A posteriori error estimates for space-time IgA approximations to parabolic initial boundary value problems

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Abstract

The paper is concerned with stabilised space-time approximations for initial boundary value problems of the parabolic type. These approximations have been presented and studied by Langer, Neumüller, and Moore (2016), who have shown that they satisfy standard a priori error estimates. The goal of this paper is to deduce a posteriori error estimates and investigate their applicability to IgA space-time approximations. The derivation is based on purely functional arguments and, therefore, the estimates do not contain mesh dependent constants and are valid for any approximation from the admissible (energy) class. In particular, they imply estimates for discrete norms associated with IgA approximations. We establish different forms of a posteriori error majorants and prove equivalence of them to the energy error norm. This property justifies efficiency and reliability of a posteriori error estimates. Another important property of the estimates is their flexibility with respect to several free parameters. Using these parameters, we can obtain estimates for different error norms and minimise the respective majorant in order to find the best possible bound of the error.

1 Introduction

Time-dependent systems governed by parabolic equations arise in various scientific and engineering applications, for instance, processes with slow evolution such as heat conduction and diffusion, changing in time processes in life and social sciences, etc. Analytic and numerical treatment of this class of problems involve several complications due to possible non-linearities of the studied processes, instabilities of numerical schemes causing blow-ups in simulations, and increasing an amount of data due to extra dimensionality. Therefore, remaining open questions (from theoretical as well as applied viewpoints) have triggered active investigations of such models in mathematical and numerical modelling and large-scale scientific computing.

Time-stepping methods, which have become quite popular in industrial software packages, allow combining various discretisation techniques in space (e.g., finite element method, finite difference method, finite volume method) with marching in time. Usually, it is common to distinguish between two different time-stepping methods, i.e., horizontal and vertical methods of lines. In the first one, also known as Rothe’s method, one starts from discretisation w.r.t. time variable [37], whereas the vertical method performs first the discretisation in space and then in time [68]. For both of these approaches, development of efficient and fully adaptive schemes becomes complicated because of the separation of time and space discretisations. It also affects negatively the parallelisation of the solver due to the curse of sequentiality.

Due to the fast development of parallel computers with hundreds of thousands of cores, treating time as yet another dimension in space in the evolutionary equations became quite natural. Moreover, space-time approach does not have the above-mentioned drawbacks of time-marching schemes. On the contrary, it becomes quite advantageous when efficient parallel methods and their implementation on massively parallel computers are concerned. The simplest ideas for space-time solvers are based on time-parallel integration techniques for ordinary differential equations (the comprehensive overview on the history of this approach can be found in [17]). Time-parallel multigrid methods for parabolic problems have also a long history starting from the first introduction in [21]. Later, parallel multigrid waveform relaxation methods for parabolic initial boundary value problem (I-BVPs) was presented in [41]. The study on convergence behaviour of these time-parallel multigrid methods by means of Fourier mode...
Various approximation methods have been recently developed for space-time formulation of I-BVPs. In particular, $h$-$p$ versions of the finite element method in space with $p$ and $h$-$p$ approximations in time for parabolic I-BVPs have been originally presented in \cite{2,3}, respectively. Wavelet methodology was extended to space-time adaptive schemes in \cite{58}. Uniform stability of abstract Petrov-Galerkin discretisations of boundedly invertible operators and their applicability to space-time discretizations of linear parabolic problems is discussed in \cite{48}. Error bounds for reduced basis approximation to linear parabolic problems were proved in \cite{69}, and in \cite{64} conforming space-time finite element approximations for the same class of problems was investigated.

Increasing popularity of space-time methods has generated new methods of solving complicated engineering problems such as fluid-structure interaction, aerodynamics problems, and cardiac electro-mechanics (see \cite{66,65,26}, and the references therein). These results only confirm the great potential of space-time methods for solving time-dependent problems, models with growing and shrinking in time domains, and objects with moving boundaries or interfaces.

In this paper, we use the method presented in \cite{38}, based on special time-upwind test functions motivated by the space-time streamline diffusion method introduced in \cite{22,24,25}. IgA framework provides approximations of high accuracy and flexibility due to a high smoothness of the respective basis functions (B-splines, NURBS, or localised splines; see, e.g., \cite{67,66}). Therefore, the method presented in \cite{38}, combining full space-time approach with IgA technologies, is a pioneering work into the direction of efficient fully-adaptive and heavily parallelised schemes aiming to tackle problems oriented to industrial applications.

Investigation of effective adaptive refinement methods is highly important for the construction of fast and efficient solvers for partial differential equations (PDEs). In space-time methods (as in many others), the aspect of scheme localisation is strongly linked with reliable and quantitatively efficient a posteriori error estimation (the general overview on error estimators can be found in, e.g., monographs \cite{1,12}). In other words, adaptive algorithms rely on a posteriori error estimation tools, which suppose to identify those areas of the considered computational domain, where the approximation error is substantially higher than on the rest of it. A smart combination of solvers and error indicators makes the refinement step fully automated to the characteristics of the problem (external forces, geometries, etc.) providing at the same time discretisations with the desired accuracy in terms of the output quantity of the interest. Moreover, such automation becomes quite essential in the generation of the mesh suitable to a complicated geometry, by using an efficient refinement procedure and adapting the initial design representations.

Due to a tensor-product setting of IgA splines, mesh refinement has global effects, including a large percentage of superfluous control points in data analysis, unwanted ripples on the surface, etc. Arising from these challenges with the design process as well as complications in handling big amount of corresponding data naturally have triggered the development of local refinement strategies for IgA. There are at least three different approaches to achieve local refinements. The first one, so-called truncated B-splines (T-splines), was introduced in \cite{62,61} and analysed in \cite{6,7,59,60}. It is based on T-mesh that allows eliminating the redundant control points from NURBS model. The study of this approach has confirmed to generate efficient local refinement algorithm for analysis-suitable T-splines, which avoids excessive propagation of control points. An alternative approach, that allows local control of the refinement, is based on truncated hierarchical B-splines (THB-splines). The procedure to construct a basis of the hierarchical spline space was suggested in \cite{30} and extended in \cite{72,20}. Unlike T-spline localisation algorithm that does not eliminate the unwanted propagation of the refinement, no such propagation is observed for THB-splines (the corresponding examples can be found in \cite{51,28}). The third group of locally defined splines is called locally refined splines (LR-splines) and have been developed in \cite{13} and \cite{9}.

Local refinement techniques in IgA have been combined with various a posteriori error estimation approaches. For instance, a posteriori error estimates using the hierarchical bases (i.e., saturation assumption on the enlarged underlying space and the constants in the strengthened Cauchy inequality) was investigated in \cite{14,72}. However, according to the original paper on this method \cite{4}, the validity of this assumption depends strictly on the considered example. Moreover, an accurate estimation of constants in the strengthened Cauchy inequality requires the solution of generalised minimum eigenvalue problem, which might become quite technical. In \cite{28,73,10}, and \cite{16}, residual-based a posteriori error estimators and their modifications were exploited in order to construct efficient automated mesh refinement algorithms. These estimates require computation of constants related to Clement-type interpolation operators, which are mesh dependent. Finally, goal-oriented error estimators based on auxiliary global refinement...
steps have been considered in [70] [11] [32] [33]. Below, we use a different (functional) method that provides fully guaranteed error estimates in the various weighted norms equivalent to the global energy norm. The estimates include only global constants (independent of the mesh characteristic \( h \)) and are valid for any approximation from the admissible functional space.

Functional error estimates (so-called majorants and minorants) were originally introduced in [55] [56] [57] [53] and later applied to different mathematical models (see the monographs [52] [42]). They provide guaranteed, sharp, and fully computable upper and lower bounds of errors. This approach to error control was applied to IgA schemes in [29], where it was confirmed that the majorants also provide not only reliable and efficient upper bounds of the total energy error but a quantitatively sharp indicator of local errors.

In this paper, we deduce and study functional type a posteriori error estimates for time-dependent problems [53] in the context of the space-time IgA scheme [38]. By exploiting the universality and efficiency of the considered error estimates as well as taking an advantage of smoothness of the obtained approximations, one can construct fully adaptive fast and efficient parallelised space-time method that could tackle complicated problems inspired by industrial applications.

This paper is organised as follows: Section 2 defines the problem and its variational formulation. It also introduces the notation and some special functional spaces used throughout the paper. An overview of main ideas and definitions used in the IgA framework can be found in the subsequent section. Section 4 presents the stabilised space-time IgA scheme and establishes its main properties. In Section 5 we introduce new a posteriori error estimates on a functional type using the ideas coming from stabilised formulation of parabolic I-BVPs. Theorems 2 and 3 present two different forms of the estimates that rely on different regularity assumptions for the approximate solution and auxiliary flux. Consequently, Corollaries 1 and 2 present majorants that are tailored to the space-time IgA scheme presented in Section 4. Finally, Section 6 introduces the advanced form of the majorants (derived in Theorems 2 and 3) and shows the equivalence of these modified functional estimates to the error measured in the energy norm.

