}-oldsymbol{u})\geq eta\|oldsymbol{u}_{ heta}-oldsymbol{u}^*\|_Z^k$$

where k = 2 or 4 under coercivity or sup-linear coercivity assumptions. On the other hand, the boundedness of \mathcal{B} yields

$$\begin{split} \mathcal{L}(\boldsymbol{u}_{\theta}) - \mathcal{L}(\boldsymbol{u}^{*}) = & \mathcal{L}(\boldsymbol{u}_{\theta}) - \inf_{\hat{\boldsymbol{u}}_{\theta} \in \mathcal{F}_{\Theta}} \mathcal{L}(\hat{\boldsymbol{u}}_{\theta}) + \inf_{\hat{\boldsymbol{u}}_{\theta} \in \mathcal{F}_{\Theta}} \left(\mathcal{L}(\hat{\boldsymbol{u}}_{\theta}) - \mathcal{L}(\boldsymbol{u}^{*}) \right) \\ \leq & \delta(\boldsymbol{u}_{\theta}) + \gamma \inf_{\hat{\boldsymbol{u}}_{\theta} \in \mathcal{F}_{\Theta}} \| \hat{\boldsymbol{u}}_{\theta} - \boldsymbol{u}^{*} \|_{X}^{2} \end{split}$$

with the constant $\gamma > 0$. Hence combining the two estimates and rearranging the terms, we obtain (33) and (34).

Remark 3.1. Let $\widehat{\mathcal{L}}(u)$ be the empirical loss function corresponding to $\mathcal{L}(u)$, we furthermore decompose the error term $\delta(u_{\theta})$ as follows:

$$\begin{split} \delta(\boldsymbol{u}_{\theta}) = & \mathcal{L}(\boldsymbol{u}_{\theta}) - \widehat{\mathcal{L}}(\boldsymbol{u}_{\theta}) + \widehat{\mathcal{L}}(\boldsymbol{u}_{\theta}) - \inf_{\hat{\boldsymbol{u}}_{\theta} \in \mathcal{F}_{\Theta}} \widehat{\mathcal{L}}(\hat{\boldsymbol{u}}_{\theta}) + \inf_{\hat{\boldsymbol{u}}_{\theta} \in \mathcal{F}_{\Theta}} \widehat{\mathcal{L}}(\hat{\boldsymbol{u}}_{\theta}) - \inf_{\hat{\boldsymbol{u}}_{\theta} \in \mathcal{F}_{\Theta}} \mathcal{L}(\hat{\boldsymbol{u}}_{\theta}) \\ \lesssim \sup_{\hat{\boldsymbol{u}}_{\theta} \in \mathcal{F}_{\Theta}} |\mathcal{L}(\hat{\boldsymbol{u}}_{\theta}) - \widehat{\mathcal{L}}(\hat{\boldsymbol{u}}_{\theta})| + \big(\widehat{\mathcal{L}}(\boldsymbol{u}_{\theta}) - \inf_{\hat{\boldsymbol{u}}_{\theta} \in \mathcal{F}_{\Theta}} \widehat{\mathcal{L}}(\hat{\boldsymbol{u}}_{\theta})\big). \end{split}$$

In the last inequality, the first term is called global generalization error, and the second term is called optimization error. Combining with Lemma 3.3, our estimate is in the form of "global generalization error+optimization error+approximation error".

Next, we apply Céa's Lemma to the MIM neural networks with first-order and second-order least squares systems.

3.2.1. Application to first-order system. In this case, let the spaces $X = (H^1(\Omega) \times H^1(\Omega)^d)^n$, and we define the linear map T_α with $\alpha = D, N, R$, corresponding to the case of Dirichlet, Neumann and Robin boundary, as

$$T_{\alpha} = \begin{cases} (\mathcal{P}, S_{\alpha}), & \text{when } \alpha = D, R, \\ (\mathcal{P}, S_{\alpha}, \mathcal{I}), & \text{when } \alpha = N, \end{cases}$$

where the matrix operator \mathcal{P} and trace operator S_{α} are defined in (12), (13), and \mathcal{I} denotes the integral on Ω , i.e. $\mathcal{I}u = \int_{\Omega} u \, dx$. Moreover, we define

(35)
$$Y_{\alpha} = \begin{cases} L^{2}(\Omega) \oplus L^{2}(\partial\Omega), & \text{when } \alpha = D, R, \\ L^{2}(\Omega) \oplus L^{2}(\partial\Omega) \oplus \mathbb{R}, & \text{when } \alpha = N, \end{cases}$$

such that $T_{\alpha} : X \to Y_{\alpha}$. Then the linear map T_{α} induces a bilinear form \mathcal{B}_{α} defined in (27)-(28), and the corresponding loss function \mathcal{L}_{α} is given by (14), (16). Furthermore, set $Z = (H^1(\Omega) \times H(\operatorname{div}, \Omega))^n$, then Lemma 3.1 indicates that \mathcal{B}_{α} is coercive with respect to Z when $\alpha = D, R$, and sup-linear coercive with respect to Z when $\alpha = N$.

Now we can apply Céa's Lemma to the neural networks of first-order least squares system with the spaces and the bilinear form defined above. Suppose $u_{\alpha}^* \in B^{2n+2}(\Omega)$ is the solution to problem (4) with three different boundary conditions (5)-(7). We use the notation

$$oldsymbol{u}_{lpha}^{*}=\left(u_{lpha}^{*},\,
abla u_{lpha}^{*},\cdots,\,
abla \Delta^{n-1}u_{lpha}^{*}
ight),$$

then it follows that $\boldsymbol{u}^* \in \left(H^1(\Omega) \times H^1(\Omega)^d\right)^n$. Moreover, Let

$$\boldsymbol{u}_{\theta} = (\phi_0, \, \boldsymbol{\psi}_0, \cdots, \, \phi_{n-1}, \, \boldsymbol{\psi}_{n-1})$$

be any neural network in $\mathcal{F}_{\text{ReQU},m}$. For the sake of brevity, we denote the approximation error between u^* and u_{θ} , and the generalization error between \mathcal{L}_{α} and $\hat{\mathcal{L}}_{\alpha}$ by

(36)
$$\begin{cases} \mathcal{E}_{\mathrm{app}} = \inf_{\boldsymbol{u}_{\theta} \in \mathcal{F}_{\mathrm{ReQU},m}} \sum_{k=0}^{n-1} \|\phi_{k} - \Delta^{k} u_{\alpha}^{*}\|_{H^{1}(\Omega)}^{2} + \|\psi_{k} - \nabla(\Delta)^{k} u_{\alpha}^{*}\|_{H^{1}(\Omega)}^{2}, \\ \mathcal{E}_{\mathrm{gen}} = \sup_{\boldsymbol{u}_{\theta} \in \mathcal{F}_{\mathrm{ReQU},m}} |\mathcal{L}_{\alpha}(\boldsymbol{u}_{\theta}) - \widehat{\mathcal{L}}_{\alpha}(\boldsymbol{u}_{\theta})|, \end{cases}$$

where the empirical loss function $\widehat{\mathcal{L}}_{\alpha}$ is given by (15), (17). Hence Lemma 3.1 and Céa's Lemma together with Remark 3.1 indicate the result below.

Lemma 3.4 (First-order system). Use the notation defined above, and denote

$$\hat{\boldsymbol{u}}_{\theta} = \left(\hat{\phi}_{0}, \, \hat{\boldsymbol{\psi}}_{0}, \cdots, \hat{\phi}_{n-1}, \, \hat{\boldsymbol{\psi}}_{n-1}\right) = \arg\min_{\boldsymbol{u}_{\theta} \in \mathcal{F}_{\operatorname{ReQU},m}} \widehat{\mathcal{L}}_{\alpha}(\boldsymbol{u}_{\theta}).$$

For the Neumann and Robin boundary, i.e. $\alpha = N, R$, we have

$$\sum_{k=0}^{n-1} \|\hat{\phi}_k - \Delta^k u_\alpha^*\|_{H^1(\Omega)}^2 + \|\hat{\psi}_k - \nabla(\Delta)^k u_\alpha^*\|_{H(\operatorname{div};\Omega)}^2 \lesssim \mathcal{E}_{\operatorname{app}} + \mathcal{E}_{\operatorname{gen}}$$

For the Dirichlet boundary, it follows that

$$\sum_{k=0}^{n-1} \|\hat{\phi}_k - \Delta^k u_\alpha^*\|_{H^1(\Omega)}^2 + \|\hat{\psi}_k - \nabla(\Delta)^k u_\alpha^*\|_{H(\operatorname{div};\Omega)}^2 \lesssim \sqrt{\mathcal{E}_{\operatorname{app}}} + \sqrt{\mathcal{E}_{\operatorname{gen}}}.$$

3.2.2. Application to second-order system. By analogy with the case of the first-order system, we can define the spaces and bilinear form for the second-order system as follows. Let $X = (H^2(\Omega))^n$, and define the linear map T^*_{α} as

$$T_{\alpha}^{*} = \begin{cases} (\mathcal{P}^{*}, S_{\alpha}^{*}), & \text{when } \alpha = \mathbf{D}, \mathbf{R}, \\ (\mathcal{P}^{*}, S_{\alpha}^{*}, \mathcal{I}), & \text{when } \alpha = \mathbf{N}, \end{cases}$$

where the matrix operator \mathcal{P}^* and the trace operator S^*_{α} are defined in (20) and (21). Therefore $T^*_{\alpha}: X \to Y_{\alpha}$, where Y_{α} is the space defined in (35). In addition, the linear map T^*_{α} induces a bilinear form \mathcal{B}_{α} defined in (30)-(31) with $\alpha = D, N, R$. Define the norm space \mathcal{H} as follows:

(37)
$$\mathcal{H}(\Omega) = \left\{ v \in H^1(\Omega) \, \middle| \, \Delta v \in L^2(\Omega) \right\}$$

with the norm

$$\|v\|_{\mathcal{H}(\Omega)} = \left(\|v\|_{H^1(\Omega)}^2 + \|\Delta v\|_{L^2(\Omega)}^2\right)^{\frac{1}{2}}.$$

We set $Z = (\mathcal{H}(\Omega))^n$, then Lemma 3.2 indicates that \mathcal{B}_{α} is coercive with respect to Z when $\alpha = D, R$, and is sup-linear coercive with respect to Z when $\alpha = N$.

Subsequently, Céa's Lemma can be utilized in the neural networks of the second-order least squares system with the spaces and bilinear form defined above. Assume $u_{\alpha}^* \in \mathcal{B}^{2n+3}(\Omega)$ is the solution to problem (4) with three different boundary conditions (5)-(7). Denote the vector

$$\boldsymbol{v}_{\alpha}^{*} = \left(u_{\alpha}^{*}, \cdots, \Delta^{n-1}u_{\alpha}^{*}\right),$$

then it follows that $v_{\alpha}^* \in (H^2(\Omega))^n$. We also define the corresponding approximation error and generalization error in the following manner:

(38)
$$\begin{cases} \mathcal{E}_{app}^* = \inf_{\boldsymbol{v}_{\theta} \in \mathcal{F}_{ReCU,m}} \sum_{k=0}^{n-1} \|\varphi_k - \Delta^k u_{\alpha}^*\|_{H^2(\Omega)}^2; \\ \mathcal{E}_{gen}^* = \sup_{\boldsymbol{v}_{\theta} \in \mathcal{F}_{ReCU,m}} |\mathcal{L}_{\alpha}^*(\boldsymbol{v}_{\theta}) - \widehat{\mathcal{L}}_{\alpha}^*(\boldsymbol{v}_{\theta})|. \end{cases}$$

Therefore, by applying Lemma 3.1 and Céa Lemma, we can directly infer the following result.

Lemma 3.5 (Second-order system). Assume u_{α}^* is the solution to problem (4) with three different boundary conditions (5)-(7). Let

$$\boldsymbol{v}_{\hat{ heta}} = \left(\hat{arphi}_0, \cdots, \, \hat{arphi}_{n-1}
ight) = rg \min_{\boldsymbol{v}_{ heta} \in \mathcal{F}_{\operatorname{ReCU},m}} \widehat{\mathcal{L}}(\boldsymbol{v}_{ heta}).$$

Then for the Neumann and Robin boundary, i.e. $\alpha = N, R$, one has

$$\sum_{k=0}^{n-1} \left(\|\hat{\varphi}_k - \Delta^k u^*_\alpha\|^2_{H^1(\Omega)} + \|\nabla\hat{\varphi}_k - \nabla\Delta^k u^*_\alpha\|^2_{H(\operatorname{div};\Omega)} \right) \lesssim \mathcal{E}^*_{\operatorname{app}} + \mathcal{E}^*_{\operatorname{gen}}$$

for the Dirichlet boundary, it follows that

$$\sum_{k=0}^{n-1} \left(\|\hat{\varphi}_k - \Delta^k u_{\mathrm{D}}^*\|_{H^1(\Omega)}^2 + \|\nabla\hat{\varphi}_k - \nabla\Delta^k u_{\mathrm{D}}^*\|_{H(\mathrm{div};\Omega)}^2 \right) \lesssim \sqrt{\mathcal{E}_{\mathrm{app}}^*} + \sqrt{\mathcal{E}_{\mathrm{gen}}^*}.$$

From the aforementioned Lemma 3.4 and 3.5, it can be inferred that the error between the neural network approximation and the true solution can be bounded by the approximation error and the generalization error. Therefore, our task below is to estimate these two errors.

3.3. Approximation error. Since the neural networks of both first and second-order least squares systems are considered, we introduce the following approximation error regarding ReCU and ReQU-activated neural networks, as defined earlier in (10) and (18). In addition, to address the impact of the curse of dimensionality on approximation errors, our work adopts a method based on range control in Barron space. The approximation property of neural networks using the ReQU activation function has been thoroughly discussed in [13], which is presented as follows:

Lemma 3.6. Given any function $u^* \in \mathcal{B}^{2n+2}(\Omega)$. Let the collection of ReQU-activated neural networks $\mathcal{F}_{\operatorname{ReQU},m}$ be defined in (10) associated with u^* . We use the notation $u^* = (u^*, \nabla u^*, \cdots, \nabla \Delta^{n-1} u^*)$, then there exists a network $u_m \in \mathcal{F}_{\operatorname{ReQU},m}$ such that

$$\|\boldsymbol{u}^* - \boldsymbol{u}_m\|_{H^1(\Omega)}^2 \precsim \frac{\|\boldsymbol{u}^*\|_{\mathcal{B}^{2n+2}}^2}{m}.$$

Furthermore, we give the following approximation results regarding ReCUactivated neural networks. Note that the function u^* requires a higher regularity.

