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CONSTRUCTIVE A PRIORI ERROR ESTIMATES FOR A FULL DISCRETE APPROXIMATION OF THE HEAT EQUATION

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CONSTRUCTIVE A PRIORI ERROR ESTIMATES FOR A FULL DISCRETE APPROXIMATION OF THE HEAT EQUATION*

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Abstract. In this paper, we consider the constructive a priori error estimates for a full discrete numerical solution of the heat equation. Our method is based on the finite element Galerkin method with an interpolation in time that uses the fundamental solution for semidiscretization in space. The present estimates play an essential role in the numerical verification method of exact solutions for the nonlinear parabolic equations. This implies that by utilizing the present results we could get the guaranteed a posteriori error estimates for various kinds of nonlinear evolutional problems. Our results can also be considered as an explicit optimal estimate with the limited regularity of solutions.

Key words. Parabolic problem, Galerkin methods, Constructive a priori error estimates

AMS subject classifications. 35K05, 65M15, 65M60

1. Introduction. The main aim of this paper is to obtain the constructive a priori error estimates for a full discrete approximation u_h^k of the solution u to the following heat equation with homogeneous initial and boundary conditions:

$$\begin{cases} \dfrac{\partial u}{\partial t} - \nu \triangle u = f & \text{in } \Omega \times J, \quad (1.1a) \\ u(x,t) = 0 & \text{on } \partial\Omega \times J, \quad (1.1b) \\ u(x,0) = 0 & \text{in } \Omega. \quad (1.1c) \end{cases}$$

Here, $\Omega \subset \mathbb{R}^d$, $(d \in \{1,2,3\})$ is a bounded polygonal or polyhedral domain; $J := (0,T) \subset \mathbb{R}$, (for a fixed $T < \infty$) is a bounded open interval; the diffusion coefficient ν is a positive constant; and $f \in L^2\big(J; L^2(\Omega)\big)$. In the discussion below, we refer to the a priori estimates as *'constructive'* if all the constants can be numerically determined. In particular, we try to derive the estimates with a numerically computable constant C with

$$\left\| u - u_h^k \right\|_{L^2\left(J; H_0^1(\Omega)\right)} \le C \left\| f \right\|_{L^2\left(J; L^2(\Omega)\right)}. \quad (1.2)$$

Such a bound plays an essential role in the numerical verification of solutions to the nonlinear parabolic initial-boundary value problems, which is a principal motivation for our work. Namely, by using the constructive error estimates (1.2), we can formulate the numerical enclosure method for a solution to the nonlinear problem of the form

$$\begin{cases} \dfrac{\partial u}{\partial t} - \nu \triangle u = g(t,x,u,\nabla u) & \text{in } \Omega \times J, \quad (1.3a) \\ u(x,t) = 0 & \text{on } \partial\Omega \times J, \quad (1.3b) \\ u(x,0) = 0 & \text{in } \Omega, \quad (1.3c) \end{cases}$$

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where g is a nonlinear function in u with appropriate assumptions.

We will first introduce a full discrete approximation scheme for the problem (1.1), in which we use a time interpolation scheme by using the associated fundamental matrix for a system of ordinary differential equations (ODEs) which is generated by the usual semidiscrete Galerkin method in the space direction. Next, by the use of a priori estimates for the semidiscrete approximation and the interpolation, we will derive the constructive error estimates for the full discretization.

Notice that the basic situation for the verified computation of solutions to the parabolic problems is similar to the elliptic case. Namely, the corresponding elliptic problem to (1.1) is the following Poisson equation.

$$\begin{cases} -\triangle u = f & \text{in } \Omega, \quad (1.4a) \\ u = 0 & \text{on } \partial\Omega. \quad (1.4b) \end{cases}$$

Then, the constructive error estimates for the usual finite element solution of (1.4), i.e., the H_0^1-projection of a solution u, presents the basic principle of the verified computations for nonlinear problems, corresponding to (1.3), of the form

$$\begin{cases} -\triangle u = g(x, u, \nabla u) & \text{in } \Omega, \quad (1.5a) \\ u = 0 & \text{on } \partial\Omega. \quad (1.5b) \end{cases}$$

Based on this principle, there have been several works for elliptic problems, including the Navier-Stokes equations [7, 8, 18, 19, 9, 10, 11, 1]. Therefore, if we obtain the constructive error estimates of a full discrete numerical scheme for the heat equation (1.1), we can establish the numerical verification method of solutions for the nonlinear problem (1.3).