## 2 Model Problem

Let \( \overrightarrow{Q} := Q \cup \partial Q \), \( Q := \Omega \times (0, T) \), denote the space-time cylinder, where \( \Omega \subset \mathbb{R}^d \), \( d \in \{1, 2, 3\} \), is a bounded Lipschitz domain with boundary \( \partial \Omega \), and \( (0, T) \) is a given time interval, \( 0 < T < +\infty \). Here, the cylindrical surface is defined as \( \partial Q := \Sigma = \Sigma_0 \cup \Sigma_T \) with \( \Sigma = \partial \Omega \times (0, T) \), \( \Sigma_0 = \Omega \times \{0\} \) and \( \Sigma_T = \Omega \times \{T\} \). In order to avoid non-principal technical difficulties and present the main ideas in the most transparent form, we discuss our approach to guaranteed error control of space-time approximations with the paradigm of the classical linear parabolic initial-boundary value problem: find \( u : \overrightarrow{Q} \to \mathbb{R} \) satisfying the system

\[
\begin{align*}
\partial_t u - \Delta_x u &= f & \text{in } Q, \\
u &= 0 & \text{on } \Sigma, \\
u &= u_0 & \text{on } \Sigma_0,
\end{align*}
\]

where \( \partial_t \) denotes the time derivative, \( \Delta_x \) is the Laplace operator in space, \( f \in L^2(Q) \) is a given source function, and \( u_0 \in H^1_0(\Sigma_0) \) is a given initial state, satisfying zero boundary condition on \( \partial \Sigma_0 = \partial \Omega \times \{0\} \). Here, \( L^2(Q) \) denotes the space of square-integrable functions over \( Q \). The respective norm and scalar product are denoted by \( \| v \|_Q := \| v \|_{L^2(Q)} \) and \( \langle v, w \rangle_Q := \int_Q v(x, t)w(x, t)\,dxdt, \forall v, w \in L^2(Q) \), respectively, with similar notation used for spaces of vector-valued fields.

By \( H^k(Q), k \geq 1 \), we denote spaces of functions having generalised square-summable derivatives of the order \( k \) with respect to (w.r.t.) space and time. Next, we introduce the following Sobolev spaces:

\[
\begin{align*}
V_0 := H^1_0(Q) := \left\{ u \in H^1(Q) : u = 0 \text{ on } \Sigma, \right\}, \\
H^1_0(Q) := \left\{ u \in H^1(Q) : u = 0 \text{ on } \Sigma_T, \right\}, \\
H^1_0(\Sigma_0) := \left\{ u \in H^1(Q) : u = 0 \text{ on } \Sigma_0, \right\}, \\
V_0^\Delta := H^1_0(Q) := \left\{ u \in H^1_0(Q) : \Delta_x u \in L^2(Q), \right\},
\end{align*}
\]

and

\[
H^s_0(Q) := H^s(Q) \cap H^1_0(Q),
\]

where \( s \in \mathbb{R} \).

3
In addition, we introduce Hilbert spaces for auxiliary vector-valued functions (which are used in the derivation of the a posteriori error estimates):

$$H^{\text{div}, 0}(Q) := \left\{ y \in [L^2(Q)]^d : \text{div}_x y \in L^2(Q) \right\}$$

and

$$H^{\text{div}, 1}(Q) := \left\{ y \in [L^2(Q)]^d : \text{div}_x y \in L^2(Q), \partial_t y \in [L^2(Q)]^d \right\}.$$  

These spaces are supplied with the natural norm and semi-norm

$$\| y \|_{H^{\text{div}, 0}}^2 := \| \text{div}_x y \|_{Q}^2$$

and

$$\| y \|_{H^{\text{div}, 1}}^2 := \| \text{div}_x y \|_{Q}^2 + \| \partial_t y \|_{Q}^2.$$  

In what follows, $C_F$ denotes the constant in the Friedrichs inequality

$$\| w \|_Q \leq C_F \| \nabla_x w \|_Q, \quad \forall w \in H^{1,0}_0(Q) := \left\{ u \in L^2(Q) : \nabla_x u \in [L^2(Q)]^d, u = 0 \text{ on } \Sigma \right\}.$$  

It is also well-known that if $f \in L^2(Q)$ and $u_0 \in H^1_0(\Sigma_0)$, the problem (14–16) is uniquely solvable in $V^\Delta_x$, and the solution $u$ depends continuously on $f$ in the norm $H^1_0(\Omega)$ (see, e.g., [34] and [36, Theorem 2.1]). Moreover, according to [36, Remark 2.2], $\| u_x(\cdot, t) \|_Q^2$ is an absolutely continuous function of $t \in [0, T]$ for any $u \in V^\Delta_x$. If the initial condition $u_0 \in L^2(\Sigma_0)$, then the problem has a unique solution $u \in H^{1,0}_0(Q)$, that satisfies the generalised statement of the problem

$$a(u, w) = l(w), \quad \forall w \in H^{1,0}_0(Q),$$

with the bilinear form

$$a(u, w) := (\nabla_x u, \nabla_x w)_{Q} - (u, \partial_t w)_Q,$$

and the linear functional

$$l(w) := (f, w)_Q + (u_0, w)_{\Sigma_0}.$$  

Here and later on $(u_0, w)_{\Sigma_0} := \int_{\Sigma_0} u_0(x) w(x, 0) dx = \int_{\Omega} u_0(x) w(x, 0) dx$. According to the well-establish arguments (see [34] [35] [74]), without loss of generality, we homogenise the problem, i.e., consider the problem with zero initial conditions $u_0 = 0$.

In order to be able to provide efficient discretisation method, we introduce a stabilised weak formulation of (11) with time-upwind test functions

$$\lambda w + \mu \partial_t w, \quad w \in V^\Delta_x := \left\{ w \in V_0^\Delta : \nabla_x \partial_t w \in L^2(Q) \right\}, \quad \lambda, \mu \geq 0.$$  

where $\lambda$ and $\mu$ are positive constants. We arrive at the following space-time formulation [22] [24] [25]: find $u \in V_0$ satisfying

$$a_s(u, w) = l_s(w), \quad \forall w \in V_0,$$

where

$$a_s(u, w) := (\partial_t u, \lambda w + \mu \partial_t w)_Q + (\nabla_x u, \nabla_x (\lambda w + \mu \partial_t w))_Q$$

and

$$l_s(w) := (f, \lambda w + \mu \partial_t w)_Q.$$  

**Remark 1** Notice that the approach presented in this paper (related to approximations and a posteriori error estimates) can be extended to more general parabolic equations, e.g., to those containing the term $\text{div}_x (D(x, t)\nabla_x u(x, t))$ (where $D(x, t)$ is a positive definite matrix of diffusion coefficients) instead of $\Delta_x u(x, t)$ in (11).

Our main goal is to derive fully computable estimates for space IgA approximations of this class of the problems. For this purpose, we use the functional approach to a posteriori error estimates. Initially, their simplest form have been obtained for a heat equation in [53]. In [16], these estimates have been tested for generalised diffusion equation with a focus on an algorithmic part as well as on the comparison of two different forms of majorants. Evolutionary convection-diffusion equations and majorants for the approximations with jumps with respect to time variable has been considered in the paper [54]. Finally, functional a posteriori error estimates for parabolic time-periodic BVPs as well as for optimal control problems have been studied in [39] and [40].
This approach has been extended to a wide class of problems. Paper [16] analyses the robustness of the majorant in the cases with drastic changes in values of the reaction parameter in reaction-diffusion time-dependent problems. It also discusses the quality of the indicator that follows from the functional error estimate. Moreover, it introduces the minorant of the error that is tested in several numerical examples and compared to the majorant. In order to make the estimates applicable to problems in domains with complicated geometry, the domain decomposition technique in combination with local Poincaré inequalities can be used (see [14]). The question on the constants in above-mentioned local inequalities is addressed in [47], where sharp bounds of them have been found for some simplexes that are typically used in numerical methods. Numerical properties of above-mentioned error estimates w.r.t. the time-marching and space-time method are discussed in [43].

3 Overview of the IgA framework

For the convenience of the reader, we first recall the general concept of the IgA approach, the definition of B-splines (NURBS) and their use in the geometrical representation of the space-time cylinder $Q$, as well as the construction of the IgA trial spaces, which are used to approximate solutions satisfying the variational formulation of (6).

Let $p \geq 2$ be a polynomial degree and $n$ denote the number of basis functions used to construct a $B$-spline curve. The knot-vector in one dimension is a non-decreasing set of coordinates in the parameter domain, written as $\Xi = \{\xi_1, \ldots, \xi_{n+p+1}\}, \xi_i \in \mathbb{R}$, where $\xi_1 = 0$ and $\xi_{n+p+1} = 1$. The knots can be repeated, and the multiplicity of the $i$-th knot is indicated by $m_i$. Throughout the paper, we consider only open knot vectors, i.e., the multiplicity of the first and the last knots are equal to $m_1 = m_{n+p+1} = p+1$. For example, for the one-dimensional parametric domain $\hat{Q} = (0, 1)$, there is an underlying mesh $\hat{K}_h$ of elements $\hat{K} \in \hat{K}_h$, such that each of them is constructed by the distinct neighbouring knots. The global size of $\hat{K}_h$ is denoted by

$$\hat{h} := \max_{\hat{K} \in \hat{K}_h} \{\hat{h}_{\hat{K}}\}, \quad \text{where} \quad \hat{h}_{\hat{K}} := \text{diam}(\hat{K}).$$

For the time being, we assume locally quasi-uniform meshes, i.e., the ratio of two neighbouring elements $\hat{K}_i$ and $\hat{K}_j$ satisfies the inequality $c_1 \leq \frac{h_{\hat{K}_i}}{h_{\hat{K}_j}} \leq c_2$, where $c_1, c_2 > 0$.