Lemma 3.7. Given any function $u^* \in \mathcal{B}^{2n+3}(\Omega)$. Let the collection of ReCU-activated neural networks $\mathcal{F}_{\operatorname{ReCU},m}$ be defined in (18) associated with u^* . We use the notation $u^* = (u^*, \Delta u^*, \cdots, \Delta^{n-1}u^*)$, then there exists a network $u_m \in \mathcal{F}_{\operatorname{ReCU},m}$ such that

$$\|\boldsymbol{u}^* - \boldsymbol{u}_m\|_{H^1(\Omega)}^2 \precsim \frac{\|\boldsymbol{u}^*\|_{\mathcal{B}^{2n+3}}^2}{m}.$$

We refer to the work [13] for the proof of Lemma 3.6. The proof of Lemma 3.7 is shown in Appendix A, where we apply a technique similar to [13]. More precisely, we construct ReCU-activated networks by utilizing ReLU and ReQU-activated networks. During the construction process, the coefficients rely on the higher regularity of u^* , hence in Lemma 3.7 the assumption $u^* \in \mathcal{B}^{2n+3}(\Omega)$ is necessary.

15

A general work on the density of ReLU^k -activated network in Barron space is studied in [14]. Compared to [14], we provide a sharper bound on the approximation error, where the constants in our estimates are independent of dimension d.

3.4. Generalization error. We will illustrate that the quadrature error trained on a finite dataset $\{X_i\}_{i=1}^N$ can be estimated by the Rademacher complexity.

Definition 3.1. Let $X = \{X_i\}_{i=1}^N$ be a set of random variables in Ω that is independently distributed, and $\varepsilon = \{\varepsilon_i\}_{i=1}^N$ be independent Rademacher random variables that take values +1 or -1 with equal probability. Then the **empirical Rademacher Complexity** of the function class S is a random variable given by

$$\hat{R}_N(\mathcal{S}) := \mathbb{E}_{\varepsilon} \Big[\sup_{f \in \mathcal{S}} \Big| \frac{1}{N} \sum_{i=1}^n \varepsilon_i f(X_i) \Big| \Big].$$

Taking its expectation in terms of X yields the **Rademacher Complexity** of the function class \mathcal{F}

$$R_N(\mathcal{S}) = \mathbb{E}_X \mathbb{E}_{\varepsilon} \Big[\sup_{f \in \mathcal{S}} \Big| \frac{1}{N} \sum_{i=1}^N \varepsilon_i f(X_i) \Big| \Big].$$

In the following, we explore the relation between the generalization error and the Rademacher complexity. Given a network $u \in \mathcal{F}$, we denote an expected loss function $\mathcal{L}(u)$ of the form:

(39)
$$\mathcal{L}(u) = \int_{\Omega} l(u(x)) d\mu(x),$$

where l(y) is a function that measures how well the network output y = u(x) fits a given criterion, and $\mu(x)$ is a probability measure. The following lemma from [13] fills up the gap between the Rademacher complexity and the quadrature error.

Lemma 3.8. Let \mathcal{F} be a set of functions, $X = \{X_i\}_{i=1}^N$ be i.i.d. random variables following the distribution $\mu(x)$. Then

(40)
$$\mathbb{E}_X \sup_{u \in \mathcal{F}} \left| \frac{\mathcal{L}(u)}{|\Omega|} - \frac{1}{N} \sum_{i=1}^N l(u(X_i)) \right| \le 2R_N(\mathcal{S}).$$

Here, $S := \{l(u) | u \in F\}$ is referred to as loss function class.

Lemma 3.8 indicates that generalization error can be bounded by Rademacher complexity. In the following. we provide an estimation of the Rademacher complexity for the loss function class regarding both first-order and second-order systems.

For the case of the first-order system, let $l(\boldsymbol{u}_{\theta}) = |\mathcal{P}\boldsymbol{u}_{\theta} - \boldsymbol{f}|^2$, we define the interior loss function class:

(41)
$$\mathcal{S} = \{ |\mathcal{P}\boldsymbol{u}_{\theta} - \boldsymbol{f}|^2 \, \big| \, \boldsymbol{u}_{\theta} \in \mathcal{F}_{\mathrm{ReQU},m} \},$$

and let $l(\boldsymbol{u}_{\theta}) = |S_{\alpha}\boldsymbol{u}_{\theta} - \boldsymbol{g}_{\alpha}|^2$. We define the boundary loss function class:

(42)
$$\mathcal{S}_{\alpha} = \left\{ |S_{\alpha} \boldsymbol{u}_{\theta} - \boldsymbol{g}_{\alpha}|^{2} \, \big| \, \boldsymbol{u}_{\theta} \in \mathcal{F}_{\text{ReQU},m} \right\}.$$

By Lemma SM4.7 in [13], we can directly get

Lemma 3.9. Denote by N and \widehat{N} the number of sample points in Ω and on $\partial\Omega$, respectively. Assume that $\widehat{N} = O(\frac{N}{d^2})$. The function classes $\mathcal{S}, \mathcal{S}_{\alpha}$ satisfy

(43)
$$R_N(\mathcal{S}) + R_{\widehat{N}}(\mathcal{S}_\alpha) \le \frac{C \|u^*\|_{\mathcal{B}^{2n+2}}^2}{\sqrt{N}},$$

where C depends polynomially on dimension d.

On the other hand, for the case of the second-order system, we similarly define the function classes:

(44)
$$\mathcal{S}^* = \left\{ |\mathcal{P}^* \boldsymbol{v}_{\theta} - \boldsymbol{f}|^2 \, \big| \, \boldsymbol{v}_{\theta} \in \mathcal{F}_{\operatorname{ReCU},m} \right\},$$

and boundary loss function class:

(45)
$$\mathcal{S}_{\alpha}^{*} = \left\{ |S_{\alpha}^{*} \boldsymbol{v}_{\theta} - \boldsymbol{g}_{\alpha}|^{2} \, \big| \, \boldsymbol{v}_{\theta} \in \mathcal{F}_{\operatorname{ReCU},m} \right\}$$

Lemma 3.10. Assume that the number of boundary and interior sample points satisfies $\hat{N} = O(\frac{N}{d^2})$. The function classes S^* , S^*_{α} satisfy

(46)
$$R_N(\mathcal{S}^*) + R_{\widehat{N}}(\mathcal{S}^*_{\alpha}) \le \frac{C \|u^*\|_{\mathcal{B}^{2n+3}}^2}{\sqrt{N}},$$

where C depends polynomially on dimension d.

To keep the presentation concise, the proof of this lemma will be provided in Appendix (A.2).

3.5. **Proof of main theorems.** Now, we can utilize the previous results to prove the main theorems. Here we only present the proof of Theorem 2.1, while Theorem 2.2 can be proved in the same way.

Proof of Theorem 2.1. For Neumann and Robin boundary, from Lemma 3.4, we conclude that the total error $\|\hat{\phi}_k - \Delta^k u^*_{\alpha}\|^2_{H^1(\Omega)}$ and $\|\hat{\psi}_k - \nabla(\Delta)^k u^*_{\alpha}\|^2_{H(\operatorname{div};\Omega)}$, where $k = 0, 1, \cdots, n-1$, can be bounded by generalization error

$$\mathcal{E}_{ ext{gen}} = \sup_{oldsymbol{u}_{ heta} \in \mathcal{F}_{ ext{ReQU},m}} |\mathcal{L}_{lpha}(oldsymbol{u}_{ heta}) - \widehat{\mathcal{L}}_{lpha}(oldsymbol{u}_{ heta})|,$$

and approximation error

$$\mathcal{E}_{\text{app}} = \inf_{u_{\theta} \in \mathcal{F}_{\text{ReQU},m}} \sum_{k=0}^{n-1} \|\phi_k - \Delta^k u_{\alpha}^*\|_{H^1(\Omega)}^2 + \|\psi_k - \nabla(\Delta)^k u_{\alpha}^*\|_{H^1(\Omega)}^2.$$

By Lemma 3.6, since $u_{\alpha}^* \in \mathcal{B}^{2n+2}(\Omega)$, we derive the estimate for the approximation error

$$\mathcal{E}_{\mathrm{app}} \precsim \frac{\|u_{\alpha}^*\|_{\mathcal{B}^{2n+2}(\Omega)}^2}{m}.$$

Furthermore, for the generalization error, we apply Lemma 3.8 and 3.9 to deduce that the estimate holds for $u_{\theta} \in \mathcal{F}_{\text{ReQU},m}$:

$$\mathcal{E}_{\text{gen}} \precsim \mathbb{E} |\mathcal{L}_{\alpha}(\boldsymbol{u}_{\theta}) - \widehat{\mathcal{L}}_{\alpha}(\boldsymbol{u}_{\theta})| \le 2|\Omega| (R_{N}(\mathcal{S}) + R_{\widehat{N}}(\mathcal{S}_{\alpha})) \precsim \frac{\|\boldsymbol{u}^{*}\|_{\mathcal{B}^{2n+2}}^{2}}{\sqrt{N}},$$

where the expectation is taken on the random sampling of training data in Ω and $\partial\Omega$, and we take $\hat{N} \geq \frac{N}{d^2}$. The constant in the inequality is at most polynomially dependent on d.

Note that for the Neumann case, an additional zero-mean penalty is applied, thus the Rademacher complexity $R_N(\mathcal{S}')$ for an extra function class $\mathcal{S}' = \{ u_{\theta} | u_{\theta} \in \mathcal{F}_{\text{ReQU},m} \}$ need to be estimated, which is clearly bounded by $R_N(\mathcal{S})$.

Finally, applying Lemma 3.4, the theorem is proved.

4. First-order system for the 2n-order elliptic equation

In this section, we provide the proof of the coercivity estimates for the bilinear form (27) and (28), induced from the first-order least squares system of the 2*n*-order elliptic equation. Suppose $\boldsymbol{u} \in \mathbb{R}^{n(d+1)}$ with the form:

$$\boldsymbol{u} = (\phi_0, \, \boldsymbol{\psi}_0, \cdots, \, \phi_{n-1}, \, \boldsymbol{\psi}_{n-1}).$$

Lemma 4.1. The bilinear form (27)-(28) are coercive with respect to $(H^1(\Omega) \times H(\operatorname{div}; \Omega))^n$ in the following sense. For the Neumann and Robin boundary, *i.e.* $\alpha = N, R$, there exists a constant C > 0 such that

(47)
$$\mathcal{B}_{\alpha}(\boldsymbol{u},\boldsymbol{u}) \geq C \sum_{k=0}^{n-1} \left(\|\boldsymbol{\psi}_k\|_{H(\operatorname{div};\Omega)}^2 + \|\boldsymbol{\phi}_k\|_{H^1(\Omega)}^2 \right)$$

and, for the Dirichlet boundary, there exists a constant C > 0 such that (48)

$$\Big(\mathcal{B}_{\mathrm{D}}^{\frac{1}{2}}(\boldsymbol{u},\boldsymbol{u}) + \sum_{k=0}^{n-1} \|\boldsymbol{\psi}_k\|_{L^2(\partial\Omega)} \Big) \mathcal{B}_{\mathrm{D}}^{\frac{1}{2}}(\boldsymbol{u},\boldsymbol{u}) \ge C \sum_{k=0}^{n-1} \Big(\|\boldsymbol{\psi}_k\|_{H(\mathrm{div};\Omega)}^2 + \|\boldsymbol{\phi}_k\|_{H^1(\Omega)}^2 \Big).$$

4.1. Some useful inequalies. In this subsection, we introduce some important inequalities for the proof of our results. Since our work involves various non-homogeneous boundary conditions, let us first introduce the trace inequalities. Functions of $H(\operatorname{div}; \Omega)$ admit a well-defined normal trace on $\partial\Omega$. This normal trace $\boldsymbol{v} \cdot \boldsymbol{n}$ lies in $H^{-\frac{1}{2}}(\partial\Omega)$, i.e.