One of us has already obtained some constructive error estimates [12, 14], but the actual computations lacked efficiency. In our previous work [15], in which we combined the a priori error estimates for a semidiscrete approximation with the a priori estimates for the ODEs, we obtained a technique that enabled us to formulate a verification method for nonlinear problems. However, it also has computational difficulties because the corresponding linear ODEs are very stiff for a small mesh size in the spatial direction. If we use the present results to implement a new verification method, we would expect to overcome these difficulties and to improve the computational cost for the verification of solutions for the nonlinear problem (1.3). We have already confirmed that this method greatly reduces the computational cost, which will be published in a forthcoming paper [3]. Also, we emphasize that our a priori error estimates of the form (1.2) should be the optimal order for the associated norms and, as far as we know, there have been no such constructive estimates yet derived.

The contents of this paper are as follows: In Section 2, we introduce some function spaces, operators, and other notation. In Section 3, we propose a new full discretization scheme for the heat equation. For later use, we present some constructive a priori estimates for the semidiscrete approximation in Section 4. The results of this section are already known, but we describe them in order to make our arguments self-contained. In Section 5, we derive constructive a priori error estimates for the new full discretization scheme which was introduced in Section 3. We also attached an auxiliary result in an appendix.

2. Notation. We denote by $L^2(\Omega)$ and $H^1(\Omega)$ the usual Lebesgue and Sobolev spaces on Ω, respectively, and by $(u, v)_{L^2(\Omega)} := \int_\Omega u(x)v(x)\,dx$ the natural inner

product of u, v in $L^2(\Omega)$. By considering the boundary and initial conditions, we define the following subspaces of $H^1(\Omega)$ and $H^1(J)$ as

$$H_0^1(\Omega) := \big\{u \in H^1(\Omega)\ ;\ u = 0 \text{ on } \partial\Omega\big\} \quad \text{and} \quad V^1(J) := \big\{u \in H^1(J)\ ;\ u(0) = 0\big\},$$

respectively. These are Hilbert spaces with inner products

$$(u, v)_{H_0^1(\Omega)} := (\nabla u, \nabla v)_{L^2(\Omega)^d} \quad \text{and} \quad (u, v)_{V^1(J)} := \left(\frac{\partial u}{\partial t}, \frac{\partial u}{\partial t}\right)_{L^2(J)}.$$

Let $X(\Omega)$ be a subspace of $L^2(\Omega)$ defined by $X(\Omega) := \big\{u \in L^2(\Omega)\ ;\ \triangle u \in L^2(\Omega)\big\}$. We define the time-dependent Sobolev spaces as usual, and define

$$V^1\big(J; L^2(\Omega)\big) := \left\{u \in L^2\big(J; L^2(\Omega)\big)\ ;\ \frac{\partial u}{\partial t} \in L^2\big(J; L^2(\Omega)\big)\right\},$$

with inner product $(u, v)_{V^1(J;L^2(\Omega))} := \big(\frac{\partial u}{\partial t}, \frac{\partial v}{\partial t}\big)_{L^2(J;L^2(\Omega))}$. In the following discussion, abbreviations like $L^2H_0^1$ for $L^2\big(J; H_0^1(\Omega)\big)$ will often be used. We set $V := V^1\big(J; L^2(\Omega)\big) \cap L^2\big(J; H_0^1(\Omega)\big)$. Moreover, we denote the partial differential operator $\triangle_t : V \cap L^2\big(J; X(\Omega)\big) \to L^2\big(J; L^2(\Omega)\big)$ by $\triangle_t := \frac{\partial}{\partial t} - \nu\triangle$.