The univariate B-spline basis functions $\hat{B}_{i,p} : \hat{Q} \rightarrow \mathbb{R}$ are defined by means of Cox-de Boor recursion formula as follows:

$$\hat{B}_{i,p}(\xi) := \begin{cases} \frac{\xi - \xi_i}{\xi_{i+p} - \xi_i} \hat{B}_{i,p-1}(\xi) + \frac{\xi_{i+p+1} - \xi}{\xi_{i+p+1} - \xi_{i+1}} \hat{B}_{i+1,p-1}(\xi), & \text{if } \xi_i \leq \xi \leq \xi_{i+1}, \\ 0 & \text{otherwise}, \end{cases} \quad \hat{B}_{i,0}(\xi) := \begin{cases} 1 & \xi = \xi_i, \\ 0 & \text{otherwise}, \end{cases} \quad (13)$$

where a division by zero is defined to be zero. One of the most crucial properties of these basis functions is that they are $(p-m_i)$-times continuously differentiable across the $i$-th knot with multiplicity $m_i$. Hence, if, for instance, $m_i = 1$ for every inner knot, B-splines of a degree $p$ are $C^{p-1}$ continuous. For the knots lying on the boundary of the parametric domain, where the multiplicity is $p+1$, the B-spline is discontinuous ($C^{-1}$ function). We note, that analysis of this paper is only concerned with a single-patch domain. The extension to the multi-patch case (the case, in which the physical domain is decomposed into several simple patches) will be a focus of a subsequent paper.

Consider also the multivariate B-splines on the space-time parameter domain $\hat{Q} := (0, 1)^{d+1}, \ d = \{1, 2, 3\}$, as a tensor-product of the corresponding univariate B-splines basis functions. For that, we define the knot vector dependent on the space-time direction $\Xi^\alpha = \{\xi_1^\alpha, \ldots, \xi_{n+p+1}^\alpha\}, \xi_i^\alpha \in \mathbb{R}$, where $\alpha = 1, \ldots, d+1$ is the index indicating the direction in space or time. Furthermore, we introduce the set of multi-indices

$$\mathcal{I} = \{ i = (i_1, \ldots, i_{d+1}) : i_\alpha = 1, \ldots, n_\alpha; \alpha = 1, \ldots, d+1 \},$$

and multi-indices standing for the order of polynomials $p := (p_1, \ldots, p_{d+1})$. The tensor-product of the univariate B-spline basis functions generates multivariate B-spline basis functions

$$\hat{B}_{i,p}(\xi) := \prod_{\alpha=1}^{d+1} \hat{B}_{i_\alpha,p_\alpha}(\xi^\alpha), \quad \text{where} \quad \xi = (\xi^1, \ldots, \xi^{d+1}) \in \hat{Q}. \quad (14)$$

The univariate and multivariate NURBS basis functions are defined in the parametric domain by means of the corresponding B-spline basis functions $\{\hat{B}_{i,p}\}_{i \in \mathcal{I}}$. For given $p := (p_1, \ldots, p_{d+1})$ and for any $i \in \mathcal{I}$, we define the
NURBS basis functions $\tilde{R}_{i,p}$ as follows:

$$\tilde{R}_{i,p} : \widehat{Q} \rightarrow \mathbb{R}, \quad \tilde{R}_{i,p}(\xi) := \frac{w_i \tilde{B}_{i,p}(\xi)}{W(\xi)},$$

(15)

with a weighting function

$$W : \widehat{Q} \rightarrow \mathbb{R}, \quad W(\xi) := \sum_{i \in \mathcal{I}} w_i \tilde{B}_{i,p}(\xi),$$

(16)

where $w_i$ are positive real numbers.

The physical space-time domain $Q \subset \mathbb{R}^{d+1}$ is defined from the parametric domain $\widehat{Q} = (0,1)^{d+1}$ by the geometrical mapping:

$$\Phi : \widehat{Q} \rightarrow Q := \Phi(\widehat{Q}) \subset \mathbb{R}^{d+1}, \quad \Phi(\xi) := \sum_{i \in \mathcal{I}} \tilde{R}_{i,p}(\xi) P_i,$$

(17)

where $\{P_i\}_{i \in \mathcal{I}} \in \mathbb{R}^{d+1}$ are the control points. For simplicity, we assume below the same polynomial degree for all coordinate directions, i.e., $p_\alpha = p$ for all $\alpha = 1, \ldots, d + 1$.

By means of latter geometrical mapping (17), the physical mesh $\mathcal{K}_h$ is defined on the space-time domain $Q$, whose elements are images of elements of $\widehat{\mathcal{K}}_h$, i.e., $\mathcal{K}_h := \{ K = \Phi(\widehat{K}) : \widehat{K} \in \widehat{\mathcal{K}}_h \}$. The global mesh size is denoted by

$$h := \max_{K \in \mathcal{K}_h} \{ h_K \}, \quad h_K := \| \nabla \Phi \|_{L^\infty(K)} h_{\widehat{K}}.$$

(18)

Moreover, we assume that the physical mesh is also quasi-uniform, i.e., there exists a positive constant $C_u$ independent of $h$, such that

$$h_K \leq h \leq C_u h_K.$$

(19)

The discretisation spaces on $Q$ are constructed by a push-forward of the NURBS basis functions

$$V_h := \text{span} \{ \phi_{h,i} := \tilde{R}_{i,p} \circ \Phi^{-1} \}_{i \in \mathcal{I}},$$

(20)

where we assume that the geometrical mapping $\Phi$ is invertible in $Q$, with smooth inverse on each element $K \in \mathcal{K}_h$ (see [64] and [5] for more details). Moreover, we introduce the subspaces

$$V_{0h} := V_h \cap V_{0,\widehat{Q}}$$

for the functions fulfilling homogeneous boundary condition.

Let us recall two fundamental inequalities, i.e., scaled trace and inverse inequalities, that are important for the derivation of a priori error estimates of the space-time IgA scheme presented in the further sections.

**Lemma 1** [15, Theorem 3.2] Let $K \in \mathcal{K}_h$, then the scaled trace inequality

$$\| v \|_{\partial K} \leq C_{tr} h_K^{-1/2} (\| v \|_K + h_K \| \nabla_x v \|_K)$$

(21)

holds for all $v \in H^1(K)$, where $h_K$ is the diameter of the element $K \in \mathcal{K}_h$, and $C_{tr}$ is a positive constant independent of $K \in \mathcal{K}_h$.
Lemma 2 [5, Theorem 4.1] and [15, Theorem 4.2] Let $K \in K_h$, then the inverse inequalities

$$\|\nabla v_h\|_K \leq C_{inv,1} h^{-1}_K \|v_h\|_K$$

(22)

and

$$\|v_h\|_{\partial K} \leq C_{inv,0} h^{-1/2}_K \|v_h\|_K$$

(23)

hold for all $v_h \in V_h$, where $C_{inv,0}$ and $C_{inv,1}$ are positive constants independent of $K \in K_h$.

Remark 2 Inequality (22) yields inequalities with partial derivatives in space and time

$$\|\partial_x v_h\|_K \leq C_{inv,1} h^{-1}_K \|v_h\|_K, \quad i = 1, \ldots, d, \quad \text{and} \quad \|\partial_t v_h\|_K \leq C_{inv,1} h^{-1}_K \|v_h\|_K,$$

(24)

since $\nabla v_h = (\nabla_x v_h, \partial_t v_h)$. Nevertheless, for the anisotropic case (w.r.t. to spatial and time derivatives) the constant $C_{inv,1}$ will depend on the direction, i.e.,

$$\|\partial_x v_h\|_K \leq C_{inv,1}^x h^{-1}_K \|v_h\|_K \quad \text{and} \quad \|\partial_t v_h\|_K \leq C_{inv,1}^t h^{-1}_K \|v_h\|_K.$$

(25)

Remark 3 Due to the higher smoothness of basis functions ($p \geq 2$), the obtained approximations are generally $C^{p-1}$-continuous, provided that the inner knots have the multiplicity 1. Moreover, basis functions of degree $p \geq 2$ are at least $C^1$-continuous if the multiplicity of the inner knots is less than or equal to $p-1$. This automatically implies that their gradients are in $H^{div,0}(Q)$. Therefore, there is no need for constructing the projection of $\nabla_x u_h \in [L^2(Q)]^d$ into $H^{div,0}(Q)$.

4 Discretisation of stabilised weak formulation

Stable space-time IgA scheme for parabolic equations have been presented and analysed in [38], where the authors proved its efficiency for fixed and moving spatial computational domains. In particular, it was shown that the corresponding discrete bilinear form is elliptic on the IgA space (w.r.t. a discrete energy norm), bounded, consistent. Moreover, the approximation results for the IgA spaces yields an a priori discretisation error estimate w.r.t. the same norm. In our work, we consider slightly modified energy norm and prove that the same properties of the scheme remain valid.