(49)
$$\|\boldsymbol{n}\cdot\boldsymbol{v}\|_{H^{-\frac{1}{2}}(\partial\Omega)} \leq \|\boldsymbol{v}\|_{H(\operatorname{div};\Omega)}, \text{ for all } \boldsymbol{v}\in H(\operatorname{div};\Omega),$$

where n is the outer normal vector. And we have the following inequality from Theorem 1.5 of [8],

(50)
$$\|v\|_{H^{\frac{1}{2}}(\partial\Omega)} \le C_T \|v\|_{H^1(\Omega)}, \quad \text{for all } v \in H^1(\Omega)$$

Moreover, we introduce the Poincaré-Friedrichs inequality (Theorem 1.9 of [24]): For any $v \in H^1(\Omega)$, there exists a constant C_F such that

(51)
$$\|v\|_{H^1(\Omega)}^2 \le C_F \big(\|\nabla v\|_{L^2(\Omega)}^2 + \|v\|_{L^2(\partial\Omega)}^2\big),$$

Furthermore, we introduce another Poincaré-Friedrichs inequality of the form:

(52)
$$||v||_{H^1(\Omega)}^2 \le C_F \Big(||\nabla v||_{L^2(\Omega)}^2 + |\int_{\Omega} v \, \mathrm{d}\boldsymbol{x}|^2 \Big).$$

4.2. **Perturbation method.** The difficulty in the coercivity analysis arises from the cross term in \mathcal{B}_{α} . To address this issue, one can use the perturbation method by applying some small coefficients. To this end, we introduce the following parameter series. Given any integer $n \geq 1$, denote $0 < \delta < 1$, we define the series $0 < \delta_k \leq 1, k = 1, 2, \ldots, 2n + 1$, by

(53)
$$\delta_k = \frac{1}{k+1} \delta^k.$$

Moreover, given $a, b \ge 0$, for k = 2, ..., 2n, one can apply Young's inequality to derive

$$\delta_k ab \le \frac{1}{2} \left(\delta \sqrt{\frac{k}{k+2}} \right) \delta_k a^2 + \frac{1}{2} \left(\delta \sqrt{\frac{k}{k+2}} \right)^{-1} \delta_k b^2 = \frac{\epsilon_k}{2} \left(\delta_{k+1} a^2 + \delta_{k-1} b^2 \right),$$

where we set

$$\epsilon_k = \left(\frac{(k+1)^2 - 1}{(k+1)^2}\right)^{\frac{1}{2}}.$$

Hence using the monotony of ϵ_k yields the estimate:

(54)
$$\delta_k ab \leq \frac{\epsilon_{2n}}{2} \left(\delta_{k+1} a^2 + \delta_{k-1} b^2 \right)$$

Let us define the weighted energy

(55)
$$\mathcal{E}_{\delta,n} = \sum_{k=0}^{n-1} \delta_{2(n-k)-1} \| \operatorname{div} \psi_k \|_{L^2(\Omega)}^2 + \sum_{k=0}^{n-1} \delta_{2(n-k)} \| \nabla \phi_k \|_{L^2(\Omega)}^2, \\ + \sum_{k=0}^{n-1} \delta_{2(n-k)} \| \psi_k \|_{L^2(\Omega)}^2 + \sum_{k=1}^{n-1} \delta_{2(n-k)+1} \| \phi_k \|_{L^2(\Omega)}^2.$$

Then we have the following estimate.

Lemma 4.2. For the bilinear form (27)-(28), we have

(56)
$$\mathcal{B}_{\alpha}(\boldsymbol{u};\boldsymbol{u}) \geq (1-\epsilon_{2n})\mathcal{E}_{\delta,n} - \epsilon_{2n}\delta_{2n+1} \|\phi_0\|_{L^2(\Omega)}^2 + \mathcal{T}_{\mathbf{b},\alpha},$$

where the boundary term $\mathcal{T}_{\mathbf{b},\alpha}$ is defined by (57) $\mathcal{T}_{\mathbf{b},\alpha} = \lambda (S_{\alpha} \boldsymbol{u}, S_{\alpha} \boldsymbol{u})_{\partial \Omega} + \tau_{\alpha}$

$$\begin{split} \delta_{b,\alpha} &= \lambda (S_{\alpha} \boldsymbol{u}, S_{\alpha} \boldsymbol{u})_{\partial \Omega} + \tau_{\alpha} \\ &- 2 \sum_{k=0}^{n-2} \delta_{2(n-k)-1} (\boldsymbol{n} \cdot \boldsymbol{\psi}_k, \phi_{k+1})_{\partial \Omega} - 2 \sum_{k=0}^{n-1} \delta_{2(n-k)} (\phi_k, \boldsymbol{n} \cdot \boldsymbol{\psi}_k)_{\partial \Omega}. \end{split}$$

Here, the term τ_{α} is the zero-mean penalty that only appears in the Neumann boundary case, i.e.

$$\tau_{\alpha} = \begin{cases} \mu \big| \int_{\Omega} \phi_0 \, \mathrm{d} \boldsymbol{x} \big|^2, & \text{when } \alpha = \mathrm{N}, \\ 0, & \text{when } \alpha = \mathrm{D}, \mathrm{R}. \end{cases}$$

Proof. For convenience, let us denote the matrix operator $\mathcal{P} = \mathcal{P}_1 - \mathcal{P}_2$, where $\mathcal{P}_1, \mathcal{P}_2$ are $n(d+1) \times n(d+1)$ matrix given by

$$\mathcal{P}_{1} = \begin{pmatrix} \nabla & 0 & \cdots & 0 & 0 \\ 0 & \operatorname{div} & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & \nabla & 0 \\ 0 & 0 & \cdots & 0 & \operatorname{div} \end{pmatrix}, \quad \mathcal{P}_{2} = \begin{pmatrix} 0 & I_{d \times d} & 0 & \cdots & 0 \\ 0 & 0 & I & \cdots & 0 \\ \vdots & \vdots & \ddots & \ddots & \vdots \\ 0 & 0 & \cdots & 0 & I_{d \times d} \\ 0 & 0 & \cdots & 0 & 0 \end{pmatrix},$$

Then the bilinear form \mathcal{B}_{α} in (27)-(28) can be written as

(58)
$$\mathcal{B}_{\alpha}(\boldsymbol{u};\boldsymbol{u}) = \left((\mathcal{P}_1 - \mathcal{P}_2)\boldsymbol{u}, (\mathcal{P}_1 - \mathcal{P}_2)\boldsymbol{u} \right) + \lambda (S_{\alpha}\boldsymbol{u}, S_{\alpha}\boldsymbol{u})_{\partial\Omega} + \tau_{\alpha}$$

Moreover, we apply the parameters (53) and define the $n(d+1) \times n(d+1)$ weighting matrix:

(59)
$$W_{\delta,n} = \begin{pmatrix} \delta_{2n} I_{d \times d} & 0 & \cdots & 0 & 0\\ 0 & \delta_{2n-1} & \cdots & 0 & 0\\ \vdots & \vdots & \ddots & \vdots & \vdots\\ 0 & 0 & \cdots & \delta_{2} I_{d \times d} & 0\\ 0 & 0 & \cdots & 0 & \delta_{1} \end{pmatrix},$$

then it follows that

(60)
$$\mathcal{B}_{\alpha}(\boldsymbol{u};\boldsymbol{u}) \geq \left((\mathcal{P}_{1} - \mathcal{P}_{2})\boldsymbol{u}, W_{\delta,n}(\mathcal{P}_{1} - \mathcal{P}_{2})\boldsymbol{u} \right) + \lambda(S_{\alpha}\boldsymbol{u}, S_{\alpha}\boldsymbol{u})_{\partial\Omega} + \tau_{\alpha}$$
$$= \left(\mathcal{P}_{1}\boldsymbol{u}, W_{\delta,n}\mathcal{P}_{1}\boldsymbol{u} \right) + \left(\mathcal{P}_{2}\boldsymbol{u}, W_{\delta,n}\mathcal{P}_{2}\boldsymbol{u} \right) \\ - 2\left(\mathcal{P}_{1}\boldsymbol{u}, W_{\delta}\mathcal{P}_{2}\boldsymbol{u} \right) + \lambda(S_{\alpha}\boldsymbol{u}, S_{\alpha}\boldsymbol{u})_{\partial\Omega} + \tau_{\alpha}.$$

Here, the first two terms on RHS are positive and are equivalent to the weighted energy we defined in (55):

$$(\mathcal{P}_1 \boldsymbol{u}, W_{\delta,n} \mathcal{P}_1 \boldsymbol{u}) + (\mathcal{P}_2 \boldsymbol{u}, W_{\delta,n} \mathcal{P}_2 \boldsymbol{u}) = \mathcal{E}_{\delta,n}.$$

Now we estimate the cross term:

$$-2(\mathcal{P}_{1}\boldsymbol{u}, W_{\delta,n}\mathcal{P}_{2}\boldsymbol{u}) = -2\sum_{k=0}^{n-2}\delta_{2(n-k)-1}(\operatorname{div}\boldsymbol{\psi}_{k}, \phi_{k+1}) - 2\sum_{k=0}^{n-1}\delta_{2(n-k)}(\nabla\phi_{k}, \boldsymbol{\psi}_{k})$$

Integrating by parts, one has

$$(61) \quad \begin{aligned} &-2\left(\mathcal{P}_{1}\boldsymbol{u}, W_{\delta,n}\mathcal{P}_{2}\boldsymbol{u}\right) \\ &=& 2\sum_{k=0}^{n-2}\delta_{2(n-k)-1}(\boldsymbol{\psi}_{k}, \nabla\phi_{k+1}) + 2\sum_{k=0}^{n-1}\delta_{2(n-k)}(\phi_{k}, \operatorname{div}\boldsymbol{\psi}_{k}) \\ &-& 2\sum_{k=0}^{n-2}\delta_{2(n-k)-1}(\boldsymbol{n}\cdot\boldsymbol{\psi}_{k}, \phi_{k+1})_{\partial\Omega} - 2\sum_{k=0}^{n-1}\delta_{2(n-k)}(\phi_{k}, \boldsymbol{n}\cdot\boldsymbol{\psi}_{k})_{\partial\Omega}. \end{aligned}$$

Utilizing estimate (54), the first two terms can be estimated by

$$\begin{cases} 2\delta_{2(n-k)-1}(\boldsymbol{\psi}_{k},\nabla\phi_{k+1}) \geq -\epsilon_{2n} \Big(\delta_{2(n-k)} \|\boldsymbol{\psi}_{k}\|_{L^{2}(\Omega)}^{2} + \delta_{2(n-k)-2} \|\nabla\phi_{k+1}\|_{L^{2}(\Omega)}^{2} \Big),\\ 2\delta_{2(n-k)}(\phi_{k},\operatorname{div} \boldsymbol{\psi}_{k}) \geq -\epsilon_{2n} \Big(\delta_{2(n-k)+1} \|\phi_{k}\|_{L^{2}(\Omega)}^{2} + \delta_{2(n-k)-1} \|\operatorname{div} \boldsymbol{\psi}_{k}\|_{L^{2}(\Omega)}^{2} \Big). \end{cases}$$

Substituting the estimate into (61), and using notation (55), it follows that

$$-2(\mathcal{P}_{1}\boldsymbol{u}, W_{\delta,n}\mathcal{P}_{2}\boldsymbol{u})$$

$$\geq -\epsilon_{2n}\mathcal{E}_{\delta,n} - \epsilon_{2n}\delta_{2n+1} \|\phi_{0}\|_{L^{2}(\Omega)}^{2}$$

$$-2\sum_{k=0}^{n-2} \delta_{2(n-k)-1}(\boldsymbol{n}\cdot\boldsymbol{\psi}_{k}, \phi_{k+1})_{\partial\Omega} - 2\sum_{k=0}^{n-1} \delta_{2(n-k)}(\phi_{k}, \boldsymbol{n}\cdot\boldsymbol{\psi}_{k})_{\partial\Omega}$$

Combining the estimate above and plugging into (60) finally leads to (56). \Box

4.3. Estimate of boundary term. The boundary term $\mathcal{T}_{b,\alpha}$ defined in (57) can be estimated in the following lemma.

Lemma 4.3. For the boundary term $\mathcal{T}_{b,\alpha}$, we have

• Neumann boundary.

(62)
$$\mathcal{T}_{\mathrm{b,N}} \geq -C\delta \mathcal{E}_{\delta,n} - \epsilon_{2n}\delta_{2n+1} \|\phi_0\|_{L^2(\Omega)}^2 + \mu \Big| \int_{\Omega} \phi_0 \,\mathrm{d} \boldsymbol{x} \Big|^2.$$

• Robin boundary.

(63)
$$\mathcal{T}_{b,R} \ge \left(2(1-\epsilon_{2n}) - C\delta\right) \sum_{k=0}^{n-1} \delta_{2(n-k)} \|\phi_k\|_{L^2(\partial\Omega)}^2$$

• Dirichlet boundary.

(64)
$$\mathcal{T}_{b,D} \ge \lambda \sum_{k=0}^{n-1} \|\phi_k\|_{L^2(\partial\Omega)}^2 - \sum_{k=0}^{n-1} \|\psi_k\|_{L^2(\partial\Omega)} \|\phi_k\|_{L^2(\partial\Omega)},$$

Proof. Case i. Neumann boundary. In the case of the Neumann boundary condition, we apply Young's inequality and estimate the third term in

(57) by
$$25$$
 ($x - t - t - 3$)

$$-2\delta_{2(n-k)-1}(\boldsymbol{n}\cdot\boldsymbol{\psi}_{k},\phi_{k+1})_{\partial\Omega} \geq -\frac{\lambda}{2}\|\boldsymbol{n}\cdot\boldsymbol{\psi}_{k}\|_{L^{2}(\partial\Omega)}^{2} - C\delta_{2(n-k)-1}^{2}\|\phi_{k+1}\|_{L^{2}(\partial\Omega)}^{2}$$
$$\geq -\frac{\lambda}{2}\|\boldsymbol{n}\cdot\boldsymbol{\psi}_{k}\|_{L^{2}(\partial\Omega)}^{2} - C\delta_{2(n-k)-1}^{2}\|\phi_{k+1}\|_{H^{1}(\Omega)}^{2},$$

where in the last line, the trace theorem is used. Applying the fact $\delta_{2(n-k)-1} \leq \delta_{2(n-k)-2} \leq \delta$ for $0 \leq k \leq n-2$, we have

$$-2\delta_{2(n-k)-1}(\boldsymbol{n}\cdot\boldsymbol{\psi}_{k},\phi_{k+1})_{\partial\Omega}$$

$$\geq -\frac{\lambda}{2}\|\boldsymbol{n}\cdot\boldsymbol{\psi}_{k}\|_{L^{2}(\partial\Omega)}^{2} - C\delta(\delta_{2(n-k)-2}\|\nabla\phi_{k+1}\|_{L^{2}(\Omega)}^{2} - \delta_{2(n-k)-1}\|\phi_{k+1}\|_{L^{2}(\Omega)}^{2}).$$

We apply the same argument to the last term in (57). For $0 \le k \le n-1$, we have:

$$\begin{aligned} &-2\delta_{2(n-k)}(\phi_k, \boldsymbol{n} \cdot \boldsymbol{\psi}_k)_{\partial\Omega} \\ &\geq -\frac{\lambda}{2} \|\boldsymbol{n} \cdot \boldsymbol{\psi}_k\|_{L^2(\partial\Omega)}^2 - C\delta_{2(n-k)}^2 \|\phi_k\|_{L^2(\partial\Omega)}^2 \\ &\geq -\frac{\lambda}{2} \|\boldsymbol{n} \cdot \boldsymbol{\psi}_k\|_{L^2(\partial\Omega)}^2 - C\delta(\delta_{2(n-k)} \|\nabla\phi_k\|_{L^2(\Omega)}^2 + \delta_{2(n-k)+1} \|\phi_k\|_{L^2(\Omega)}^2). \end{aligned}$$