Now let $S_h(\Omega)$ be a finite-dimensional subspace of $H_0^1(\Omega)$ dependent on the parameter h. For example, $S_h(\Omega)$ is considered to be a finite element space with mesh size h. Let n be the degrees of freedom for $S_h(\Omega)$, and let $\{\phi_i\}_{i=1}^n \subset H_0^1(\Omega)$ be the basis functions of $S_h(\Omega)$. Similarly, let $V_k^1(J)$ be an approximation subspace of $V^1(J)$ dependent on the parameter k. Let m be the degrees of freedom for $V_k^1(J)$, and let $\{\psi_i\}_{i=1}^m \subset V_k^1(J)$ be the basis functions of $V_k^1(J)$. Let $V^1\big(J; S_h(\Omega)\big)$ be a subspace of V corresponding to the semidiscretized approximation in the spatial direction, and the space $V_k^1\big(J; S_h(\Omega)\big)$ is defined as the tensor product $V_k^1(J) \otimes S_h(\Omega)$, which corresponds to a full discretization. We define the H_0^1-projection $P_h^1 u \in S_h(\Omega)$ of any element $u \in H_0^1(\Omega)$ by the following variational equation:

$$\big(\nabla(u - P_h^1 u), \nabla v_h\big)_{L^2(\Omega)^d} = 0, \quad \forall v_h \in S_h(\Omega). \tag{2.1}$$

The V^1-projection $P_1^k : V^1(J) \to V_k^1(J)$ is similarly defined.

Now let $\Pi_k : V^1(J) \to V_k^1(J)$ be an interpolation operator. Namely, if the nodal points of J are given by $0 = t_0 < t_1 < \cdots < t_m = T$, then for an arbitrary $u \in V^1(J)$, the interpolation $\Pi_k u$ is defined as the function in $V_k^1(J)$ satisfying:

$$u(t_i) = \big(\Pi_k u\big)(t_i), \quad \forall i \in \{1, \ldots, m\}. \tag{2.2}$$

From [2, Lemma 2.2], if $V_k^1(J)$ is the P1 finite element space (i.e., the basis functions ψ_i are piecewise linear functions), then P_1^k coincides with Π_k. For any element $u \in V$, we define the semidiscrete projection $P_h u \in V^1\big(J; S_h(\Omega)\big)$ by the following weak form:

$$\left(\frac{\partial}{\partial t}\big(u(t) - P_h u(t)\big), v_h\right)_{L^2(\Omega)} + \nu\left(\nabla\big(u(t) - P_h u(t)\big), \nabla v_h\right)_{L^2(\Omega)^d} = 0, \tag{2.3}$$
$$\forall v_h \in S_h(\Omega), \quad \text{a.e. } t \in J.$$

Finally, we define the full discretization operator $P_h^k : V \to V_k^1\big(J; S_h(\Omega)\big)$ by $P_h^k := \Pi_k P_h$.

3. Full Discretization Scheme. In this section, we describe how to compute the full discretization approximation for (1.1). Since the full discretization scheme in this paper uses interpolation in the time variable, this method of computing $P_h^k u$ is somewhat different from the usual Galerkin procedure. But note that this principle enables us to remove the stiff property coming from the spatial discretization. In the derivation procedure of this scheme, we consider the fundamental matrix of solutions for the ODEs associated with the semidiscrete approximation $P_h u$.

Now, for each $f \in L^2\big(J; L^2(\Omega)\big)$, we define the semidiscretization by $u_h \in V^1\big(J; S_h(\Omega)\big)$ by the following variational form for a.e. $t \in J$:

$$\left(\frac{\partial u_h}{\partial t}(t), v_h\right)_{L^2(\Omega)} + \nu\left(\nabla u_h(t), \nabla v_h\right)_{L^2(\Omega)^d} = \left(f(t), v_h\right)_{L^2(\Omega)}, \quad \forall v_h \in S_h(\Omega). \tag{3.1}$$

Note that, from (2.3), we have $u_h = P_h u$.