We assume that the used spline-basis have a sufficiently high order, such that

$$w_h \in V_{0h} \subset V_{0,q}$$

(26)

In order to derive a stable discrete IgA space-time scheme for (15), we set the parameters in (11) to $\lambda = 1$ and $\mu = \delta_{s,h} = \theta h$, where $\theta$ is a positive constant and $h$ is the mesh-size defined in (13), such that

$$w_h + \delta_{s,h} \partial_t w_h, \quad \delta_{s,h} = \theta h, \quad w_h \in V_{0h}.$$  

(27)

Hence, (12) implies the discrete stabilised space-time problem: find $u_h \in V_{0h}$ satisfying

$$a_{s,h}(u_h, w_h) = l_h(w_h), \quad \forall w_h \in V_{0h},$$

(28)

where

$$a_{s,h}(u_h, w_h) := (\partial_t u_h, w_h)_Q + \delta_{s,h} (\partial_t u_h, \partial_t w_h)_Q + (\nabla_x u_h, \nabla_x w_h)_Q + \delta_{s,h} (\nabla_x u_h, \partial_t (\nabla_x w_h))_Q$$

and

$$l_h(v_h) := (f, w_h + \delta_{s,h} \partial_w v_h)_Q.$$  

$V_{0h}$-coercivity of $a_{s,h}(\cdot, \cdot) : V_{0h} \times V_{0h} \to \mathbb{R}$ w.r.t. the norm

$$\|v_h\|_{a,h}^2 := \|\nabla_x v_h\|_2^2 + \delta_{s,h} \|\partial_t v_h\|_0^2 + \|v_h\|_{\Sigma_T}^2 + \delta_{s,h} \|\nabla_x v_h\|_{\Sigma_T}^2,$$

(29)

follows from Lemma below.

Lemma 3 The form $a_{s,h}(\cdot, \cdot) : V_{0h} \times V_{0h} \to \mathbb{R}$ is strongly $V_{0h}$-coercive w.r.t. the norm $\|\cdot\|_{a,h}^2$, i.e., there exists a positive constant $\mu_c$ such that

$$a_{s,h}(w_h, w_h) \geq \mu_c \|w_h\|_{a,h}^2, \quad \forall w_h \in V_{0h},$$

where $\mu_c = \frac{4}{7}$.  

7
Proof: By considering \( a_{s,h}(w, w) \), we arrive at
\[
a_{s,h}(w_h, w_h) = \lambda \| \nabla_x w_h \|_Q^2 + \mu \| \partial_t w_h \|_Q^2 + \frac{1}{2} \| w_h \|_{\Sigma_T}^2 + \frac{1}{2} \| \nabla_x w_h \|_{\Sigma_T}^2 \geq \frac{1}{2} \| w_h \|_{s,h}^2.
\]

The latter property implies the existence and uniqueness of the discrete solution \( u_h \in V_{0h} \), which can be written as
\[
u_h(x, t) = u_h(x_1, ..., x_d, x_{d+1}) := \sum_{i \in I} \phi_{h,i}.
\]

Here, \( u_h := [\phi_{h,i}]_{i \in I} \in R^{|I|} \) is a vector of unknowns (degrees of freedom) defined by a system of equations
\[
K_h u_h = f_h
\]
with the matrix \( K_h := [K_{h,ij} = a_{s,h}(\phi_{h,i}, \phi_{h,j})]_{i,j \in I} \) and the right-hand side (RHS) \( f_h := [f_{h,i} = l_i(\phi_{h,i})]_{i \in I} \in R^{|I|} \) (generated by IgA discretisation for elliptic problems). From Lemma 3, it also follows that the matrix \( K_h \) is regular (the condition number of \( K_h \) is bounded by a constant independent of \( h \)).

Several results, crucial for an a priori error estimation, can be shown using [33, Lemma 2, 3].

Lemma 4 The bilinear form \( a_{s,h}(\cdot, \cdot) \) is uniformly bounded on \( V_{0h,*} \times V_{0h} \), where \( V_{0h,*} := H^2_0(Q) + V_{0h} \), i.e.,
\[
|a_{s,h}(w, w_h)| \leq \mu_h \| w \|_{s,h}^2 \| w_h \|_{s,h}^2, \quad \forall v \in V_{0h,*}, \forall v_h \in V_{0h},
\]

where
\[
\| w \|_{s,h}^2 := \| w \|_h^2 + \delta_{s,h}^{-1} \| w \|_Q^2, \quad \forall w \in V_{0h,*},
\]
and \( \mu_h \) is a positive constant, independent of \( h \).

Proof: The proof follows the lines of the proof in [33], where \( |a_{s,h}(w, w_h)| \) is estimated term by term. First, we integrate \( (\partial_t w, w_h)_Q \) by parts, i.e.,
\[
(\partial_t w, w_h)_Q = (w_h, \partial_t w)_\Sigma_T - (w, \partial_t w_h)_Q,
\]
and then estimate each of the terms in the RHS of (30) by the Hölder inequality:
\[
(\partial_t w, w_h)_Q - (w, \partial_t v_h)_Q \leq \left( \| w \|_{\Sigma_T}^2 + \| \nabla_x w \|_{\Sigma_T}^2 \right)^{1/2} \left( \| w \|_{\Sigma_T}^2 + \| \nabla_x w \|_{\Sigma_T}^2 \right)^{1/2} \left( \delta_{s,h} \| \partial_t w_h \|_Q^2 \right)^{1/2}.
\]
The second and the third terms in \( a_{s,h}(w, w_h) \) are estimated analogously, whereas for the forth term, [33] suggests applying the inverse inequality (22) and the condition for quasi-uniform meshes introduced in (19). If we summarise all the estimates and use the fact that both \( \delta_{s,h} \| \nabla_x w_h \|_{\Sigma_T} \) and \( \delta_{s,h} \| \nabla_x w \|_{\Sigma_T} \) are positive quantities (which can be added to the RHS), we arrive at the relation
\[
|a_{s,h}(w, w_h)| \leq \left( \| w \|_{\Sigma_T}^2 + \| \nabla_x w \|_{\Sigma_T}^2 \right)^{1/2} \left( \| w \|_{\Sigma_T}^2 + \| \nabla_x w \|_{\Sigma_T}^2 \right)^{1/2} \left( \delta_{s,h} \| \partial_t w_h \|_Q^2 \right)^{1/2} + \left( C_u^2 C_{inv,1}^2 \theta^2 \| \nabla_x w_h \|_Q^2 \right)^{1/2}
\]
\[
\leq \mu_h \| w \|_{s,h}^2 \| w_h \|_h,
\]
where \( \mu_h = \left( \max \left( 1 + C_u^2 C_{inv,1}^2 \theta^2, 2 \right) \right)^{1/2} \).

For the completeness, it is worth recalling basic results on the approximation properties of spaces generated by B-splines (NURBS) that follow from [3] Section 3] and [64] Section 4]. They state the existences of a projection operator \( \Pi_h : H^1_0(Q) \rightarrow V_h \), \( s \in \mathbb{N}, s \geq 0 \), that provide the asymptotically optimal approximation result.
Lemma 5 Let \( l, s \in \mathbb{N} \) be \( 0 \leq l \leq s \leq p + 1 \), and \( w \in H_{0,\Omega}^s(Q) \). Then, there exists a projection operator \( \Pi_h : H_{0,\Omega}^s(Q) \rightarrow V_{0h} \) and a positive constant \( C_s \) such that

\[
\sum_{K \in \mathcal{T}_h} \| w - \Pi_h w \|_{H^l(K)}^2 \leq C_s^2 h^{2(s-l)} \| w \|_{H^s(Q)}^2.
\]

(31)

where \( h \) is a global mesh size defined by \([13]\) and \( C_s \) is a constant only dependent on degrees \( s, l, \) and \( p \), the shape regularity of \( Q \), described by \( \Phi \) and its gradient.

Proof: The proof follows the lines of \([5, \text{Subsection 3.3, 3.4}]\), \([64, \text{Proposition 3.1}]\), and \([8, \text{Chapter 4}]\). □

If the multiplicity of each inner knot \( m_i \leq p + 1 - l \), \( \Pi_h w \) belongs to \( H_{0,\Omega}^s(Q) \). Then, Lemma 5 yields the global estimate

\[
\| w - \Pi_h w \|_{H^l(Q)} \leq C_s h^{s-l} \| w \|_{H^s(Q)}.
\]

(32)

Both interpolation estimates \([31]\) and \([32]\) yield a priori estimates of the interpolation error \( e_h = w - \Pi_h w \), measured in terms of the \( L^2 \)-norm and the discrete norms \( \| \cdot \|_h \) and \( \| \cdot \|_{h,s} \), which we later need in order to obtain an a priori estimate for the discretisation error \( u - u_h \).