Here, the inequality $\delta_{2(n-k)}^2 \leq \delta \delta_{2(n-k)+1}$ is used in the last line. Combining the estimates above, and using notation (55), we obtain

$$-2\sum_{k=0}^{n-2}\delta_{2(n-k)-1}(\boldsymbol{n}\cdot\boldsymbol{\psi}_{k},\phi_{k+1})\partial_{\Omega}-2\sum_{k=0}^{n-1}\delta_{2(n-k)}(\phi_{k},\boldsymbol{n}\cdot\boldsymbol{\psi}_{k})\partial_{\Omega}$$
$$\geq -\lambda\sum_{k=0}^{n-1}\|\boldsymbol{n}\cdot\boldsymbol{\psi}_{k}\|_{L^{2}(\partial\Omega)}^{2}-C\delta\mathcal{E}_{\delta,n}-\epsilon_{2n}\delta_{2n+1}\|\phi_{0}\|_{L^{2}(\Omega)}^{2}.$$

Substituting into (57), we can derive the estimate (62). **Case ii. Robin boundary**. For the case of the Robin boundary condition, we can rewrite the third term in (57) as

$$-2\delta_{2(n-k)-1}(\boldsymbol{n}\cdot\boldsymbol{\psi}_k,\phi_{k+1})_{\partial\Omega} = -2\delta_{2(n-k)-1}(\boldsymbol{n}\cdot\boldsymbol{\psi}_k+\phi_k,\phi_{k+1})_{\partial\Omega} + 2\delta_{2(n-k)-1}(\phi_k,\phi_{k+1})_{\partial\Omega}.$$

Applying Young's inequality and estimate (54), it follows that

$$-2\delta_{2(n-k)-1}(\boldsymbol{n}\cdot\boldsymbol{\psi}_{k},\phi_{k+1})_{\partial\Omega} \geq -\frac{\lambda}{2}\|\boldsymbol{n}\cdot\boldsymbol{\psi}_{k}+\phi_{k}\|_{L^{2}(\partial\Omega)}^{2}-C\delta_{2(n-k)-1}^{2}\|\phi_{k+1}\|_{L^{2}(\partial\Omega)}^{2}\\-\epsilon_{2n}\delta_{2(n-k)}\|\phi_{k}\|_{L^{2}(\partial\Omega)}^{2}-\epsilon_{2n}\delta_{2(n-k)-2}\|\phi_{k+1}\|_{L^{2}(\partial\Omega)}^{2}.$$

We use the fact $\delta_{2(n-k)-1} \leq \delta_{2(n-k)-2} \leq \delta$ and sum up the inequality for $k = 0, \ldots, n-2$, then it follows that (65)

$$= 2\sum_{k=0}^{n-2} \delta_{2(n-k)-1} (\boldsymbol{n} \cdot \boldsymbol{\psi}_k, \phi_{k+1})_{\partial\Omega}$$

$$\ge -\frac{\lambda}{2} \sum_{k=0}^{n-2} \|\boldsymbol{n} \cdot \boldsymbol{\psi}_k + \phi_k\|_{L^2(\partial\Omega)}^2 - (C\delta + 2\epsilon_{2n}) \sum_{k=0}^{n-1} \delta_{2(n-k)} \|\phi_k\|_{L^2(\partial\Omega)}^2 .$$

As for the last term in (57), for $0 \le k \le n-1$, we have:

$$-2\delta_{2(n-k)}(\phi_k, \boldsymbol{n} \cdot \boldsymbol{\psi}_k)_{\partial\Omega}$$

= $-2\delta_{2(n-k)}(\phi_k, \boldsymbol{n} \cdot \boldsymbol{\psi}_k + \phi_k)_{\partial\Omega} + 2\delta_{2(n-k)} \|\phi_k\|_{L^2(\partial\Omega)}^2$
$$\geq -\frac{\lambda}{2} \|\boldsymbol{n} \cdot \boldsymbol{\psi}_k + \phi_k\|_{L^2(\partial\Omega)}^2 - C\delta_{2(n-k)}^2 \|\phi_k\|_{L^2(\partial\Omega)}^2 + 2\delta_{2(n-k)} \|\phi_k\|_{L^2(\partial\Omega)}^2.$$

Summing up for k = 0, ..., n - 1, note that $\delta_{2(n-k)} \leq \delta$, we can obtain

$$-2\sum_{k=0}^{n-1} \delta_{2(n-k)}(\phi_k, \mathbf{n} \cdot \boldsymbol{\psi}_k)_{\partial\Omega}$$

$$\geq -\frac{\lambda}{2}\sum_{k=0}^{n-1} \|\mathbf{n} \cdot \boldsymbol{\psi}_k + \phi_k\|_{L^2(\partial\Omega)}^2 + \sum_{k=0}^{n-1} (2 - C\delta) \delta_{2(n-k)} \|\phi_k\|_{L^2(\partial\Omega)}^2.$$

Combining it with (57), (65), we can finally derive (63).

Case iii. Dirichlet boundary. For the case of the Dirichlet boundary condition, the boundary term in (57) can be estimated by

$$-2\delta_{2(n-k)-1}(\boldsymbol{n}\cdot\boldsymbol{\psi}_{k+1},\phi_k)_{\partial\Omega} \ge -2\delta\|\boldsymbol{n}\cdot\boldsymbol{\psi}_{k+1}\|_{L^2(\partial\Omega)}\|\phi_k\|_{L^2(\partial\Omega)},\\\delta_{2(n-k)}(\phi_k,\boldsymbol{n}\cdot\boldsymbol{\psi}_k)_{\partial\Omega} \ge -2\delta\|\boldsymbol{n}\cdot\boldsymbol{\psi}_k\|_{L^2(\partial\Omega)}\|\phi_k\|_{L^2(\partial\Omega)}.$$

Hence the estimate (63) follows.

4.4. **Proof of Lemma 4.1.** Now let us prove the Lemma 4.1 by applying the results above. For the Neumann case, we substitute (62) into (56) to derive that, for $\alpha = N$,

(66)

$$\mathcal{B}_{\alpha}(\boldsymbol{u};\boldsymbol{u}) \geq (1-\epsilon_{2n}-C\delta)\mathcal{E}_{\delta,n} - 2\epsilon_{2n}\delta_{2n+1} \|\phi_0\|_{L^2(\Omega)}^2 + \mu \Big| \int_{\Omega} \phi_0 \,\mathrm{d}\boldsymbol{x} \Big|^2.$$

We can utilizing the Poincaré-Friedrichs inequality (52) to deduce

$$\begin{aligned} 3\epsilon_{2n}\delta_{2n+1} \|\phi_0\|_{L^2(\Omega)}^2 &\leq 3C\epsilon_{2n}\delta_{2n+1} \Big(\|\nabla\phi_0\|_{L^2(\Omega)}^2 + \Big| \int_{\Omega} \phi_0 \,\mathrm{d}\boldsymbol{x} \Big|^2 \Big) \\ &= 3C\sqrt{\frac{k-1}{k+1}}\delta\delta_{2n} \Big(\|\nabla\phi_0\|_{L^2(\Omega)}^2 + \Big| \int_{\Omega} \phi_0 \,\mathrm{d}\boldsymbol{x} \Big|^2 \Big) \\ &\leq C^*\delta\Big(\mathcal{E}_{\delta,n} + \Big| \int_{\Omega} \phi_0 \,\mathrm{d}\boldsymbol{x} \Big|^2 \Big). \end{aligned}$$

Using the result above, it follows from (66) that

$$\mathcal{B}_{\alpha}(\boldsymbol{u};\boldsymbol{u}) \geq (1-\epsilon_{2n}-C^*\delta)\mathcal{E}_{\delta,n}+\epsilon_{2n}\delta_{2n+1}\|\phi_0\|_{L^2(\Omega)}^2+(\mu-C^*\delta)\Big|\int_{\Omega}\phi_0\,\mathrm{d}\boldsymbol{x}\Big|^2.$$

Therefore (47) is derived for $\alpha = N$.

For the Robin case, we substitute (63) into (56) to derive that, for $\alpha = R$,

(67)
$$\mathcal{B}_{\alpha}(\boldsymbol{u};\boldsymbol{u}) \geq (1-\epsilon_{2n})\mathcal{E}_{\delta,n} - \epsilon_{2n}\delta_{2n+1} \|\phi_0\|_{L^2(\Omega)}^2 + \left(2(1-\epsilon_{2n}) - C\delta\right)\sum_{k=0}^{n-1} \delta_{2(n-k)} \|\phi_k\|_{L^2(\partial\Omega)}^2.$$

Note that by Poincaré-Friedrichs inequality (51), we have

(68)
$$2\epsilon_{2n}\delta_{2n+1} \|\phi_0\|_{L^2(\Omega)}^2 \leq 2C\epsilon_{2n}\delta_{2n+1} \left(\|\nabla\phi_0\|_{L^2(\Omega)}^2 + \|\phi_0\|_{L^2(\partial\Omega)}^2 \right)$$
$$= 2C\sqrt{\frac{k-1}{k+1}}\delta\delta_{2n} \left(\|\nabla\phi_0\|_{L^2(\Omega)}^2 + \|\phi_0\|_{L^2(\partial\Omega)}^2 \right)$$
$$\leq C^*\delta \left(\mathcal{E}_{\delta,n} + \delta_{2n} \|\phi_0\|_{L^2(\partial\Omega)}^2 \right).$$

Substituting into (67), it leads to

(69)
$$\mathcal{B}_{\alpha}(\boldsymbol{u};\boldsymbol{u}) \geq (1 - \epsilon_{2n} - C^* \delta) \mathcal{E}_{\delta,n} + \epsilon_{2n} \delta_{2n+1} \|\phi_0\|_{L^2(\Omega)}^2 + \left(2(1 - \epsilon_{2n}) - C\delta - C^*\delta\right) \sum_{k=0}^{n-1} \delta_{2(n-k)} \|\phi_k\|_{L^2(\partial\Omega)}^2.$$

Hence (47) is derived for $\alpha = R$.

For the Dirichlet case, one can substitute (64) into (56) to derive that, for $\alpha = D$,

$$\mathcal{B}_{\alpha}(\boldsymbol{u};\boldsymbol{u}) \geq (1-\epsilon_{2n})\mathcal{E}_{\delta,n} - \epsilon_{2n}\delta_{2n+1} \|\phi_0\|_{L^2(\Omega)}^2 + \lambda \sum_{k=0}^{n-1} \|\phi_k\|_{L^2(\partial\Omega)}^2 - \sum_{k=0}^{n-1} \|\boldsymbol{\psi}_k\|_{L^2(\partial\Omega)} \|\phi_k\|_{L^2(\partial\Omega)}.$$

Utilizing the result in (68), it follows that

$$\mathcal{B}_{\alpha}(\boldsymbol{u};\boldsymbol{u}) \geq (1 - \epsilon_{2n} - C^* \delta) \mathcal{E}_{\delta,n} + \epsilon_{2n} \delta_{2n+1} \|\phi_0\|_{L^2(\Omega)}^2 + (\lambda - C^* \delta) \sum_{k=0}^{n-1} \|\phi_k\|_{L^2(\partial\Omega)}^2 - \sum_{k=0}^{n-1} \|\psi_k\|_{L^2(\partial\Omega)} \|\phi_k\|_{L^2(\partial\Omega)}.$$

Moreover, we note the fact

$$\|\phi_k\|_{L^2(\partial\Omega)} \leq \mathcal{B}^{\frac{1}{2}}_{\alpha}(\boldsymbol{u};\boldsymbol{u}),$$

we finally obtain

$$\mathcal{B}_{\alpha}(\boldsymbol{u};\boldsymbol{u}) + \sum_{k=0}^{n-1} \|\boldsymbol{\psi}_{k}\|_{L^{2}(\partial\Omega)} \mathcal{B}_{\alpha}^{\frac{1}{2}}(\boldsymbol{u};\boldsymbol{u})$$

$$\geq (1 - \epsilon_{2n} - C^{*}\delta) \mathcal{E}_{\delta,n} + \epsilon_{2n} \delta_{2n+1} \|\phi_{0}\|_{L^{2}(\Omega)}^{2} + (\lambda - C^{*}\delta) \sum_{k=0}^{n-1} \|\phi_{k}\|_{L^{2}(\partial\Omega)}^{2}.$$

5. Second-order system for 2n-order elliptic equation

In this section, we give the proof of the coercivity estimates for the bilinear form (30) and (31), induced from the second-order least squares system of the 2*n*-order elliptic equation. Suppose $v \in \mathbb{R}^n$ with the form:

$$\boldsymbol{v} = (\varphi_0, \dots, \varphi_{n-1}).$$

Lemma 5.1. The bilinear form (30)-(31) is coercive with respect to $(\mathcal{H}(\Omega))^n$ defined in (37) in the following sense. For the Neumann and Robin boundary, i.e. $\alpha = N, R$, there exists a constant C > 0 such that

(70)
$$\mathcal{B}_{\alpha}(\boldsymbol{v},\boldsymbol{v}) \geq C \sum_{k=0}^{n-1} \left(\|\nabla \varphi_k\|_{H(\operatorname{div};\Omega)}^2 + \|\varphi_k\|_{H^1(\Omega)}^2 \right)$$

And for the Dirichlet boundary, there exists a constant C > 0 such that (71)

$$\left(\mathcal{B}_{\mathrm{D}}^{\frac{1}{2}}(\boldsymbol{v},\boldsymbol{v}) + \sum_{k=0}^{n-1} \|\nabla\varphi_k\|_{L^2(\partial\Omega)}\right) \mathcal{B}_{\mathrm{D}}^{\frac{1}{2}}(\boldsymbol{v},\boldsymbol{v}) \ge C \sum_{k=0}^{n-1} \left(\|\nabla\varphi_k\|_{H(\operatorname{div};\Omega)}^2 + \|\varphi_k\|_{H^1(\Omega)}^2\right)$$