We now define the symmetric and positive definite matrices L_ϕ and D_ϕ in $\mathbb{R}^{n\times n}$ by

$$L_{\phi,i,j} := \left(\phi_j, \phi_i\right)_{L^2(\Omega)}, \quad D_{\phi,i,j} := \left(\nabla\phi_j, \nabla\phi_i\right)_{L^2(\Omega)^d}, \quad \forall i, j \in \{1, \dots, n\}.$$

Let $\mathfrak{f} := (\mathfrak{f}_1, \dots, \mathfrak{f}_n)^T \in L^2(J)^n$ be a vector function defined by $\mathfrak{f}_i := (f, \phi_i)_{L^2(\Omega)}$. From the fact that $u_h \in V^1\big(J; S_h(\Omega)\big)$, there exists a coefficient vector $\mathfrak{u} := (\mathfrak{u}_1, \dots, \mathfrak{u}_n)^T \in V^1(J)^n$ such that

$$u_h(x,t) = \sum_{j=1}^{n} \phi_i(x)\mathfrak{u}_j(t) = \phi(x)^T\mathfrak{u}(t),$$

where $\phi := (\phi_1, \dots, \phi_n)^T$. Then, the variational equation (3.1) is equivalent to the following system of linear ODEs:

$$L_\phi \mathfrak{u}' + \nu D_\phi \mathfrak{u} = \mathfrak{f}. \tag{3.2}$$

Noting that (3.2) is a system of nonhomogeneous linear ODEs with constant coefficients, by using the fundamental matrix of the system, we obtain

$$\mathfrak{u}(t) = \int_0^t \exp\left((s-t)\nu L_\phi^{-1} D_\phi\right) L_\phi^{-1}\mathfrak{f}(s)\, ds. \tag{3.3}$$

Here, 'exp' means the exponential of a matrix. Taking notice of this representation, we define the full discretization $u_h^k \in V_k^1\big(J; S_h(\Omega)\big)$ of (1.1) by the interpolation

$$u_h^k(x, t_i) = \big(\Pi_k u_h\big)(x, t_i), \quad \forall x \in \Omega, \quad \forall i \in \{1, \dots, m\}. \tag{3.4}$$

Then, by definition, we have $u_h^k = P_h^k u$, and the actual computational procedure to get u_h^k is as follows.

First, we define the matrix $F \in \mathbb{R}^{n\times m}$ whose i-th column is given by

$$F_i := \int_0^{t_i} \exp\left((s-t_i)\nu L_\phi^{-1} D_\phi\right) L_\phi^{-1}\mathfrak{f}(s)\, ds, \quad \forall i \in \{1, \dots, m\}. \tag{3.5}$$

Next, noting that $u_h^k \in V_k^1\big(J; S_h(\Omega)\big)$, there exists a coefficient matrix U in $\mathbb{R}^{n\times m}$ such that $u_h^k = \phi^T U\psi$, where $\psi := (\psi_1, \dots, \psi_m)^T$. Therefore, from the definition (3.4), and by the use of (3.3), we have

$$\phi(x)^T U\psi(t_i) = \phi(x)^T\mathfrak{u}(t_i), \qquad \forall x \in \Omega, \quad \forall i \in \{1, \dots, m\}. \tag{3.6}$$

Let $\Psi \in \mathbb{R}^{m\times m}$ be the matrix whose elements are defined by $\Psi_{j,i} := \psi_j(t_i)$. Then the functional equation (3.6) is equivalent to the following linear system of equations:

$$U\Psi = F. \tag{3.7}$$

Thus by solving (3.7), i.e., computing $F\Psi^{-1}$, we can determine the full discrete approximation u_h^k.

REMARK 3.1. *If the basis functions ψ_j satisfy $\psi_j(t_i) = \delta_{j,i}$, where δ means the Kronecker delta, then the matrix Ψ is the unit matrix in $\mathbb{R}^{m\times m}$. Therefore, it is not necessary to solve the linear system of equations.*

Now we will give some consideration to the actual computation of the integral in (3.5) because it looks complicated due to the exponential of a matrix. First, note that we have the following proposition.