Lemma 6 Let \( l, s \in \mathbb{N} \) be \( 1 \leq l \leq s \leq p + 1 \), and \( v \in H_{0,\Omega}^s(Q) \). Then, there exists a projection operator \( \Pi_h : H_{0,\Omega}^s(Q) \rightarrow V_{0h} \) (see Lemma 5) and positive constants \( C_1, C_2, C_3, C_4 \), such that the following a priori error estimates hold

\[
\| w - \Pi_h w \|_{\partial Q} \leq C_1 h^{s/2} \| w \|_{H^s(Q)},
\]

(33)

\[
\delta_h^{1/2} \| \nabla_{x}(w - \Pi_h w) \|_{\partial Q} \leq C_2 h^{s-1} \| w \|_{H^s(Q)},
\]

(34)

\[
\| w - \Pi_h w \|_h \leq C_3 h^{s-1} \| w \|_{H^s(Q)},
\]

(35)

\[
\| w - \Pi_h w \|_{s,h} \leq C_4 h^{s-1} \| w \|_{H^s(Q)}.
\]

(36)

Proof: Estimate (33) follows straightforwardly from the proof of Lemma 6 in \([38]\). Let us show that estimate (34) holds:

\[
\delta_{s,h} \| \nabla_{x}(w - \Pi_h w) \|_{\partial Q}^2 \leq \theta h \sum_{K \in \mathcal{T}_h} \sum_{i=1}^{d} \| \partial_{x_i}(w - \Pi_h w) \|_{\partial K \cap \partial Q}^2
\]

\[
\leq 2 \theta h \sum_{K \in \mathcal{T}_h} \sum_{i=1}^{d} \left( C_{0,\text{inv}}^2 h_K^{-1} \left( \| \partial_{x_i}(w - \Pi_h w) \|_{\partial K}^2 + h_K^2 \| \partial_{x_i}(w - \Pi_h w) \|_{\partial K}^2 \right) \right)
\]

\[
\leq 2 \theta h \sum_{K \in \mathcal{T}_h} \sum_{i=1}^{d} \left( C_{0,\text{inv}}^2 C_u h^{-1} \left( \| \partial_{x_i}(w - \Pi_h w) \|_{\partial K}^2 + h^2 \| \partial_{x_i}(w - \Pi_h w) \|_{\partial K}^2 \right) \right)
\]

\[
\leq 2 C_{0,\text{inv}}^2 C_u \theta \left( \| \nabla_{x}(w - \Pi_h w) \|_{\partial Q}^2 + h^2 \sum_{j=1}^{d+1} \| \partial_{x_j}(w - \Pi_h w) \|_{\partial Q}^2 \right)
\]

\[
\leq 2 C_u \theta (1 + d(d+1)) C_{0,\text{inv}}^2 C_s^2 h^{2(s-1)} \| w \|_{H^s(Q)}^2
\]

Since \( \| \nabla_{x}(w - \Pi_h w) \|_{\Sigma_T} \leq \| \nabla_{x}(w - \Pi_h w) \|_{\partial Q} \), the relations (35) and (36) hold. □

Lemma 7 If the solution \( u \in H_{0,\Omega}^{1,0}(Q) \cap H^2(Q) \), then it satisfies the consistency identity \( a_{s,h}(u, v_h) = l_h(w_h) \), \( \forall w_h \in V_{0h} \).

Proof: The proof follows the steps of the lines of Lemma 7 in \([38]\). □

The main result of this section, namely, the a priori error estimate in the discrete norm \( \| \cdot \|_h \), is formulated in the following theorem.

Theorem 1 Let \( u \in H_{0}^s(Q) := H^s(Q) \cap H_{0,\Omega}^{1,0}(Q) \) with \( s \in \mathbb{N}, s \geq 2, \) be the exact solution of \([38]\), and let \( u_h \in V_{0h} \) be a solution of the space-time IgA scheme \([28]\) with some fixed parameter \( \theta \). Then, the discretisation error estimate

\[
\| u - u_h \|_h \leq C h^{r-1} \| u \|_{H^r(Q)}
\]

(37)

holds, where \( C \) is a constant independent of \( h \) and \( r = \min \{s, p + 1\} \).
5 Error majorant

In this section, we derive error majorants of the functional type for stabilised weak formulations of parabolic I-BVPs with time-upwind test functions. These error estimates are used to obtain a posteriori error estimates for the distance \( e = u - v \) between \( u \in V_{0,0}^{\Delta t} \) and any \( v \in V_{0,0}^{\Delta t} (V_{0,0}^{\Delta t}) \) (in particular, approximations produced by the space-time IgA method presented in the previous section) measured in terms of the norm

\[
\| e \|_{\nu_i} := \nu_1 \| \nabla_x e \|_Q^2 + \nu_2 \| \partial_t e \|_{\Sigma_T}^2 + \nu_3 \| \nabla_x e \|_{\Sigma_T}^2 + \nu_4 \| e \|_{\Sigma_T}^2,
\]  (38)

where \( \nu_i > 0, i = 1, \ldots, 4, \) are some weights (introduced throughout the derivation process).

To obtain guaranteed error bounds of (33), we apply a method similar to the one developed in [33] for parabolic I-BVPs. For the derivation process, we consider space of smoother functions \( V_{\nu_i}^{\Delta t} \) (cf. (11)) equipped with the norm

\[
\| w \|_{\nu_i} := \sup_{t \in [0,T]} \| \nabla_x w(t) \|_Q^2 + \| w \|_{\nu_i}^2,
\]

where

\[
\| w \|_{V_{\nu_i}^{\Delta t}} := \| \Delta_x w \|_Q^2 + \| \partial_t w \|_Q^2
\]

which is dense in \( V_{\nu_i}^{\Delta t} \). According to [33], Remark 2.2, norms \( \| \cdot \|_{V_{\nu_i}^{\Delta t}} \approx \| \cdot \|_{V_{\nu_i}^{\Delta t}} \).

Consider the sequence \( u_n \in V_{\nu_i}^{\Delta t} \). Then, the corresponding stabilised identity is formulated as follows:

\[
a_x(u_n, w) = (f_n, \lambda w + \partial_t w)_Q, \quad \text{where} \quad f_n = (u_n)_t - \Delta_x u_n \in L^2(Q).
\]  (39)

By subtracting \( a_x(u_n, v_n), v_n \in V_{\nu_i}^{\Delta t}, \) from (39), and by setting \( w = e_n = u_n - v_n \in V_{\nu_i}^{\Delta t} \), we arrive at the so-called ‘error-identity’

\[
\lambda \| \nabla_x e_n \|_Q^2 + \mu \| \partial_t e_n \|_Q^2 + \frac{1}{2} (\mu \| \nabla_x e_n \|_{\Sigma_T}^2 + \lambda \| e_n \|_{\Sigma_T}^2)
\]

\[
= \lambda\left( (f_n - \partial_t v_n, e_n)_Q - (\nabla_x v_n, \nabla_x e_n)_Q \right) + \mu\left( (f_n - \partial_t v_n, \partial_t e_n)_Q - (\nabla_x v_n, \nabla_x \partial_t e_n)_Q \right),
\]

which is used in the derivation of the majorants of (39) in Theorems 2 and 3.

**Theorem 2** For any \( v \in V_0^{\Delta t} \) and \( y \in H_{\text{div},0}(Q) \), the following estimate holds:

\[
(2 - \frac{1}{2}) (\lambda \| \nabla_x e \|_Q^2 + \mu \| \partial_t e \|_Q^2 + \mu \| \nabla_x e \|_{\Sigma_T}^2 + \lambda \| e \|_{\Sigma_T}^2) \leq M^T(v, y; \gamma, \alpha_i)
\]

\[
:= \gamma \left\{ \lambda \left( 1 + \alpha_1 \right) \| r_{\text{eq}} \|_Q^2 + (1 + \frac{1}{\alpha_1}) C_F^\gamma \| r_{\text{eq}} \|_Q^2 \right\} + \mu \left( (1 + \alpha_2) \| \text{div}_x r_d \|_Q^2 + (1 + \frac{1}{\alpha_2}) \| r_{\text{eq}} \|_Q^2 \right),
\]  (40)

where \( r_{\text{eq}} \) and \( r_d \) are defined by relations

\[
r_{\text{eq}}(v, y) := f - \partial_t v + \text{div}_x y \quad \text{and} \quad r_d(v, y) := y - \nabla_x v,
\]  (41)

\( C_F \) is the Friedrichs constant, \( \lambda \) and \( \mu \) are positive weights introduced in (11), \( \gamma \in [\frac{1}{2}, +\infty) \), and \( \alpha_i > 0, i = 1, 2. \)

**Proof:** The RHS of the error-identity is modified by means of the relation

\[
(\text{div}_x y, \lambda e_n + \mu \partial_t e_n)_Q + (y, \nabla_x (\lambda e_n + \mu \partial_t e_n))_Q = 0.
\]

The obtained result can be presented as follows:

\[
\lambda \| \nabla_x e_n \|_Q^2 + \mu \| \partial_t e_n \|_Q^2 + \frac{1}{2} (\mu \| \nabla_x e_n \|_{\Sigma_T}^2 + \lambda \| e_n \|_{\Sigma_T}^2)
\]

\[
= \lambda\left( (f_n - \partial_t v_n, e_n)_Q - (\nabla_x v_n, \nabla_x e_n)_Q \right) + \mu\left( (f_n - \partial_t v_n, \partial_t e_n)_Q - (\nabla_x v_n, \nabla_x \partial_t e_n)_Q \right) + \mu \left( (f_n - \partial_t v_n, \partial_t e_n)_Q - (\nabla_x v_n, \nabla_x \partial_t e_n)_Q \right).
\]  (42)

We proceed further by integrating by parts the term \( (r_d, \nabla_x \partial_t e_n)_Q \):

\[
\mu (r_d, \nabla_x (\partial_t e_n))_Q = \mu (r_d, \partial_t e_n)_Q - \mu (\text{div}_x (y - \nabla_x v_n), \partial_t e_n)_Q = -\mu (\text{div}_x y - \Delta_x v_n, \partial_t e_n)_Q.
\]
Using density arguments, i.e., \( u_n \to u, v_n \to v \in V_{0,T}^{1,1/2} \), and \( f_n \to f \in L^2(Q) \) for \( n \to \infty \), we arrive at the identity formulated for \( e = u - v \) with \( u, v \in V_{0,T}^{1,1/2} \), i.e.,

\[
\lambda \|\nabla_x e\|_Q^2 + \mu \|\partial_t e\|_Q^2 + \frac{1}{2} (\mu \|\nabla_x e\|_{\Sigma_T}^2 + \lambda \|e\|_{\Sigma_T}^2)
\]

\[
= \lambda \left( (r_{eq}, e)_Q + (r_d, \nabla_v e)_Q \right) + \mu \left( (r_{eq}, \partial_t e)_Q - \mu (\text{div}_x r_d, \partial_t e)_Q \right). \tag{43}
\]