5.1. **Perturbation method.** Utilizing the notation δ_k defined in (53), we introduce the weighted energy

(72)
$$\mathcal{E}_{\delta,n}^{*} = \sum_{k=1}^{n-1} \delta_{n-k+1} \|\varphi_k\|_{L^2(\Omega)}^2 + \sum_{k=0}^{n-1} \delta_{n-k} \|\Delta\varphi_k\|_{L^2(\Omega)}^2.$$

Then we have the following estimate:

Lemma 5.2. For the bilinear form (30), we have

(73)
$$\mathcal{B}_{\alpha}(\boldsymbol{v};\boldsymbol{v}) \geq (1-\epsilon_n)\mathcal{E}^*_{\delta,n} - \epsilon_n \delta_{n+1} \|\varphi_0\|^2_{L^2(\Omega)} + \mathcal{T}_{\mathbf{b},\alpha},$$

where the boundary term $\mathcal{T}_{b,\alpha}$ is defined by

$$\mathcal{T}_{\mathbf{b},\alpha} = \lambda (S^*_{\alpha} \boldsymbol{v}, S^*_{\alpha} \boldsymbol{v})_{\partial \Omega} + \tau_{\alpha}$$

(74)
$$-2\sum_{k=0}^{n-2}\delta_{n-k}\Big((\partial_{\boldsymbol{n}}\varphi_{k},\varphi_{k+1})_{\partial\Omega}-(\varphi_{k},\partial_{\boldsymbol{n}}\varphi_{k+1})_{\partial\Omega}\Big).$$

Here, τ_{α} is zero-mean penalty that appears in the Neumann boundary case, *i.e.*

$$\tau_{\alpha} = \begin{cases} \mu \big| \int_{\Omega} \varphi_0 \, \mathrm{d} \boldsymbol{x} \big|^2, & \text{when } \alpha = \mathrm{N}, \\ 0, & \text{when } \alpha = \mathrm{D}, \mathrm{R}. \end{cases}$$

Proof. Let us denote the $n \times n$ matrix

$$\mathcal{P}_{1}^{*} = \begin{pmatrix} \Delta & 0 & \cdots & 0 & 0 \\ 0 & \Delta & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & \Delta & 0 \\ 0 & 0 & \cdots & 0 & \Delta \end{pmatrix}, \quad \mathcal{P}_{2}^{*} = \begin{pmatrix} 0 & I & 0 & \cdots & 0 \\ 0 & 0 & I & \cdots & 0 \\ \vdots & \vdots & \ddots & \ddots & \vdots \\ 0 & 0 & \cdots & 0 & I \\ 0 & 0 & \cdots & 0 & 0 \end{pmatrix}.$$

Then the bilinear form can be written as

(75)
$$\mathcal{B}_{\alpha}(\boldsymbol{v};\boldsymbol{v}) = \left((\mathcal{P}_1^* - \mathcal{P}_2^*)\boldsymbol{v}, (\mathcal{P}_1^* - \mathcal{P}_2^*)\boldsymbol{v} \right) + \lambda (S_{\alpha}^*\boldsymbol{v}, S_{\alpha}^*\boldsymbol{v})_{\partial\Omega} + \tau_{\alpha}.$$

Similarly to the proof of the first-order system, we recall parameters δ_i in (53) and introduce the $n \times n$ weighting matrix $W^*_{\delta,n}$ defined by

(76)
$$W_{\delta,n}^* = \begin{pmatrix} \delta_n & 0 & \cdots & 0 & 0\\ 0 & \delta_{n-1} & \cdots & 0 & 0\\ \vdots & \vdots & \ddots & \vdots & \vdots\\ 0 & 0 & \cdots & \delta_2 & 0\\ 0 & 0 & \cdots & 0 & \delta_1 \end{pmatrix}.$$

,

Then one can derive that

(77)
$$\mathcal{B}_{\alpha}(\boldsymbol{v};\boldsymbol{v}) \geq \left((\mathcal{P}_{1}^{*} - \mathcal{P}_{2}^{*})\boldsymbol{v}, W_{\delta,n}^{*}(\mathcal{P}_{1}^{*} - \mathcal{P}_{2}^{*})\boldsymbol{v} \right) + \lambda(S_{\alpha}^{*}\boldsymbol{v}, S_{\alpha}^{*}\boldsymbol{v})_{\partial\Omega} + \tau_{\alpha} \\ = \left(\mathcal{P}_{1}^{*}\boldsymbol{v}, W_{\delta,n}^{*}\mathcal{P}_{1}^{*}\boldsymbol{v} \right) + \left(\mathcal{P}_{2}^{*}\boldsymbol{v}, W_{\delta,n}^{*}\mathcal{P}_{2}^{*}\boldsymbol{v} \right) \\ - 2\left(\mathcal{P}_{1}^{*}\boldsymbol{v}, W_{\delta,n}^{*}\mathcal{P}_{2}^{*}\boldsymbol{v} \right) + \lambda(S_{\alpha}^{*}\boldsymbol{v}, S_{\alpha}^{*}\boldsymbol{v})_{\partial\Omega} + \tau_{\alpha}.$$

Here, the first two terms on RHS are equivalent to the weighted energy defined in (72):

$$\left(\mathcal{P}_1^*\boldsymbol{v}, W_{\delta.n}^*\mathcal{P}_1^*\boldsymbol{v}\right) + \left(\mathcal{P}_2^*\boldsymbol{v}, W_{\delta.n}^*\mathcal{P}_2^*\boldsymbol{v}\right) = \mathcal{E}_{\delta,n}^*.$$

Now we estimate the cross term:

$$-2\left(\mathcal{P}_{1}^{*}\boldsymbol{v}, W_{\delta,n}^{*}\mathcal{P}_{2}^{*}\boldsymbol{v}\right) = -2\sum_{k=0}^{n-2}\delta_{n-k}(\Delta\varphi_{k}, \varphi_{k+1}).$$

Note that by integration by parts, one has

$$-2(\mathcal{P}_{1}^{*}\boldsymbol{v}, W_{\delta,n}^{*}\mathcal{P}_{2}^{*}\boldsymbol{v}) = -2\sum_{k=0}^{n-2} \delta_{n-k} \Big((\varphi_{k}, \Delta \varphi_{k+1}) \\ + (\partial_{\boldsymbol{n}}\varphi_{k}, \varphi_{k+1})_{\partial\Omega} - (\varphi_{k}, \partial_{\boldsymbol{n}}\varphi_{k+1})_{\partial\Omega} \Big).$$

Utilizing estimate (54), one can deduce that

$$-2\delta_{n-k}(\varphi_k,\Delta\varphi_{k+1}) \ge -\epsilon_n \Big(\delta_{n-k+1} \|\varphi_k\|_{L^2(\Omega)}^2 + \delta_{n-k-1} \|\Delta\varphi_{k+1}\|_{L^2(\Omega)}^2\Big).$$

Then using the notation (72), it leads to

$$2(\mathcal{P}_{1}^{*}\boldsymbol{v}, W_{\delta,n}^{*}\mathcal{P}_{2}^{*}\boldsymbol{v}) \geq -\epsilon_{n}\mathcal{E}_{\delta,n}^{*} - \epsilon_{n}\delta_{n+1} \|\varphi_{0}\|_{L^{2}(\Omega)}^{2} \\ -2\sum_{k=0}^{n-2}\delta_{n-k}\Big((\partial_{n}\varphi_{k}, \varphi_{k+1})_{\partial\Omega} - (\varphi_{k}, \partial_{n}\varphi_{k+1})_{\partial\Omega}\Big).$$

Combining the estimate above, and plugging into (77), it finally leads to

$$\mathcal{B}_{\alpha}(\boldsymbol{v};\boldsymbol{v}) \geq (1-\epsilon_{n})\mathcal{E}_{\delta,n}^{*} - \epsilon_{n}\delta_{n+1} \|\varphi_{0}\|_{L^{2}(\Omega)}^{2} + \lambda(S_{\alpha}^{*}\boldsymbol{v},S_{\alpha}^{*}\boldsymbol{v})_{\partial\Omega} + \tau_{\alpha} \\ - 2\sum_{k=0}^{n-2} \delta_{n-k} \Big((\partial_{\boldsymbol{n}}\varphi_{k},\varphi_{k+1})_{\partial\Omega} - (\varphi_{k},\partial_{\boldsymbol{n}}\varphi_{k+1})_{\partial\Omega} \Big).$$

The Lemma is proved.

5.2. Estimate of boundary term. Now let us estimate the boundary term $\mathcal{T}_{b,\alpha}$ in (74).

Lemma 5.3. For the boundary term $\mathcal{T}_{b,\alpha}$, we have

• Neumann boundary.

(78)

$$\mathcal{T}_{\mathrm{b,N}} \geq -C\delta \mathcal{E}_{\delta,n}^{*} - \epsilon_{n} \delta_{n+1} \|\varphi_{0}\|_{L^{2}(\Omega)}^{2} + \left(\frac{\lambda}{2} - C\delta\right) \sum_{k=0}^{n-1} \|\partial_{n}\varphi_{k}\|_{L^{2}(\partial\Omega)}^{2} + \mu \Big| \int_{\Omega} \varphi_{0} \,\mathrm{d}\boldsymbol{x} \Big|^{2}.$$

• Robin boundary.

(79)
$$\mathcal{T}_{\mathbf{b},\mathbf{R}} \ge -C\delta\mathcal{E}_{\delta,n}^* + \left(\frac{\lambda}{2} - C\delta\right)\sum_{k=0}^{n-1} \|\varphi_k + \partial_n\varphi_k\|_{L^2(\partial\Omega)}^2$$

• Dirichlet boundary.

(80)
$$\mathcal{T}_{\mathbf{b},\mathbf{D}} \ge \lambda \sum_{k=0}^{n-1} \|\varphi_k\|_{L^2(\partial\Omega)}^2 - \sum_{k=0}^{n-1} \|\partial_{\boldsymbol{n}}\varphi_{k+1}\|_{L^2(\partial\Omega)} \|\varphi_k\|_{L^2(\partial\Omega)}.$$

Proof. Case i. Neumann boundary. For the Neumann boundary case, we utilize Young's inequality and trace theorem for the third term in (74) and derive the estimate

$$2\delta_{n-k}(\partial_{\boldsymbol{n}}\varphi_{k},\varphi_{k+1})_{\partial\Omega} \geq -C\delta_{n-k}^{2}\|\varphi_{k+1}\|_{L^{2}(\partial\Omega)}^{2} - \frac{\lambda}{4}\|\partial_{\boldsymbol{n}}\varphi_{k}\|_{L^{2}(\partial\Omega)}^{2}$$
$$\geq -C\delta_{n-k}^{2}\|\varphi_{k+1}\|_{H^{1}(\Omega)}^{2} - \frac{\lambda}{4}\|\partial_{\boldsymbol{n}}\varphi_{k}\|_{L^{2}(\partial\Omega)}^{2}.$$

Moreover, we apply the standard elliptic estimate of Neumann problem, see Proposition 2.10 of [7]:

(81)
$$\|\nabla \varphi_k\|_{L^2(\Omega)}^2 \le C(\|\Delta \varphi_k\|_{L^2(\Omega)}^2 + \|\partial_n \varphi_k\|_{L^2(\partial\Omega)}^2).$$

27

Note the fact $\delta_{n-k} \leq \delta_{n-k-1} \leq \delta$ for $0 \leq k \leq n-2$, it follows that

$$2\delta_{n-k}(\partial_{\boldsymbol{n}}\varphi_{k},\varphi_{k+1})_{\partial\Omega} \geq -C\delta\left(\delta_{n-k-1}\|\Delta\varphi_{k+1}\|_{L^{2}(\Omega)}^{2}+\delta_{n-k}\|\varphi_{k+1}\|_{L^{2}(\Omega)}^{2}\right)$$
$$-C\delta\delta_{n-k-1}\|\partial_{\boldsymbol{n}}\varphi_{k+1}\|_{L^{2}(\partial\Omega)}^{2}-\frac{\lambda}{4}\|\partial_{\boldsymbol{n}}\varphi_{k}\|_{L^{2}(\partial\Omega)}^{2}.$$

We apply the same argument to the last term in (74):

$$-2\delta_{n-k}(\varphi_k,\partial_n\varphi_{k+1})_{\partial\Omega} \ge -C\delta_{n-k}^2 \|\varphi_k\|_{H^1(\Omega)}^2 - \frac{\lambda}{4} \|\partial_n\varphi_{k+1}\|_{L^2(\partial\Omega)}^2$$
$$\ge -C\delta(\delta_{n-k}\|\Delta\varphi_k\|_{L^2(\Omega)}^2 + \delta_{n-k+1}\|\varphi_k\|_{L^2(\Omega)}^2)$$
$$-C\delta\delta_{n-k}\|\partial_n\varphi_k\|_{L^2(\partial\Omega)}^2 - \frac{\lambda}{4} \|\partial_n\varphi_{k+1}\|_{L^2(\partial\Omega)}^2.$$

Here, the inequality $\delta_{n-k}^2 \leq \delta \delta_{n-k+1}$ for $0 \leq k \leq n-2$ is used in the last line. Combining the estimates above and using notation (72), we obtain

$$2\sum_{k=0}^{n-2} \delta_{n-k} \Big((\partial_{\boldsymbol{n}} \varphi_{k}, \varphi_{k+1})_{\partial \Omega} - (\varphi_{k}, \partial_{\boldsymbol{n}} \varphi_{k+1})_{\partial \Omega} \Big)$$

$$\geq -C\delta \mathcal{E}_{\delta,n}^{*} - \epsilon_{n} \delta_{n+1} \|\varphi_{0}\|_{L^{2}(\Omega)}^{2} - \Big(\frac{\lambda}{2} + C\delta\Big) \sum_{k=0}^{n-1} \|\partial_{\boldsymbol{n}} \varphi_{k}\|_{L^{2}(\partial\Omega)}^{2}.$$

Therefore the substituting into the boundary term (74) deduces the estimate (78).