PROPOSITION 3.2. *For any A and B in $\mathbb{R}^{n\times n}$, if they are symmetric and positive definite, then all the eigenvalues of $A^{-1}B$ are positive.*

Indeed, let (λ, v) be an eigenpair of $A^{-1}B$. Then,

$$Bv = \lambda Av.$$

Therefore, we have

$$0 < v^*Bv = \lambda v^*Av,$$

which implies $\lambda > 0$ by the positive definiteness of A.

Hence if $L_\phi^{-1}D_\phi$ is numerically diagonalizable, then the computations in (3.5) should not be difficult. We can prove this property for L_ϕ and D_ϕ by the following lemma.

LEMMA 3.3. *If A is a symmetric nonsingular matrix, and B is a symmetric positive definite matrix in $\mathbb{R}^{n\times n}$, then all eigenvalues of $A^{-1}B$ are real, and $A^{-1}B$ is diagonalizable.*

Proof. From the symmetric positive definiteness of B, it is Cholesky decomposable with $B = B^{1/2}B^{T/2}$, where $B^{T/2} := \left(B^{1/2}\right)^T$. Then, for any eigenpair (λ, ν) of $A^{-1}B$, we have

$$\left(B^{T/2}A^{-1}B^{1/2}\right)\left(B^{T/2}v\right) = \lambda\left(B^{T/2}v\right). \tag{3.8}$$

Since A is symmetric, $B^{T/2}A^{-1}B^{1/2}$ is also symmetric. Hence (λ, v) is real. Moreover, $B^{T/2}A^{-1}B^{1/2}$ can be diagonalized by some orthogonal matrix $P \in \mathbb{R}^{n\times n}$ such that $P^T\left(B^{T/2}A^{-1}B^{1/2}\right)P = \Lambda$, where Λ is a diagonal matrix generated by the eigenvalues of $B^{T/2}A^{-1}B^{1/2}$. Then, we have

$$A^{-1}B = \left(P^TB^{T/2}\right)^{-1}\Lambda\left(P^TB^{T/2}\right),$$

which proves the lemma. □

Let $V_\phi^{-1}\Lambda_\phi V_\phi$ be the diagonalization of $L_\phi^{-1}D_\phi$, where $\Lambda_{\phi,k,k} = \lambda_k$ are the eigenvalues of $L_\phi^{-1}D_\phi$. For each matrix $A = (A_{i,j}) \in \mathbb{R}^{m\times m}$, we set $\overrightarrow{\operatorname{diag}}(A) := (A_{1,1}, \ldots, A_{n,n})^T \in \mathbb{R}^n$. Then, for all $i \in \{1, \ldots, m\}$, we have by (3.5)

$$F_{i,j} = \left(V_\phi^{-1}\overrightarrow{\operatorname{diag}}\left(V_\phi L_\phi^{-1}C^i\right)\right)_j,$$

$$\text{where} \qquad C^i_{j,k} = \int_0^{t_i} \exp\left((s-t_i)\nu\lambda_k\right) \mathfrak{f}_j(s)\, ds, \quad \forall j,k \in \{1,\dots,n\}. \tag{3.9}$$

In the present case, since each λ_k in (3.9) is positive from the above proposition, the computation of F_i is not difficult.

REMARK 3.4. *If Ω is a rectangular domain, and $S_h(\Omega)$ is a Q1 finite element space with uniform mesh, then $L_\phi^{-1}D_\phi$ is a symmetric positive definite matrix (see Section A). Therefore, the diagonalization of $L_\phi^{-1}D_\phi$ is easily obtained in this case. For guaranteed computations of linear algebraic problems, including diagonalization and Cholesky decomposition, we can use a convenient software package such as INTLAB (http://www.ti3.tu-harburg.de/rump/intlab/) [16].*

4. Estimates for semi discretization. In this section, we describe for later use the a priori estimates for the solution u of (1.1) and the semidiscrete projection $P_h u$. Several of the results presented below have been previously used [15], but, for the sake of completeness, we present the proofs.