The first term on the RHS of (43) is estimated by the Hölder and Friedrichs inequalities

\[
\lambda (r_{eq}, e)_Q \leq C_F \lambda \|r_{eq}\|_Q \|\nabla v e\|_Q.
\]

The second, third, and fourth terms can be treated analogously. Therefore, (43) yields the estimate

\[
\lambda \|\nabla_x e\|_Q^2 + \mu \|\partial_t e\|_Q^2 + \frac{1}{2} (\mu \|\nabla_x e\|_{\Sigma_T}^2 + \lambda \|e\|_{\Sigma_T}^2)
\]

\[
\leq \lambda \left( \|r_d\|_Q + C_F \|r_{eq}\|_Q \right) \|\nabla_v e\|_Q + \mu \left( (\text{div}_x r_d)_Q + \|r_{eq}\|_Q \right) \|\partial_t e\|_Q
\]

\[
\leq \left( \lambda \left( \|r_d\|_Q + C_F \|r_{eq}\|_Q \right)^2 + \mu (\|\text{div}_x r_d\|_Q + \|r_{eq}\|_Q)^2 \right)^{1/2} (\lambda \|\nabla_v e\|_Q^2 + \mu \|\partial_t e\|_Q^2)^{1/2}. \tag{44}
\]

In order to regroup the terms on the RHS of (44), we apply the Young inequality with positive scalar-valued parameters \( \gamma, \alpha_1, \) and \( \alpha_2 \) and deduce the estimate

\[
\left( \lambda \left( \|r_d\|_Q + C_F \|r_{eq}\|_Q \right)^2 + \mu (\|\text{div}_x r_d\|_Q + \|r_{eq}\|_Q)^2 \right)^{1/2} (\lambda \|\nabla_v e\|_Q^2 + \mu \|\partial_t e\|_Q^2)^{1/2}
\]

\[
\leq \frac{\gamma}{2} \left( \lambda \left( \|r_d\|_Q + C_F \|r_{eq}\|_Q \right)^2 + \mu (\|\text{div}_x r_d\|_Q + \|r_{eq}\|_Q)^2 \right) + \frac{1}{2} \lambda \|\nabla_v e\|_Q^2 + \mu \|\partial_t e\|_Q^2
\]

\[
\leq \gamma \left( \left( 1 + \alpha_1 \right) \|r_d\|_Q^2 + \left( \frac{1}{\alpha_1} \right) C_F^2 \|r_{eq}\|_Q^2 \right) + \mu \left( \left( 1 + \alpha_2 \right) \|\text{div}_x r_d\|_Q^2 + \left( 1 + \frac{1}{\alpha_2} \right) \|r_{eq}\|_Q^2 \right)
\]

\[
+ \frac{1}{2} \gamma \left( \lambda \|\nabla_v e\|_Q^2 + \mu \|\partial_t e\|_Q^2 \right),
\]

where \( \gamma, \alpha_1, \) and \( \alpha_2 \) are positive scalar-valued parameters. Then, the obtained inequality yields (40). \( \Box \)

The next Theorem requires higher regularity for both \( v \) and \( y \) with respect to time.

**Theorem 3** For any \( v \in V_{0,T}^{1,1/2} \) and any \( y \in H^{\text{div},1}(Q) \), the following inequality holds:

\[
(2 - \frac{1}{2}) \lambda \left( \|\nabla_x e\|_Q^2 + \mu \|\partial_t e\|_Q^2 \right)^{1/2} + \mu (\|\text{div}_x r_d\|_Q + \|r_{eq}\|_Q)^2 \right)^{1/2} (\lambda \|\nabla_v e\|_Q^2 + \mu \|\partial_t e\|_Q^2)^{1/2}
\]

\[
\leq \frac{\gamma}{2} \left( \lambda \left( \|r_d\|_Q + C_F \|r_{eq}\|_Q \right)^2 + \mu (\|\text{div}_x r_d\|_Q + \|r_{eq}\|_Q)^2 \right) + \frac{1}{2} \lambda \|\nabla_v e\|_Q^2 + \mu \|\partial_t e\|_Q^2
\]

\[
\leq \gamma \left( \left( 1 + \alpha_1 \right) \|r_d\|_Q^2 + \left( \frac{1}{\alpha_1} \right) C_F^2 \|r_{eq}\|_Q^2 \right) + \mu \left( \left( 1 + \alpha_2 \right) \|\text{div}_x r_d\|_Q^2 + \left( 1 + \frac{1}{\alpha_2} \right) \|r_{eq}\|_Q^2 \right)
\]

\[
+ \frac{1}{2} \gamma \left( \lambda \|\nabla_v e\|_Q^2 + \mu \|\partial_t e\|_Q^2 \right), \tag{45}
\]

where \( r_{eq}(v, y) \) and \( r_d(v, y) \) are defined in (13), \( C_F \) is the Friedrichs constant, and \( \lambda \) and \( \mu \) are positive weights introduced in (11), \( C_F \) is the Friedrichs constant, \( \lambda \) and \( \mu \) are positive weights introduced in (11), \( \gamma \in \left[ \frac{1}{2}, +\infty \right) \), \( \alpha \in \left[ 1, +\infty \right) \), and \( \beta_i > 0 \), \( i = 1, 2 \).

**Proof:** Now, we use a different transformation of the last term in the RHS of (42):

\[
\mu \left( r_d, \nabla_x (\partial_t e_n) \right)_Q = \mu \left( r_d, \nabla_x e_n n_t \right)_T - \mu \left( \partial_t r_d, \nabla_x e_n \right)_Q, \tag{46}
\]

where \( n_t \mid_{\Sigma_T} = 1 \). Analogously to the proof of Theorem 2, we use density arguments to obtain

\[
\lambda \|\nabla_x e\|_Q^2 + \mu \|\partial_t e\|_Q^2 + \frac{1}{2} (\mu \|\nabla_x e\|_{\Sigma_T}^2 + \lambda \|e\|_{\Sigma_T}^2)
\]

\[
= \lambda \left( (r_{eq}, e)_Q + (r_d, \nabla_v e)_Q \right) + \mu \left( (r_{eq}, \partial_t e)_Q (r_d, \nabla_v e n_t)_{\Sigma_T} - (\partial_t r_d, \nabla_v e)_Q \right). \tag{47}
\]

Since

\[
\mu \left( r_d, \nabla_v e \right)_{\Sigma_T} \leq \frac{\epsilon}{2} (\frac{1}{2} \|\nabla_v e\|_{\Sigma_T}^2 + \|r_d\|_{\Sigma_T}^2), \quad \epsilon > 0,
\]

and

\[-\mu \left( \partial_t r_d, \nabla_v e \right)_Q \leq \mu \|\partial_t r_d\|_Q \|\nabla_v e\|_Q,
\]
we obtain
\[
\lambda \| \nabla_x e \|^2_Q + \mu \| \partial_t e \|^2_Q + \frac{1}{2} (\lambda \| e \|^2_{2, T} + \mu \| \nabla_x e \|^2_{2, T}) \\
\leq \frac{\mu}{2} (\frac{1}{r} \| \nabla_x e \|^2 + \epsilon \| \partial_t e \|^2) + \left( \lambda (\| \partial_t \|_Q + C_F \| \text{refl} \|_Q) + \mu \| \partial_t \|_Q \right) \| \nabla_x e \|_Q + \mu \| \text{refl} \|_Q \| \partial_t e \|_Q \\
\leq \frac{\mu}{2} (\frac{1}{r} \| \nabla_x e \|^2 + \epsilon \| \partial_t e \|^2) + \left( \lambda (\| \partial_t \|_Q + C_F \| \text{refl} \|_Q) + \frac{\mu}{2} \| \partial_t \|_Q \right)^2 + \mu \| \text{refl} \|_Q \right)^{1/2} (\lambda \| \nabla_x e \|^2_Q + \mu \| \partial_t e \|^2_Q)^{1/2} \\
\leq \frac{\mu}{2} (\frac{1}{r} \| \nabla_x e \|^2 + \epsilon \| \partial_t e \|^2) + \frac{1}{2} (\lambda \| \nabla_x e \|^2_Q + \mu \| \partial_t e \|^2_Q) \\
\quad + \frac{\epsilon}{2} \left( \lambda (1 + \beta_1) (1 + \beta_2) \| \partial_t \|_Q + (1 + \frac{1}{2\epsilon}) C_F \| \text{refl} \|_Q) + \frac{\mu}{2} \right) \| \partial_t \|_Q \right) + \mu \| \text{refl} \|_Q^2 \right). \\
\]
This estimate yields \( [50] \). \qed

In Corollaries below, we consider a particular case related to the choice \( \lambda = 1 \) and \( \mu = \delta_{s,h} \).