Case ii. Robin boundary. For the Robin boundary case, we utilize Young's inequality. The last two terms in (74) can be written as

(82)
$$2\delta_{n-k}(\partial_{n}\varphi_{k},\varphi_{k+1})_{\partial\Omega} - 2\delta_{n-k}(\varphi_{k},\partial_{n}\varphi_{k+1})_{\partial\Omega} = 2\delta_{n-k}(\varphi_{k}+\partial_{n}\varphi_{k},\varphi_{k+1})_{\partial\Omega} - 2\delta_{n-k}(\varphi_{k},\varphi_{k+1}+\partial_{n}\varphi_{k+1})_{\partial\Omega}$$

The first term on the right-hand side of (82) yields the estimate

$$2\delta_{n-k}(\varphi_k + \partial_{\mathbf{n}}\varphi_k, \varphi_{k+1})_{\partial\Omega} \ge -C\delta_{n-k}^2 \|\varphi_{k+1}\|_{L^2(\partial\Omega)}^2 - \frac{\lambda}{4} \|\varphi_k + \partial_{\mathbf{n}}\varphi_k\|_{L^2(\partial\Omega)}^2$$
$$\ge -C\delta_{n-k}^2 \|\varphi_{k+1}\|_{H^1(\Omega)}^2 - \frac{\lambda}{4} \|\varphi_k + \partial_{\mathbf{n}}\varphi_k\|_{L^2(\partial\Omega)}^2.$$

Note the fact $\delta_{n-k} \leq \delta_{n-k-1} \leq \delta$ for $0 \leq k \leq n-2$, it follows that

$$2\delta_{n-k}(\varphi_k + \partial_n \varphi_k, \varphi_{k+1})_{\partial\Omega} \ge -C\delta\delta_{n-k-1} \|\varphi_{k+1}\|_{H^1(\Omega)}^2 - \frac{\lambda}{4} \|\varphi_k + \partial_n \varphi_k\|_{L^2(\partial\Omega)}^2$$

Moreover, we apply the elliptic estimate of Robin problem:

(83)
$$\|\varphi_k\|_{H^1(\Omega)}^2 \le C(\|\Delta\varphi_k\|_{L^2(\Omega)}^2 + \|\varphi_k + \partial_n\varphi_k\|_{L^2(\partial\Omega)}^2).$$

Then it finally leads to

$$2\delta_{n-k}(\varphi_k + \partial_n \varphi_k, \varphi_{k+1})_{\partial\Omega} \ge -C\delta\delta_{n-k-1} \|\Delta\varphi_{k+1}\|_{L^2(\Omega)}^2$$
$$-C\delta \|\varphi_{k+1} + \partial_n \varphi_{k+1}\|_{L^2(\partial\Omega)}^2 - \frac{\lambda}{4} \|\varphi_k + \partial_n \varphi_k\|_{L^2(\partial\Omega)}^2.$$

29

We apply the same argument to the second term on the right-hand side of (82):

$$-2\delta_{n-k}(\varphi_k,\varphi_{k+1}+\partial_n\varphi_{k+1})_{\partial\Omega}$$

$$\geq -C\delta\delta_{n-k}\|\varphi_k\|_{H^1(\Omega)}^2 - \frac{\lambda}{4}\|\varphi_{k+1}+\partial_n\varphi_{k+1}\|_{L^2(\partial\Omega)}^2$$

$$\geq -C\delta\delta_{n-k}\|\Delta\varphi_k\|_{L^2(\Omega)}^2 - C\delta\|\varphi_k+\partial_n\varphi_k\|_{L^2(\partial\Omega)}^2 - \frac{\lambda}{4}\|\varphi_{k+1}+\partial_n\varphi_{k+1}\|_{L^2(\partial\Omega)}^2.$$

Combining the estimates above, and using notation (72), we obtain

$$-2\sum_{k=0}^{n-2} \delta_{n-k} \Big((\partial_{n}\varphi_{k}, \varphi_{k+1})_{\partial\Omega} - (\varphi_{k}, \partial_{n}\varphi_{k+1})_{\partial\Omega} \Big)$$

$$\geq -C\delta \mathcal{E}_{\delta,n}^{*} - \Big(\frac{\lambda}{2} + C\delta\Big) \sum_{k=0}^{n-1} \|\varphi_{k} + \partial_{n}\varphi_{k}\|_{L^{2}(\partial\Omega)}^{2}.$$

Case iii. Dirichlet boundary. For the case of the Dirichlet boundary condition, the last two terms in (57) can be estimated by

$$2\delta_{n-k}(\partial_{\boldsymbol{n}}\varphi_{k},\varphi_{k+1})_{\partial\Omega} \geq -2\delta \|\partial_{\boldsymbol{n}}\varphi_{k}\|_{L^{2}(\partial\Omega)} \|\varphi_{k+1}\|_{L^{2}(\partial\Omega)},$$

$$-2\delta_{n-k}(\varphi_{k},\partial_{\boldsymbol{n}}\varphi_{k+1})_{\partial\Omega} \geq -2\delta \|\partial_{\boldsymbol{n}}\varphi_{k+1}\|_{L^{2}(\partial\Omega)} \|\varphi_{k}\|_{L^{2}(\partial\Omega)}.$$

Hence the estimate (80) follows.

5.3. Proof of Lemma 5.1. For the Neumann case, we substitute (78) into (73) to derive that, for $\alpha = N$,

(84)
$$\mathcal{B}_{\alpha}(\boldsymbol{v};\boldsymbol{v}) \geq (1-\epsilon_{n}-C\delta)\mathcal{E}_{\delta,n}^{*}-2\epsilon_{n}\delta_{n+1}\|\varphi_{0}\|_{L^{2}(\Omega)}^{2} + \left(\frac{\lambda}{2}-C\delta\right)\sum_{k=0}^{n-1}\|\partial_{\boldsymbol{n}}\varphi_{k}\|_{L^{2}(\partial\Omega)}^{2} + \mu\Big|\int_{\Omega}\varphi_{0}\,\mathrm{d}\boldsymbol{x}\Big|^{2}.$$

We utilize the inequality (81) and the Poincaré-Friedrichs inequality (52) to deduce

$$2\epsilon_{n}\delta_{n+1}\|\varphi_{0}\|_{L^{2}(\Omega)}^{2} \leq \epsilon_{n}\delta_{n+1}C\Big(\|\Delta\varphi_{0}\|_{L^{2}(\Omega)}^{2} + \|\partial_{n}\varphi_{0}\|_{L^{2}(\partial\Omega)}^{2} + \Big|\int_{\Omega}\varphi_{0} \,\mathrm{d}\boldsymbol{x}\Big|^{2}\Big)$$
$$\leq C\delta\Big(\mathcal{E}_{\delta,n}^{*} + \|\partial_{n}\varphi_{0}\|_{L^{2}(\partial\Omega)}^{2} + \Big|\int_{\Omega}\varphi_{0} \,\mathrm{d}\boldsymbol{x}\Big|^{2}\Big).$$

Using the result above, it follows from (84) that

$$\mathcal{B}_{\alpha}(\boldsymbol{v};\boldsymbol{v}) \geq (1-\epsilon_{n}-C\delta)\mathcal{E}_{\delta,n}+\epsilon_{n}\delta_{n+1}\|\varphi_{0}\|_{L^{2}(\Omega)}^{2} \\ +\left(\frac{\lambda}{2}-C\delta\right)\sum_{k=0}^{n-1}\|\partial_{n}\varphi_{k}\|_{L^{2}(\partial\Omega)}^{2}+(\mu-C\delta)\Big|\int_{\Omega}\varphi_{0}\,\mathrm{d}\boldsymbol{x}\Big|^{2}.$$

Therefore (70) is derived for $\alpha = N$.

For the case of the Robin boundary, Combining (73) and (79) to derive

$$\begin{aligned} \mathcal{B}_{\alpha}(\boldsymbol{v};\boldsymbol{v}) \geq & \left(1-\epsilon_{n}-C\delta\right)\mathcal{E}_{\delta,n}^{*} \\ & -\epsilon_{n}\delta_{n+1}\|\varphi_{0}\|_{L^{2}(\Omega)}^{2} + \left(\frac{\lambda}{2}-C\delta\right)\sum_{k=0}^{n-1}\|\varphi_{k}+\partial_{\boldsymbol{n}}\varphi_{k}\|_{L^{2}(\partial\Omega)}^{2}. \end{aligned}$$

In addition. Applying the elliptic estimate (83), we have

$$2\epsilon_{n}\delta_{n+1}\|\varphi_{0}\|_{L^{2}(\Omega)}^{2} \leq \epsilon_{n}\delta_{n+1}C(\|\Delta\varphi_{0}\|_{L^{2}(\Omega)}^{2} + \|\varphi_{0} + \partial_{n}\varphi_{0}\|_{L^{2}(\partial\Omega)}^{2})$$
$$\leq C\delta(\mathcal{E}_{\delta,n}^{*} + \|\varphi_{0} + \partial_{n}\varphi_{0}\|_{L^{2}(\partial\Omega)}^{2}).$$

Hence we conclude that

$$\mathcal{B}_{\alpha}(\boldsymbol{v};\boldsymbol{v}) \geq (1-\epsilon_n - C\delta) \mathcal{E}_{\delta,n}^* + \epsilon_n \delta_{n+1} \|\varphi_0\|_{L^2(\Omega)}^2 + \left(\frac{\lambda}{2} - C\delta\right) \sum_{k=0}^{n-1} \|\varphi_k + \partial_n \varphi_k\|_{L^2(\partial\Omega)}^2.$$

For the case of Dirichlet boundary, we utilize (80) and (73) to deduce that

(85)
$$\mathcal{B}_{\alpha}(\boldsymbol{v};\boldsymbol{v}) \geq (1-\epsilon_{n})\mathcal{E}_{\delta,n}^{*} - \epsilon_{n}\delta_{n+1} \|\varphi_{0}\|_{L^{2}(\Omega)}^{2} + \lambda \sum_{k=0}^{n-1} \|\varphi_{k}\|_{L^{2}(\partial\Omega)}^{2} - \sum_{k=0}^{n-1} \|\partial_{n}\varphi_{k+1}\|_{L^{2}(\partial\Omega)} \|\varphi_{k}\|_{L^{2}(\partial\Omega)}.$$

Applying Poincaré-Friedrichs inequality (51), one can derive

$$2\epsilon_n \delta_{n+1} \|\varphi_0\|_{L^2(\Omega)}^2 \leq \epsilon_n \delta_{n+1} C(\|\nabla\varphi_0\|_{L^2(\Omega)}^2 + \|\varphi_0\|_{L^2(\partial\Omega)}^2)$$

$$\leq C\delta(\|\Delta\varphi_0\|_{L^2(\Omega)}^2 + \|\partial_n\varphi_0\|_{L^2(\partial\Omega)} \|\varphi_0\|_{L^2(\partial\Omega)} + \|\varphi_0\|_{L^2(\partial\Omega)}^2),$$

where in the last line we used the elliptic estimate for Dirichlet boundary. Then by utilizing this fact $\|\varphi_k\|_{L^2(\partial\Omega)} \leq \mathcal{B}^{\frac{1}{2}}_{\alpha}(\boldsymbol{v};\boldsymbol{v})$, it follows that

$$\mathcal{B}_{\alpha}(\boldsymbol{v};\boldsymbol{v}) + \sum_{k=0}^{n-1} \|\nabla \boldsymbol{\varphi}_{k}\|_{L^{2}(\partial\Omega)} \mathcal{B}_{\alpha}^{\frac{1}{2}}(\boldsymbol{v};\boldsymbol{v})$$

$$\geq (1 - \epsilon_{n} - C\delta) \mathcal{E}_{\delta,n}^{*} + \epsilon_{n} \delta_{n+1} \|\boldsymbol{\varphi}_{0}\|_{L^{2}(\Omega)}^{2} + (\lambda - C\delta) \sum_{k=0}^{n-1} \|\boldsymbol{\varphi}_{k}\|_{L^{2}(\partial\Omega)}^{2}.$$

6. CONCLUSION

This study delves into the error estimates of the Deep Mixed Residual method (MIM) in solving high-order elliptic equations with non-homogeneous boundary conditions, including Dirichlet, Neumann, and Robin conditions. Two types of loss functions of MIM, referred to as first-order and second-order least squares systems, are both considered. We apply a general approach in the notion of bilinear forms introduced in [32], where one can utilize Céa's Lemma by performing boundedness and coercivity analysis.

30

31

As a result, the total error is decomposed into three components: approximation error, generalization error, and optimization error. Through the Barron space theory and Rademacher complexity, an a priori error is derived regarding the training samples and network size that are exempt from the curse of dimensionality. Our results reveal that MIM significantly reduces the regularity requirements for activation functions compared to the deep Ritz method, implying the effectiveness of MIM in solving high-order equations.

The main challenge in our analysis arises from the coercivity analysis of the low-order least squares systems (Equation (2) and (3)), specifically controlling the coupling terms. We employ a perturbation technique, selecting a special sequence of small parameters, to effectively bound these cross terms by decoupled terms. In addition, when considering the Dirichlet boundary condition, using an L^2 boundary penalty will lead to a loss of regularity of 3/2. This implies that approximations in H^2 yield a posteriori estimate only in $H^{\frac{1}{2}}$. In this work, we utilize the idea in [13] and derive a priori estimate in H^1 under the Dirichlet boundary condition. This is achieved by extending the Céa's Lemma and conducting a sup-linear coercivity analysis.