LEMMA 4.1 ([15, Lemma 2]). *It holds that*

$$\|u\|_{V^1\left(J;L^2(\Omega)\right)} \le \|\triangle_t u\|_{L^2\left(J;L^2(\Omega)\right)}, \quad \forall u \in V \cap L^2\big(J;X(\Omega)\big). \tag{4.1}$$

Proof. For arbitrary $u \in C_0^\infty\big(J\times\Omega\big)$ and $t \in J$, we have

$$\begin{aligned}
\left\|\frac{\partial u}{\partial t}(t)\right\|^2_{L^2(\Omega)} + \frac{\nu}{2}\frac{d}{dt}\|\nabla u(t)\|^2_{L^2(\Omega)^d} &= (u_t,u_t)_{L^2(\Omega)} + \nu\,(\nabla u,\nabla u_t)_{L^2(\Omega)^d} \\
&= (u_t - \nu\triangle u, u_t)_{L^2(\Omega)} \\
&\le \|\triangle_t u\|_{L^2(\Omega)}\,\|u_t\|_{L^2(\Omega)} \\
&\le \frac{1}{2}\|\triangle_t u\|^2_{L^2(\Omega)} + \frac{1}{2}\|u_t\|^2_{L^2(\Omega)}.
\end{aligned}$$

Hence we have

$$\|u_t\|^2_{L^2(\Omega)} + \nu\frac{d}{dt}\|\nabla u\|^2_{L^2(\Omega)^d} \le \|\triangle_t u\|^2_{L^2(\Omega)}.$$

Integrating this on J, we get

$$\|u_t\|^2_{L^2\left(J;L^2(\Omega)\right)} + \nu\,\|\nabla u(T)\|^2_{L^2(\Omega)^d} \le \|\triangle_t u\|^2_{L^2\left(J;L^2(\Omega)\right)}.$$

From $\|\nabla u(T)\|^2_{L^2(\Omega)^d} \ge 0$, we obtain

$$\|u_t\|_{L^2\left(J;L^2(\Omega)\right)} \le \|\triangle_t u\|_{L^2\left(J;L^2(\Omega)\right)}.$$

Since $C_0^\infty\big(J\times\Omega\big)$ is dense in $V\cap L^2\big(J;X(\Omega)\big)$, (4.1) is obtained. □

The following estimates can be obtained in a similar way.

LEMMA 4.2. *It holds that*

$$\|u\|_{L^2\left(J;H_0^1(\Omega)\right)} \le \frac{C_p}{\nu}\|\triangle_t u\|_{L^2\left(J;L^2(\Omega)\right)}, \quad \forall u \in V \cap L^2\big(J;X(\Omega)\big), \tag{4.2}$$

where $C_p > 0$ is the Poincaré constant.

Proof. For arbitrary $u \in V \cap L^2\big(J; X(\Omega)\big)$ and almost everywhere $t \in J$, we have

$$\begin{aligned}\frac{1}{2}\frac{d}{dt}\left\|u(t)\right\|^2_{L^2(\Omega)} + \nu\left\|\nabla u(t)\right\|^2_{L^2(\Omega)^d} &= \left(u_t, u\right)_{L^2(\Omega)} + \nu\left(\nabla u, \nabla u\right)_{L^2(\Omega)^d} \\ &= \left(u_t - \nu\triangle u, u\right)_{L^2(\Omega)} \\ &\le \left\|\triangle_t u\right\|_{L^2(\Omega)}\left\|u\right\|_{L^2(\Omega)} \\ &\le \frac{C_p^2}{2\nu}\left\|\triangle_t u\right\|^2_{L^2(\Omega)} + \frac{\nu}{2C_p^2}\left\|u\right\|^2_{L^2(\Omega)}.\end{aligned}$$

Using Poincaré's inequality, we obtain

$$\frac{d}{dt}\left\|u(t)\right\|^2_{L^2(\Omega)} + \nu\left\|\nabla u(t)\right\|^2_{L^2(\Omega)^d} \le \frac{C_p^2}{\nu}\left\|\triangle_t u\right\|^2_{L^2(\Omega)}.$$

Integrating this on J, we get

$$\left\|u(T)\right\|^2_{L^2(\Omega)} + \nu\left\|\nabla u\right\|^2_{L^2\left(J;L^2(\Omega)\right)^d} \le \frac{C_p^2}{\nu}\left\|\triangle_t u\right\|^2_{L^2\left(J;L^2(\Omega)\right)}.$$

From $\left\|u(T)\right\|^2_{L^2(\Omega)} \ge 0$, (4.2) is obtained. □

The following lemma shows V^1L^2 stability for the semidiscretization operator P_h.