**Corollary 1** Assume that \( v \in V_{0, Q}^\Delta \) and \( y \in H^{d_1, 0}(Q) \). Then, Theorems \( [2] \) yields the estimate
\[
(2 - \frac{1}{\gamma})(\| \nabla_x e \|^2_Q + \delta_{s,h} \| \partial_t e \|^2_Q) + \delta_{s,h} \| \nabla_x e \|^2_{2, T} + \| e \|^2_{2, T} \leq M_{s,h}^d(v, y; \gamma, \alpha_i) \\
:= \gamma ((1 + \alpha_1) \| \partial_t \|_Q + (1 + \frac{1}{\alpha_1}) C_F \| \text{refl} \|_Q) + \delta_{s,h} ((1 + \alpha_2) \| \nabla_x e \|^2_Q + (1 + \frac{1}{\alpha_2}) \| \text{refl} \|_Q)), \quad (48)
\]
where \( \partial_t \) and \( \text{refl} \) are defined in \( [11] \), \( \delta_{s,h} \) is a parameter defined in \( [22] \), \( \gamma \in \left[ \frac{1}{2}, +\infty \right) \), and \( \alpha_i > 0, i = 1, 2 \). A useful particular form of \( [48] \) arises if we set \( \gamma = 1 \). Then, the estimate has the form
\[
\| \nabla_x e \|^2_Q + \delta_{s,h} \| \partial_t e \|^2_Q + \| e \|^2_{2, T} + \delta_{s,h} \| \nabla_x e \|^2_{2, T} \leq M_{s,h}^d(v, y; \alpha_i) \\
:= (1 + \alpha_1) \| \partial_t \|_Q + (1 + \frac{1}{\alpha_1}) C_F \| \text{refl} \|_Q + \delta_{s,h} ((1 + \alpha_2) \| \nabla_x e \|^2_Q + (1 + \frac{1}{\alpha_2}) \| \text{refl} \|_Q)), \quad (49)
\]
where the best \( \alpha_1 \) and \( \alpha_2 \) are defined by relations \( \alpha_1^* = \frac{C_F \| \text{refl} \|_Q}{\| \partial_t \|_Q} \) and \( \alpha_2^* = \frac{\| \text{refl} \|_Q}{\| \nabla_x e \|^2_Q} \).

**Remark 4** In general, \( \alpha_1 \) and \( \alpha_2 \) can be positive functions of \( t \). Then, \( \alpha_1^* \) and \( \alpha_2^* \) are also functionals of \( t \). In this case, the overall value of the majorant is minimal.

**Corollary 2** Let \( v \in V_{0, Q}^{\Delta t} \) and \( y \in H^{d_1, 1}(Q) \). Then, we have the estimate
\[
(2 - \frac{1}{\epsilon})(\| \nabla_x e \|^2_Q + \delta_{s,h} \| \partial_t e \|^2_Q) + \delta_{s,h} (1 - \frac{1}{\epsilon}) \| \nabla_x e \|^2_{2, T} + \| e \|^2_{2, T} \leq M_{s,h}^d(v, y; \zeta, \beta_i, \epsilon) \\
:= \epsilon \delta_{s,h} \| \partial_t \|_Q^2 + \zeta ((1 + \beta_1)(1 + \beta_2) \| \partial_t d \|^2_Q + (1 + \frac{1}{\beta_1}) C_F \| \text{refl} \|_Q^2) + (1 + \frac{1}{\beta_2}) \| \nabla_x e \|^2_Q + \delta_{s,h} \| \text{refl} \|_Q^2), \quad (50)
\]
where \( \partial_t \) and \( \text{refl} \) are defined in \( [11] \), \( \delta_{s,h} \) is a parameter defined in \( [27] \), \( \zeta \in \left[ \frac{1}{2}, +\infty \right), \epsilon \in [1, +\infty) \), and \( \beta_i > 0, i = 1, 2 \). In particular, for \( \zeta = 1 \) and \( \epsilon = 2 \), we obtain
\[
\| \nabla_x e \|^2_Q + \delta_{s,h} \| \partial_t e \|^2_Q + \| e \|^2_{2, T} + \delta_{s,h} \| \nabla_x e \|^2_{2, T} \leq M_{s,h}^d(v; \beta_i) \\
:= 2 \delta_{s,h} \| \partial_t \|_Q^2 + (1 + \beta_1)((1 + \beta_2) \| \partial_t d \|^2_Q + (1 + \frac{1}{\beta_2}) C_F \| \text{refl} \|_Q^2) + (1 + \frac{1}{\beta_1}) \| \nabla_x e \|^2_Q + \delta_{s,h} \| \text{refl} \|_Q^2, \quad (51)
\]
where the optimal parameters are given by relations
\[
\beta_1^* = \frac{\delta_{s,h} \| \partial_t \|_Q}{\sqrt{(1 + \beta_2) \| \partial_t d \|^2_Q + (1 + \frac{1}{\beta_2}) C_F \| \text{refl} \|_Q^2}} \quad \text{and} \quad \beta_2^* = \frac{C_F \| \text{refl} \|_Q}{\| \partial_t \|_Q}
\]

**Theorem 4** Functionals \( M_{s,h}^d \) and \( M_{s,h}^{\Delta t} \) (\( M_{s,h}^d \) and \( M_{s,h}^{\Delta t} \)) vanish if and only if the approximations \( v \) and \( y \) coincide with the exact solution of the problem and its exact flux, i.e., \( v = u \) and \( y = \nabla_x u \).
Remark 5 For the case $\mu = 0$, the majorants presented in Theorems 2 and 3 coincide with the estimates derived in [23]. Computational properties of these estimates have been studied in [40] and [43]. The paper [40] includes two benchmark examples, where error majorants were applied to approximations reconstructed by the space-time method. Numerical results, presented in these examples, confirm the efficient performance of the majorant (ratios between majorant and error are close to 1).

6 Modification of majorans $\overline{M}^I$ and $\overline{M}^{II}$

In this section, we deduce modified forms of $\overline{M}^I$ and $\overline{M}^{II}$, which, in general, provide sharper bounds of the error. These estimates contain an additional ‘free’ function $w \in V_{\Delta t}^0$. First, we rewrite (52) as follows:

$$\begin{align*}
\lambda \| \nabla e \|_{L^2}^2 + \mu \| \partial_t e \|_{L^2}^2 + \frac{1}{2} (\mu \| \nabla e \|_{L^2}^2 + \lambda \| e \|_{L^2}^2) \\
= \lambda \left( (\overline{r}_{eq}(v; y, w)e) + (\overline{r}_d(v; y, w), \nabla e) \right) + \mu \left( (\overline{r}_{eq}(v; y, w), \partial_t e) + (\overline{r}_d(v; y, w), \nabla \partial_t e) \right) \\
+ \lambda \left( (\partial_t w, \partial_t e) - (\nabla w, \nabla \partial_t e) \right) + \mu \left( (\partial_t w, \partial_t e) - (\nabla w, \nabla \partial_t e) \right),
\end{align*}$$

(52)

where

$$\begin{align*}
\overline{r}_{eq}(v; y, w) := f + \nabla y - \partial_t (v + w) \quad \text{and} \quad \overline{r}_d(v; y, w) := y - \nabla x (v - w)
\end{align*}$$

are modified residuals. All deducted terms are compensated by adding

$$I(e; v, y) := (\partial_t w, \lambda e + \mu \partial_t e) - (\nabla w, \nabla x (\lambda e + \mu \partial_t e)).$$

It is not difficult to see that

$$I(e; v, w) := (\partial_t w, \lambda e + \mu \partial_t e) - (\nabla w, \nabla x (\lambda e + \mu \partial_t e)).$$

(53)

Here,

$$J(v, w) := (\lambda w - \mu \partial_t w, \nabla v) + (\nabla x (\lambda w - \mu \partial_t w), \nabla v) - (\lambda w - \mu \partial_t w, f).$$

is a linear functional that mimics the residual of (8) with the test function $\lambda w - \mu \partial_t w$. The first two terms in the RHS of (53) can be estimated as follows:

$$\lambda w, e)_{\Sigma^T} \leq \frac{1}{2} \left( \rho_1 \| w \|_{L^2}^2 + \frac{1}{p_2} \| e \|_{L^2}^2 \right),$$

(54)

and

$$\mu (\nabla w, \nabla e)_{\Sigma^T} \leq \frac{1}{2} \left( \rho_2 \| \nabla w \|_{L^2}^2 + \frac{1}{p_2} \| \nabla e \|_{L^2}^2 \right),$$

(55)

where $\rho_1, \rho_2 > 0$. From (52), (53), (54), and (55), we obtain

$$\begin{align*}
\lambda \| \nabla e \|_{L^2}^2 + \mu \| \partial_t e \|_{L^2}^2 + \frac{1}{2} (\mu (1 - \frac{1}{p_2}) \| \nabla e \|_{L^2}^2 + \lambda (1 - \frac{1}{p_1}) \| e \|_{L^2}^2) \leq \frac{\rho_1}{2} \| w \|_{L^2}^2 + \frac{\rho_2}{2} \| \nabla w \|_{L^2}^2 \\
+ \lambda \left( (\overline{r}_{eq}(y, w), e) + (\overline{r}_d(y, w), \nabla e) \right) + \mu \left( (\overline{r}_{eq}(y, w), \partial_t e) + (\overline{r}_d(y, w), \nabla \partial_t e) \right) + J(v, w).
\end{align*}$$

(56)
By means of this inequality and arguments analogous those used in the proofs of Theorems 2 and 3 we deduce advanced forms of majorants.