Acknowledgements

J. Chen is supported by the NSFC Major Research Plan - Interpretable and General-purpose Next-generation Artificial Intelligence (92370205) and NSFC 12425113. R. Du is supported by NSFC grant 12271360. The authors acknowledge partial support from the Austrian Science Fund (FWF), grant DOI 10.55776/P33010 and 10.55776/F65. This work has received funding from the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation programme, ERC Advanced Grant NEUROMORPH, no. 101018153

References

- Lars-Erik Andersson, Tommy Elfving, and Gene H Golub, Solution of biharmonic equations with application to radar imaging, Journal of Computational and Applied Mathematics 94 (1998), no. 2, 153–180.
- Andrew R Barron, Universal approximation bounds for superpositions of a sigmoidal function, IEEE Transactions on Information theory 39 (1993), no. 3, 930–945.
- Zhiqiang Cai, Jingshuang Chen, Min Liu, and Xinyu Liu, Deep least-squares methods: An unsupervised learning-based numerical method for solving elliptic PDEs, Journal of Computational Physics 420 (2020), 109707.
- Zhiqiang Cai, R Lazarov, Thomas A Manteuffel, and Stephen F McCormick, Firstorder system least squares for second-order partial differential equations: Part I, SIAM Journal on Numerical Analysis 31 (1994), no. 6, 1785–1799.
- WH Duan and Chien Ming Wang, Exact solutions for axisymmetric bending of micro/nanoscale circular plates based on nonlocal plate theory, Nanotechnology 18 (2007), no. 38, 385704.
- Weinan E and Bing Yu, The deep ritz method: a deep learning-based numerical algorithm for solving variational problems, Communications in Mathematics and Statistics 6 (2018), no. 1, 1–12.

- Alexandre Ern and Jean-Luc Guermond, Theory and practice of finite elements, vol. 159, Springer, 2004.
- 8. Vivette Girault and Pierre-Arnaud Raviart, *Finite element methods for Navier–Stokes equations: theory and algorithms*, vol. 5, Springer Science & Business Media, 2012.
- Jiequn Han, Arnulf Jentzen, and Weinan E, Solving high-dimensional partial differential equations using deep learning, Proceedings of the National Academy of Sciences 115 (2018), no. 34, 8505–8510.
- 10. Qingguo Hong, Jonathan W Siegel, and Jinchao Xu, A priori analysis of stable neural network solutions to numerical PDEs, arXiv preprint arXiv:2104.02903 (2021).
- Evgeniy Khain and Leonard M Sander, Generalized Cahn-Hilliard equation for biological applications, Physical Review E—Statistical, Nonlinear, and Soft Matter Physics 77 (2008), no. 5, 051129.
- 12. Lev Davidovich Landau, LP Pitaevskii, Arnol'd Markovich Kosevich, and Evgenii Mikhailovich Lifshitz, *Theory of elasticity: volume 7*, vol. 7, Elsevier, 2012.
- Lingfeng Li, Xue-Cheng Tai, Jiang Yang, and Quanhui Zhu, A priori error estimate of deep mixed residual method for elliptic PDEs, Journal of Scientific Computing 98 (2024), no. 2, 44.
- Yuanyuan Li, Shuai Lu, Peter Mathé, and Sergei V Pereverzev, Two-layer networks with the ReLU^k activation function: Barron spaces and derivative approximation, Numerische Mathematik 156 (2024), no. 1, 319–344.
- 15. Jacques Louis Lions and Enrico Magenes, Non-homogeneous boundary value problems and applications: Vol. 1, vol. 181, Springer Science & Business Media, 2012.
- Yulong Lu, Jianfeng Lu, and Min Wang, A priori generalization analysis of the deep ritz method for solving high dimensional elliptic partial differential equations, Conference on learning theory (2021), 3196–3241.
- Liyao Lyu, Keke Wu, Rui Du, and Jingrun Chen, *Enforcing exact boundary and initial conditions in the deep mixed residual method*, CSIAM Transactions on Applied Mathematics 2 (2021), no. 4, 748–775.
- Liyao Lyu, Zhen Zhang, Minxin Chen, and Jingrun Chen, MIM: A deep mixed residual method for solving high-order partial differential equations, Journal of Computational Physics 452 (2022), 110930.
- Siddhartha Mishra and Roberto Molinaro, Estimates on the generalization error of physics informed neural networks (PINNs) for approximating a class of inverse problems for PDEs, IMA Journal of Numerical Analysis 42 (2022), no. 2, 981–1022.
- 20. _____, Estimates on the generalization error of physics-informed neural networks for approximating PDEs, IMA Journal of Numerical Analysis **43** (2023), no. 1, 1–43.
- 21. Johannes Müller and Marius Zeinhofer, Error estimates for the variational training of neural networks with boundary penalty, arXiv preprint arXiv:2103.01007 (2021).
- 22. _____, Error estimates for the deep ritz method with boundary penalty, Mathematical and Scientific Machine Learning (2022), 215–230.
- 23. _____, Notes on exact boundary values in residual minimisation, Mathematical and Scientific Machine Learning (2022), 231–240.
- 24. Jindřich Nečas, *Les méthodes directes en théorie des équations elliptiques*, Academia (1967).
- Maziar Raissi, Paris Perdikaris, and George E Karniadakis, *Physics-informed neural networks: A deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations*, Journal of Computational physics **378** (2019), 686–707.
- Martin Schechter, On L^p estimates and regularity II, Mathematica Scandinavica 13 (1963), no. 1, 47–69.
- Jonathan W Siegel, Qingguo Hong, Xianlin Jin, Wenrui Hao, and Jinchao Xu, Greedy training algorithms for neural networks and applications to PDEs, Journal of Computational Physics 484 (2023), 112084.

33

- Justin Sirignano and Konstantinos Spiliopoulos, DGM: A deep learning algorithm for solving partial differential equations, Journal of computational physics 375 (2018), 1339–1364.
- Mohammad Vahab, Ehsan Haghighat, Maryam Khaleghi, and Nasser Khalili, A physics-informed neural network approach to solution and identification of biharmonic equations of elasticity, Journal of Engineering Mechanics 148 (2022), no. 2, 04021154.
- E Weinan, Chao Ma, and Lei Wu, The Barron space and the flow-induced function spaces for neural network models, Constructive Approximation. 55 (2022), no. 1, 369– 406.
- Yaohua Zang, Gang Bao, Xiaojing Ye, and Haomin Zhou, Weak adversarial networks for high-dimensional partial differential equations, Journal of Computational Physics 411 (2020), 109409.
- Marius Zeinhofer, Rami Masri, and Kent-André Mardal, A unified framework for the error analysis of physics-informed neural networks, arXiv preprint arXiv:2311.00529 (2023).

APPENDIX A. NEURAL-NETWORK APPROXIMATION

A.1. The proof of Lemma 3.7. For simplicity, we will only provide the proof for the case when the output function is one-dimensional here. The higher-dimensional case can be directly generalized. From [16], we recall for any $s \in \mathbb{N}$, the spectral Barron space $\mathcal{B}^s(\Omega)$ given by

$$\mathcal{B}^{s}(\Omega) := \Big\{ u \in L^{1}(\Omega) \, \Big| \, \sum_{k \in \mathbb{N}_{0}^{d}} (1 + \pi^{s} |k|_{1}^{s}) |\hat{u}(k)| < \infty \Big\},$$

with associated norm $||u||_{\mathcal{B}^s(\Omega)} := \sum_{k \in \mathbb{N}_0^d} (1 + \pi^s |k|_1^s) |\hat{u}(k)|$, where $\{\hat{u}(k)\}_{k \in \mathbb{N}_0^d}$ is the expansion cofficients of u under the cosine basis functions. And for any function $u \in H^1(\Omega)$ admits the expansion

(86)
$$u(\boldsymbol{x}) := \hat{u}(0) + \int g(\boldsymbol{x}, k) \mu(\mathrm{d}k),$$

where $\mu(dk)$ is the probability measure on $\mathbb{N}_0^d/\{\mathbf{0}\}$ define by

$$\mu(\mathrm{d}k) = \sum_{\mathbb{N}_0^d / \{\mathbf{0}\}} \frac{1}{Z_u} |\hat{u}(k)| (1 + \pi^4 |k|_1^4) \delta(\mathrm{d}k),$$

with normalizing constant $Z_u = \sum_{\mathbb{N}_0^d/\{\mathbf{0}\}} |\hat{u}(k)| (1 + \pi^4 |k|_1^4) \le ||u||_{\mathcal{B}^4(\Omega)}$, and

$$g(\boldsymbol{x},k) = \frac{Z_u}{1 + \pi^4 |k|_1^4} \cdot \frac{1}{2^d} \sum_{\boldsymbol{\xi} \in \Xi} \cos\left(\pi (\boldsymbol{k}_{\boldsymbol{\xi}} \cdot \boldsymbol{x} + \theta_k)\right).$$

with $\theta(k) \in \{0, 1\}$ and $\mathbf{k}_{\xi} = (k_1 \xi_1, \cdots, k_d \xi_d)$. Let us define the function class:

$$\mathcal{F}_{\cos}(B) := \left\{ \frac{\gamma}{1 + \pi^4 |k|_1^4} \cos\left(\pi(\boldsymbol{k} \cdot \boldsymbol{x}) + b\right) \left| k \in \mathbb{Z}^d / \{\boldsymbol{0}\}, |\gamma| \le B, b \in \{0, 1\} \right\},\$$

where B > 0 is a constant. Hence if $u \in \mathcal{B}^4(\Omega)$, then $\bar{u} := u - \hat{u}(0)$ lies in the H^1 -closure of the convex hull of $\mathcal{F}_{\cos}(B)$ with $B = ||u||_{\mathcal{B}^4(\Omega)}$. Since the H^1 -norm of any function in $\mathcal{F}_{\cos}(B)$ is bounded by B, apply the following conclusion: **Lemma A.1.** [2] Suppose u belongs to the closure of the convex hull of a set \mathcal{G} in a Hilbert space. Let the Hilbert norm of each element of \mathcal{G} be bounded by B > 0. Then for every $m \in \mathbb{N}$, there exists $\{g_i\}_{i=1}^m \subset \mathcal{G}$ and $\{c_i\}_{i=1}^m \subset [0,1]$ with $\sum_{i=1}^m c_i = 1$ such that

$$\left\|u - \sum_{i=1}^{m} c_i g_i\right\|^2 \le \frac{B^2}{m}.$$

Therefore it yields the following theorem:

Theorem A.1. Let $u \in \mathcal{B}^4$. Then there exists ϕ_m which is a convex combination of m functions in $\mathcal{F}_{\cos}(B)$ with $B = ||u||_{\mathcal{B}^4(\Omega)}$ such that

$$||u - \hat{u}(0) - \phi_m||^2_{H^1(\Omega)} \le \frac{||u||^2_{\mathcal{B}^4(\Omega)}}{m}.$$

Next, we will give the reduction to the ReCU function. Notice that every function in $\mathcal{F}_{cos}(B)$ is the composition of the one dimensional function g defined on [-1,1] by

(87)
$$g(z) = \frac{\gamma}{1 + \pi^4 |k|_1^4} \cos\left(\pi(|k|_1 z + b)\right),$$

with $k \in \mathbb{Z}^d/\{\mathbf{0}\}$, $|\gamma| \leq B$ and $b \in \{0, 1\}$, and a linear function $z = \boldsymbol{w} \cdot \boldsymbol{x}$ with $\boldsymbol{w} = \boldsymbol{k}/|\boldsymbol{k}|_1$. It is clear that $g \in C^4([-1, 1])$ satisfies

$$||g^{(s)}||_{L^{\infty}[-1,1]} \le |\gamma| \le B$$
 for $s = 0, 1, \cdots, 4$.

Lemma A.2. Let $g \in C^4([-1,1])$ with $||g^{(s)}||_{L^{\infty}([-1,1])} \leq B$ for $s = 0, 1, \dots, 4$. Assume $g^{(s)} = 0$ for s = 1, 2, 3. Let $\{z_j\}_{j=0}^{2m}$ be a partition of [-1,1] with $z_0 = -1, z_m = 0, z_{2m} = 1$ and $z_{j+1} - z_j = h = 1/m$ for each $j = 0, \dots, 2m - 1$. Then there exists a two-layer ReCU networks g_m of the form

(88)
$$g_m(z) = c + \sum_{i=1}^{2m+5} a_i \operatorname{ReCU}(\epsilon_i z - b_i),$$

with c = g(0), $b_i \in [-1,1]$, $\epsilon_i \in \{-1,1\}$ for $i = 1, \dots, 2m + 5$, and $\sum_{i=1}^{2m+5} |a_i| \leq 8B$ such that

$$\|g - \hat{g}_m\|_{H^1(\Omega)} \le \frac{6B}{\sqrt{m}}.$$

Proof. From [13], There exists a two-layer ReQU activated neural networks $\hat{g}_m(z)$ of the form

(89)
$$\hat{g}_m(z) = c + \sum_{i=0}^{2m+3} \hat{a}_i \operatorname{ReQU}(\epsilon_i z - \hat{b}_i),$$

with $c = g(0), \hat{b}_i \in [-1, 1], \ \epsilon \in \{-1, 1\}, \ \text{for } i = 0, \cdots, 2m + 3, \ \text{and} \sum_{i=0}^{2m+3} |\hat{a}_i| \leq 8B \text{ such that}$

$$\|g - \hat{g}_m\|_{H^1(\Omega)} \le \frac{5B}{\sqrt{m}}.$$

In addition, an example of coefficients $\{\hat{a}_i\}_{i=0}^{2m+3}$ are given as

$$\hat{a}_{i} = \begin{cases} \frac{a_{i+1}}{4h} & i = 0, 1, \\ \frac{\tilde{a}_{i+1} - \tilde{a}_{i-1}}{4h} & 2 \le i \le m - 1, \\ -\frac{\tilde{a}_{i-1}}{4h} & i = m, m + 1, \\ \frac{\tilde{a}_{i-1}}{4h} & i = m + 2, m + 3, \\ \frac{\tilde{a}_{i-1} - \tilde{a}_{i-3}}{4h} & m + 4 \le i \le 2m + 1, \\ -\frac{\tilde{a}_{i-3}}{4h} & i = 2m + 2, 2m + 3, \end{cases}$$

with

$$\tilde{a}_{i} = \begin{cases} \frac{g(z_{m+1}) - g(z_{m})}{h}, & i = m+1, \\ \frac{g(z_{m-1}) - g(z_{m})}{h}, & i = m, \\ \frac{g(z_{i}) - 2g(z_{i-1}) + g(z_{i-2})}{h}, & i > m+1, \\ \frac{g(z_{i-1}) - 2g(z_{i}) + g(z_{i+1})}{h}, & i < m. \end{cases}$$