LEMMA 4.3 ([15, Lemma 3]). *It holds that*

$$\left\|P_h u\right\|_{V^1\left(J;L^2(\Omega)\right)} \le \left\|\triangle_t u\right\|_{L^2\left(J;L^2(\Omega)\right)}, \quad \forall u \in V \cap L^2\big(J; X(\Omega)\big). \tag{4.3}$$

Proof. For arbitrary $u \in V \cap L^2\big(J; X(\Omega)\big)$ and almost everywhere $t \in J$, by setting $v_h = (P_h u)_t$ in (2.3) we have

$$\begin{aligned}\left\|\frac{\partial P_h u}{\partial t}(t)\right\|^2_{L^2(\Omega)} + \frac{\nu}{2}\frac{d}{dt}\left\|\nabla P_h u(t)\right\|^2_{L^2(\Omega)^d} &= \left(\frac{\partial P_h u}{\partial t}, \frac{\partial P_h u}{\partial t}\right)_{L^2(\Omega)} + \nu\left(\nabla P_h u, \nabla\frac{\partial P_h u}{\partial t}\right)_{L^2(\Omega)^d} \\ &= \left(\frac{\partial u}{\partial t} - \nu\triangle u, \frac{\partial P_h u}{\partial t}\right)_{L^2(\Omega)}.\end{aligned}$$

Therefore, applying similar estimates in Lemma 4.1, the proof is completed. □

Similarly, by setting $v_h = P_h u$ in (2.3), we have the following $L^2H_0^1$ stability.

LEMMA 4.4. *It holds that*

$$\left\|P_h u\right\|_{L^2\left(J;H_0^1(\Omega)\right)} \le \frac{C_p}{\nu}\left\|\triangle_t u\right\|_{L^2\left(J;L^2(\Omega)\right)}, \quad \forall u \in V \cap L^2\big(J; X(\Omega)\big). \tag{4.4}$$

Now we can make the following assumptions about the approximation property of the H_0^1-projection P_h^1 defined in (2.1).

ASSUMPTION 4.5. *There exists a numerically computable constant $C_\Omega(h) > 0$ satisfying*

$$\left\|u - P_h^1 u\right\|_{H_0^1(\Omega)} \le C_\Omega(h)\left\|\triangle u\right\|_{L^2(\Omega)}, \quad \forall u \in H_0^1(\Omega) \cap X(\Omega), \tag{4.5}$$

$$\left\|u - P_h^1 u\right\|_{L^2(\Omega)} \le C_\Omega(h)\left\|u - P_h^1 u\right\|_{H_0^1(\Omega)}, \quad \forall u \in H_0^1(\Omega). \tag{4.6}$$

For example, if Ω is a bounded open interval in $\mathbb{R}$, and $S_h(\Omega)$ is the P1 finite element space, then Assumption 4.5 is satisfied by $C_\Omega(h) = \frac{h}{\pi}$, where h is the mesh size (see, e.g., [13]).

The following theorem is similar to [12, Lemma 2] but with a better result.