**Theorem 5**

(i) For any \( v, w \in V_{\Delta h}^1 \) and any \( y \in H^{\text{div}, 0}(Q) \), the alternative estimate holds:

\[
(2 - \frac{1}{\epsilon})(\lambda \| \nabla x e \|_Q^2 + \mu \| \partial e \|_Q^2) + (1 - \frac{1}{\rho_2}) \| \nabla x e \|_{\Sigma_T}^2 + \lambda (1 - \frac{1}{\rho_1}) \| e \|_{\Sigma_T}^2 \\
=: \| e \|_{\Sigma_T}^2 \leq \text{\( M_w \)}(v, w; \gamma, \alpha_i, \rho_1) := \rho_1 \| u \|_{\Sigma_T}^2 + \rho_2 \| \nabla x w \|_{\Sigma_T}^2 + 2 \mathcal{J}(v, w) + \gamma \left\{ \lambda \left( (1 + \alpha_1) \| \nabla x \|_Q^2 + (1 + \frac{1}{\alpha_1}) C_F^2 \| \nabla x u \|_Q^2 \right) + \mu \left( (1 + \alpha_2) \| \nabla x \|_Q^2 + (1 + \frac{1}{\alpha_2}) \| \nabla x u \|_Q^2 \right) \right\},
\]

where \( \rho_1, \rho_2, \epsilon \in [1, +\infty) \) and \( \alpha_i > 0, i = 1, 2 \), are auxiliary parameters.

(ii) For any \( v, w \in V_{\Delta h}^1 \) and any \( y \in H^{\text{div}, 1}(Q) \), the following inequality holds:

\[
(2 - \frac{1}{\epsilon})(\lambda \| \nabla x e \|_Q^2 + \mu \| \partial e \|_Q^2) + (1 - \frac{1}{\rho_2}) \| \nabla x e \|_{\Sigma_T}^2 + \lambda (1 - \frac{1}{\rho_1}) \| e \|_{\Sigma_T}^2 \\
=: \| e \|_{\Sigma_T}^2 \leq \text{\( M_w \)}(v, w; \zeta, \beta_i, \epsilon, \rho_1) := \rho_1 \| u \|_{\Sigma_T}^2 + \rho_2 \| \nabla x w \|_{\Sigma_T}^2 + \epsilon \| \nabla x \|_{\Sigma_T}^2 + 2 \mathcal{J}(v, w) + \zeta \left\{ \lambda \left( (1 + \beta_1) \| \nabla x \|_Q^2 + (1 + \frac{1}{\beta_1}) C_F^2 \| \nabla x u \|_Q^2 \right) + (1 + \frac{1}{\beta_1}) \| \nabla x u \|_Q^2 \right\},
\]

where \( \rho_1, \rho_2, \epsilon \in [1, +\infty) \), such that the combination \( 1 - \frac{1}{\rho_2} \geq 0, \gamma \in [\frac{1}{\rho_1}, +\infty) \), \( \zeta \in [\frac{1}{\beta_1}, +\infty) \), and \( \beta_i > 0, i = 1, 2 \). In both inequalities \( (60) \) and \( (61) \), \( \nabla x v; y, w \) and \( \nabla x v; y, w \) are modified residual functionals that follow from \( (1) \), and \( \lambda \) and \( \mu \) are positive weights introduced in \( (11) \).

(iii) Majorants \( M_w^1 \) and \( M_w^{11} \) satisfy the same properties that are valid for majorants \( M_w^1 \) and \( M_w^{11} \), i.e., they vanish if and only if \( v = u \), \( y = \nabla x u \), and \( w = 0 \). Moreover, the relation between both forms of the majorants can be written as follows:

\[
M_w = \inf_{w \in V_{\Delta h}^0 Q} M_w^1 \quad \text{and} \quad M_w^{11} = \inf_{w \in V_{\Delta h}^0 \nu, \nu \in Q} M_w^{11}.
\]

**Proof:** The detailed proofs can be found in works \[53, 11, 15\].

Let us prove the equivalence of modified estimate to the error measured in the energy norm \( (68) \) and majorant \( M_w^1 \). Assume that \( y = \nabla x u \) and \( w = u - v \), then:

\[
(2 - \frac{1}{\epsilon})(\lambda \| \nabla x e \|_Q^2 + \mu \| \partial e \|_Q^2) + (1 - \frac{1}{\rho_2}) \| \nabla x e \|_{\Sigma_T}^2 + \lambda (1 - \frac{1}{\rho_1}) \| e \|_{\Sigma_T}^2 \\
\leq M_w^1(v, v - u, v; \gamma, \alpha_i, \rho_1) := \rho_1 \| u - v \|_{\Sigma_T}^2 + \rho_2 \| \nabla x (v - u) \|_{\Sigma_T}^2 + \mathcal{J}(v, u - v) \\
+ \gamma \left\{ \lambda \left( (1 + \alpha_1) \| \nabla x (v - u) \|_Q^2 + (1 + \frac{1}{\alpha_1}) C_F^2 \| f + \nabla x (v - u) \|_Q^2 \right) + \mu \left( (1 + \alpha_2) \| \nabla x (v - u) \|_Q^2 \right) + (1 + \frac{1}{\alpha_2}) \| f + \nabla x (v - u) \|_Q^2 \right\},
\]

\[
= \rho_1 \| u - v \|_{\Sigma_T}^2 + \rho_2 \| \nabla x (v - u) \|_{\Sigma_T}^2 + 2 \mathcal{J}(v, u - v).
\]

Consider separately the linear functional in the RHS of \( (60) \):

\[
\mathcal{J}(v, u - v) = \left( \lambda (u - v) - \mu \partial (u - v), \partial (u - v) \right)_Q + \left( \nabla x (\lambda (u - v) - \mu \partial (u - v), \nabla x u \right)_Q - (\lambda (u - v) - \mu \partial (u - v), f)_Q \\
= (\lambda (u - v) - \mu \partial (u - v), \partial (u - v))_Q + (\nabla x (\lambda (u - v) - \mu \partial (u - v), \nabla x u \right)_Q - (\lambda (u - v) - \mu \partial (u - v), \nabla x u \right)_Q \\
= (\lambda (u - v) - \mu \partial (u - v), -\partial (u - v))_Q + (\nabla x (\lambda (u - v) - \mu \partial (u - v), \nabla x (u - v))_Q \\
= \lambda \| u - v \|_{\Sigma_T}^2 + \mu \| \partial (u - v) \|_Q^2 + \lambda \| \nabla x (u - v) \|_Q^2 + \mu \| \partial (u - v) \|_{\Sigma_T}^2. \]

(61)
In view of (61) and identity (60), we obtain
\[ \|e\|_I^2 := (2 - \frac{1}{\gamma})(\|\nabla_x e\|_{L^2}^2 + \mu(\|\partial_t e\|_{L^2}^2) + \mu (1 - \frac{1}{\rho_2})\|\nabla_x e\|_{L^2}^2 + \lambda (1 - \frac{1}{\rho_1})\|e\|_{L^2}^2) \]
\[ \leq M_w(v, \nabla_x u, e) := (2 \lambda + \rho_1)\|e\|_{L^2}^2 + (2 \mu + \rho_2)\|\nabla_x e\|_{L^2}^2 + 2 (\mu \|\partial_t e\|_{L^2}^2 + \lambda \|\nabla_x e\|_{L^2}^2) \]
\[ \leq \max \left\{ \frac{2 \gamma}{2 \gamma - 1}, \frac{\rho_1 (2 \lambda + \rho_1)}{\lambda (\rho_1 - 1)}, \frac{\rho_2 (2 \mu + \rho_2)}{\mu (\rho_2 - 1)} \right\} \left( (2 - \frac{1}{\gamma})(\|\nabla_x e\|_{L^2}^2 + \mu \|\partial_t e\|_{L^2}^2) + \mu (1 - \frac{1}{\rho_2})\|\nabla_x e\|_{L^2}^2 + \lambda (1 - \frac{1}{\rho_1})\|e\|_{L^2}^2) \right) \]
\[ = \max \left\{ \frac{2 \gamma}{2 \gamma - 1}, \frac{\rho_1 (2 \lambda + \rho_1)}{\lambda (\rho_1 - 1)}, \frac{\rho_2 (2 \mu + \rho_2)}{\mu (\rho_2 - 1)} \right\} \|e\|_{I}^2. \] (62)

The double inequality (62) states the equivalence of $\|e\|_I^2$ and $\inf_{w \in V_0^h} M_w(v, y, w; \gamma, \alpha, \rho_1)$, i.e.,
\[ 1 \leq \inf_{w \in V_0^h} \frac{M_w(v, y, w; \gamma, \alpha, \rho_1)}{\|e\|_I^2} \leq C_{eq}^I \] (63)

where the constant $C_{eq}^I := \max \left\{ \frac{2 \gamma}{2 \gamma - 1}, \frac{\rho_1 (2 \lambda + \rho_1)}{\lambda (\rho_1 - 1)}, \frac{\rho_2 (2 \mu + \rho_2)}{\mu (\rho_2 - 1)} \right\}$ is explicitly computable.

Analogous equivalence of $\|e\|_{II}^2$ and majorant $\inf_{w \in V_0^h} M_w(v, y, w; \gamma, \beta, \epsilon, \rho_1)$ can be formulated as follows:
\[ 1 \leq \inf_{w \in V_0^h} \frac{M_w(v, y, w; \gamma, \beta, \epsilon, \rho_1)}{\|e\|_{II}^2} \leq C_{eq}^{II} \] (64)

where $C_{eq}^{II} := \max \left\{ \frac{2 \gamma}{2 \gamma - 1}, \frac{\rho_1 (2 \lambda + \rho_1)}{\lambda (\rho_1 - 1)}, \frac{(2 \mu + \rho_2)}{\mu (1 - \frac{1}{\rho_2})} \right\}$ is explicitly defined.

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