And setting $\epsilon_i = -1, \hat{b}_i = -z_i$ for $i = 0, \dots, m+1$ and $\epsilon_i = 1, \hat{b}_i = z_{i-3}$ for $i = m+2, \dots, 2m+3$. Notice that

$$6\delta^2 \text{ReLU}(z) + 6\delta \text{ReQU}(z) = \text{ReCU}(z+\delta) - \text{ReCU}(z-\delta) + e(z,\delta)$$

with

0, δ,

$$\hat{e}(z;\delta) = \begin{cases} -(z+\delta)^2, & -\delta < z \le 0, \\ -(z+\delta)^2, & 0 < z \le \delta, \\ 0, & \text{otherwise,} \end{cases}$$

and

$$e(z;\delta) = \begin{cases} -(z+\delta)^3, & -\delta < z \le 0, \\ -(z+\delta)^3, & 0 < z \le \delta, \\ 0, & \text{otherwise.} \end{cases}$$

Hence we have

(90)
$$6\delta \operatorname{ReQU}(z) = \operatorname{ReCU}(z+\delta) - \operatorname{ReCU}(z-\delta) \\ - 6\delta^2 \operatorname{ReLU}(z) + e(z,\delta) - \frac{3}{2}\delta\hat{e}(z;\delta).$$

For fixed $\delta = h$, we obtain a ReCU activated neural networks $g_m(z)$ by approximating the ReQU active function in (89):

(91)
$$g_m(z) = g(0) + \sum_{i=0}^{2m+3} \frac{\hat{a}_i}{6h} (\operatorname{ReCU}(\epsilon_i z - \hat{b}_i + h) - \operatorname{ReCU}(\epsilon_i z - \hat{b}_i - h)).$$

It is easy to deduce that directly

(92)
$$\begin{aligned} \|g - g_m\|_{H^1(\Omega)} &\leq \|g - \hat{g}_m\|_{H^1(\Omega)} + \|\hat{g}_m - g_m\|_{H^1(\Omega)} \\ &\leq \frac{5B}{\sqrt{m}} + \frac{B}{\sqrt{m}} = \frac{6B}{\sqrt{m}}. \end{aligned}$$

Rearrange (91) in the form of

$$g_m(z) = g(0) + \sum_{i=1}^{m+2} a_i \operatorname{ReCU}(z_i - z) + \sum_{i=m+3}^{2m+5} a_i \operatorname{ReCU}(z - z_{i-5}),$$

where

$$a_{i} = \begin{cases} \frac{\hat{a}_{i+1} - \hat{a}_{i-1}}{9h}, & 1 \le i \le m, \\ -\frac{\hat{a}_{i-1}}{9h}, & i = m+1, m+2, \\ \frac{\hat{a}_{i-1}}{9h}, & i = m+3, m+4, \\ \frac{\hat{a}_{i-1} - \hat{a}_{i-3}}{9h}, & m+5 \le i \le 2m+4, \\ -\frac{\hat{a}_{i-3} + \hat{a}_{i-2}}{9h}, & i = 2m+5. \end{cases}$$

Furthermore, by the mean value theorem, $a_{m+1} = -\frac{\hat{a}_m}{9h} \leq |g^{(4)}h| \leq Bh$, which holds because of the assumption $g^{(s)} = 0$ for s = 1, 2, 3. It is similar to estimating the other coefficients.

Finally, by setting $\epsilon_i = -1, b_i = -z_i$ for $i = 1, \dots, m+2$ and $\epsilon_i = 1, b_i = z_{i-5}$ for $i = m+3, \dots, 2m+5$, it completes the proof of the lemma. \Box

Hence we have the following proposition:

Proposition A.1. Define the function class

 $\mathcal{F}_{\text{ReCU}}(B) := \{ c + \gamma \text{ReCU}(\boldsymbol{w} \cdot \boldsymbol{x} - t), |c| \le 2B, |\boldsymbol{w}|_1 = 1, |t| \le 1, |\gamma| \le 4B \}.$ Then for any constant \tilde{c} such that $|\tilde{c}| \le B$, the set $\tilde{c} + \mathcal{F}_{\cos}(B)$ is in the

 H^1 -closure of the convex hull of $\mathcal{F}_{\text{ReCU}}(B)$.

With Proposition A.1, we are ready to give the proof of Lemma 3.7.

Proof of Lemma 3.7. Observe that if $u \in \mathcal{F}_{\text{ReCU}}(B)$, then

$$||u||_{H^1(\Omega)}^2 \le (c+8\gamma)^2 + 144\gamma^2.$$

Therefore Lemma 3.7 follows directly from Theorem A.1 and Proposition A.1. $\hfill \Box$

A.2. The proof of lemma 3.10. Next, we will effectively use Rademacher complexity to derive an upper bound on the generalization error. First, let us review some important properties of Rademacher complexity from [13]:

Lemma A.3. Let \mathcal{F}, \mathcal{G} be function classes and a, b be constants. Then

- (1) $R_N(\mathcal{F} + \mathcal{G}) \leq R_N(\mathcal{F}) + R_N(\mathcal{G}).$
- (2) $R_N(a\mathcal{F}) = |a|R_N(\mathcal{F}).$
- (3) Assume g is a fixed function and $||g||_{L^{\infty}} \leq b$, then $R_{N}(\mathcal{G}) \leq \frac{b}{\sqrt{N}}$.
- (4) Assume that $\sigma : \mathbb{R} \to \mathbb{R}$ is *l*-Lipschitz with $\sigma(0) = 0$, then $R_N(\sigma(\mathcal{F})) \leq 2lR_N(\mathcal{F})$.
- (5) $R_N(\mathcal{F}^2) \leq 4 \sup_{f \in \mathcal{F}} \|f\|_{L^{\infty}} R_N(\mathcal{F}).$
- (6) $R_N(\mathcal{FG}) \le 6 \sup_{f \in \mathcal{F} \cup \mathcal{G}} \|f\|_{L^{\infty}} (R_N(\mathcal{F}) + R_N(\mathcal{G})).$

With the calculation rules prepared, we are ready to estimate the complexity of the neural network function classes.

Lemma A.4. [13] Let \mathcal{G} be the linear transformation function class defined by

(93) $\mathcal{G} := \{ \boldsymbol{\omega} \cdot \boldsymbol{x} + b \, | \, \| \boldsymbol{w} \|_2 = 1, \, |b| \le 1 \}.$

Then we have

(94)
$$R_N(\mathcal{G}) \le \frac{\sqrt{2d\log d} + 1}{\sqrt{N}}$$

Similar to the function class $\mathcal{F}_{\text{ReCU},m}$ in [13], we give an estimate of the Rademacher complexity for the function class $\mathcal{F}_{\text{ReCU},m}$. The estimate of the complexity of a two-layer neural network depends on the activation function. Since $\sigma = \text{ReCU}$ is three times three times continuously differentiable, we can make the following assumptions:

$$\sup |\sigma^{(k)}| \le \ell_k, \quad k = 0, 1, 2, 3$$

Lemma A.5. The Rademacher complexity of $\mathcal{F}_{\text{ReCU},m}$ is bounded by

(95)
$$R_N(\mathcal{F}_{\text{ReCU},m}) \le \frac{C \|u\|_{\mathcal{B}^{2n+3}}}{\sqrt{N}}$$

where C > 0 is a constant dependent on d.

Proof. Using properties (1) and (3), the Rademacher complexity of $\mathcal{F}_{\text{ReCU},m}$ is broken down into the sum of the Rademacher complexity of each neuron, i.e.

$$R_N(\mathcal{F}_{\text{ReCU},m}) \leq \frac{2\|u\|_{\mathcal{B}^{2n+3}}}{\sqrt{N}} + \sum_{i=1}^m |\boldsymbol{a}_i| R_N(\sigma(\mathcal{G})).$$

Since σ is ℓ_1 -Lipschitz and $\sigma(0) = 0$, property (4) tells us

$$R_N(\sigma(\mathcal{G})) \leq 2\ell_1 R_N(\mathcal{G}).$$

Hence combining lemma A.4, we can conclude

$$R_N(\mathcal{F}_{\text{ReCU},m}) \le \frac{(2+8\ell_1+8\ell_1\sqrt{2d\log d})\|u\|_{\mathcal{B}^{2n+3}}}{\sqrt{N}}.$$

With the preparation above, we will now prove Lemma 3.10.

The proof of lemma 3.10. By the definition of $\mathcal{F}_{\text{ReCU},m}$ neural network, for $1 \leq j \leq d$, we deduce that the first-order derivation is

$$\frac{\partial \boldsymbol{v}_{\theta}}{\partial x_j} = \sum_{i=1}^m \boldsymbol{a}_i \cdot W_{i,j} \sigma^{(1)} (W_i \boldsymbol{x} + \boldsymbol{b}_i),$$

and second-order derivation is

$$\frac{\partial^2 \boldsymbol{v}_{\theta}}{\partial^2 x_j} = \sum_{i=1}^m \boldsymbol{a}_i \cdot |W_{i,j}|^2 \sigma^{(2)} (W_i \boldsymbol{x} + \boldsymbol{b}_i).$$

Hence we have

(96)
$$\left\|\frac{\partial^{k}\boldsymbol{v}_{\theta}}{\partial^{k}x_{j}}\right\|_{L^{\infty}(\Omega)} \leq C \|\boldsymbol{u}\|_{\mathcal{B}^{2n+3}}, \quad \text{for } k = 0, 1, 2.$$

Recall the definition (20) of \mathcal{P}^* , it follows that

(97)
$$|\mathcal{P}^*\boldsymbol{v}_{\theta} - \boldsymbol{f}|^2 = |\Delta\varphi_{n-1} - \boldsymbol{f}|^2 + \sum_{i=0}^{n-2} |\varphi_{i+1} - \Delta\varphi_i|^2.$$

It follows that from property (5)

(98)

$$R_{N}(L^{*}) \leq 4 \sup_{\boldsymbol{v}_{\theta} \in \mathcal{F}_{\text{ReCU},m}} \|\mathcal{P}^{*}\boldsymbol{v}_{\theta} - \boldsymbol{f}\|_{L^{\infty}(\Omega)} \Big(R_{N}(f) + \sum_{i=1}^{m} \sum_{j=1}^{d} |\boldsymbol{a}_{i}| |W_{i,j}|^{2} R_{N} \big(\sigma^{(2)}(\mathcal{G})\big) \Big).$$

According to the definition of the neural network and (96), we have

$$\sup_{\boldsymbol{v}_{\theta}\in\mathcal{F}_{\operatorname{ReCU},m}} \|\mathcal{P}^*\boldsymbol{v}_{\theta} - \boldsymbol{f}\|_{L^{\infty}(\Omega)} \leq C \|\boldsymbol{u}^*\|_{\mathcal{B}^{2m+3}},$$

and

$$\sum_{j=1}^{d} \sum_{i=1}^{m} |\boldsymbol{a}_{i}| |W_{i,j}|^{2} R_{N}(\sigma^{(2)}(\mathcal{G})) \leq \sum_{i=1}^{m} d|\boldsymbol{a}_{i}| ||W_{i}||_{2}^{2} R_{N}(\sigma^{(2)}(\mathcal{G}))$$
$$\leq C d ||\boldsymbol{u}^{*}||_{\mathcal{B}^{2m+3}} R_{N}(\mathcal{G}),$$

where the last inequality holds by the property (4). Combining lemma A.4, it yields that

(99)
$$R_N(L^*) \le C\sqrt{\frac{2d^3 \log d}{N}} \|u^*\|_{\mathcal{B}^{2m+3}}^2.$$

Moreover, we estimate the function classes $L_{b,\alpha}^*$ with respect to the boundary conditions. In the same manner, for $\alpha = D$, we have

(100)
$$R_{\widehat{N}}(L_{\alpha}^*) \leq 4 \sup_{\boldsymbol{v}_{\theta} \in \mathcal{F}_{\operatorname{ReCU},m}} \|S_{\alpha}\boldsymbol{v}_{\theta} - \boldsymbol{g}_{\alpha}\|_{L^{\infty}} (R_{\widehat{N}}(\mathcal{F}_{\operatorname{ReCU},m}) + R_{\widehat{N}}(\boldsymbol{g}_{\alpha})),$$

39

where use the fact (96) to get

(101)
$$\sup_{\boldsymbol{v}_{\theta} \in \mathcal{F}_{\operatorname{ReCU},m}} \|S_{\alpha} \boldsymbol{v}_{\theta} - \boldsymbol{g}_{\alpha}\|_{L^{\infty}} \leq C \|\boldsymbol{u}^*\|_{\mathcal{B}^{2m+3}}.$$

Therefore, Combining lemma A.4 and A.5, we deduce that

(102)
$$R_{\widehat{N}}(L^*_{\alpha}) \le C_{\sqrt{\frac{2d\log d}{\widehat{N}}}} \|u^*\|^2_{\mathcal{B}^{2m+3}}$$

Hence taking $\widehat{N} = \frac{N}{d^2}$ will not change the upper bound of the Rademacher complexity. The situation for other boundary conditions can be obtained similarly.

School of Mathematical Sciences, Soochow University, Suzhou, 215006, China

Email address: mjbai@stu.suda.edu.cn

SCHOOL OF MATHEMATICAL SCIENCES AND SUZHOU INSTITUTE FOR ADVANCED RE-SEARCH, UNIVERSITY OF SCIENCE AND TECHNOLOGY OF CHINA, SUZHOU, 215123, CHINA *Email address:* jingrunchen@ustc.edu.cn

SCHOOL OF MATHEMATICAL SCIENCES AND MATHEMATICAL CENTER FOR INTERDIS-CIPLINARY RESEARCH, SOOCHOW UNIVERSITY, SUZHOU, 215006, CHINA *Email address*: durui@suda.edu.cn

Institute of Analysis and Scientific Computing, TU Wien, Wiedner Hauptstraße $8{-}10,\ 1040$ Wien, Austria

Email address: zhiwei.sun@asc.tuwien.ac.at