THEOREM 4.6 ([15, Theorem 4]). *Under Assumption 4.5, the following constructive a priori error estimate holds,*

$$\|u - P_h u\|_{L^2\left(J;H_0^1(\Omega)\right)} \le \frac{2}{\nu} C_\Omega(h) \|\triangle_t u\|_{L^2\left(J;L^2(\Omega)\right)}, \quad \forall u \in V \cap L^2\big(J; X(\Omega)\big). \tag{4.7}$$

Proof. For arbitrary $u \in V \cap L^2\big(J; X(\Omega)\big)$, we denote $u_\perp := u - P_h u$. Then, for almost everywhere $t \in J$, we have

$$\begin{aligned}
\frac{1}{2}\frac{d}{dt}\|u_\perp(t)\|_{L^2(\Omega)}^2 + \nu \|u_\perp(t)\|_{H_0^1(\Omega)}^2 &= \left(\frac{\partial u_\perp}{\partial t}(t), u_\perp(t)\right)_{L^2(\Omega)} + \nu \left(u_\perp(t), u_\perp(t)\right)_{H_0^1(\Omega)} \\
&= \left(\frac{\partial u_\perp}{\partial t}(t), u(t) - P_h^1 u(t)\right)_{L^2(\Omega)} + \nu \left(u_\perp(t), u(t) - P_h^1 u(t)\right)_{H_0^1(\Omega)},
\end{aligned}$$

where we have used (2.3). Thus, by using the property of H_0^1-projection, we obtain

$$\begin{aligned}
\frac{1}{2}\frac{d}{dt}\|u_\perp\|_{L^2(\Omega)}^2 + \nu \|u_\perp\|_{H_0^1(\Omega)}^2 &= \left(\frac{\partial u}{\partial t}, u - P_h^1 u\right)_{L^2(\Omega)} + \nu \left(u, u - P_h^1 u\right)_{H_0^1(\Omega)} - \left(\frac{\partial P_h u}{\partial t}, u - P_h^1 u\right)_{L^2(\Omega)} \\
&= \left(\frac{\partial u}{\partial t} - \nu\triangle u, u - P_h^1 u\right)_{L^2(\Omega)} - \left(\frac{\partial P_h u}{\partial t}, u - P_h^1 u\right)_{L^2(\Omega)} \\
&\le \left(\left\|\frac{\partial u}{\partial t} - \nu\triangle u\right\|_{L^2(\Omega)} + \left\|\frac{\partial P_h u}{\partial t}\right\|_{L^2(\Omega)}\right) \|u - P_h^1 u\|_{L^2(\Omega)}.
\end{aligned} \tag{4.8}$$

From (4.5) and (4.6) in Assumption 4.5, we have

$$\begin{aligned}
\left\|u(t) - P_h^1 u(t)\right\|_{L^2(\Omega)} &\le C_\Omega(h)^2 \|\triangle u(t)\|_{L^2(\Omega)}, \quad \text{a.e. } t \in J, \\
&= \frac{C_\Omega(h)^2}{\nu} \left\|\frac{\partial u}{\partial t}(t) - \nu\triangle u(t) - \frac{\partial u}{\partial t}(t)\right\|_{L^2(\Omega)} \\
&\le \frac{C_\Omega(h)^2}{\nu} \left(\|\triangle_t u\|_{L^2(\Omega)} + \|u_t\|_{L^2(\Omega)}\right).
\end{aligned}$$

Therefore, we have by (4.8)

$$\begin{aligned}
\frac{1}{2}\frac{d}{dt}\|u_\perp\|_{L^2(\Omega)}^2 + \nu \|u_\perp\|_{H_0^1(\Omega)}^2 &\le \frac{C_\Omega(h)^2}{\nu} \left(\|\triangle_t u\|_{L^2(\Omega)} + \left\|\frac{\partial P_h u}{\partial t}\right\|_{L^2(\Omega)}\right) \left(\|\triangle_t u\|_{L^2(\Omega)} + \left\|\frac{\partial u}{\partial t}\right\|_{L^2(\Omega)}\right) \\
&\le \frac{C_\Omega(h)^2}{\nu} \left(2\|\triangle_t u\|_{L^2(\Omega)}^2 + \left\|\frac{\partial P_h u}{\partial t}\right\|_{L^2(\Omega)}^2 + \left\|\frac{\partial u}{\partial t}\right\|_{L^2(\Omega)}^2\right).
\end{aligned}$$

Integrating this on J, from (4.1) and (4.3), we get

$$\begin{aligned}
\frac{1}{2}\|u_\perp(T)\|_{L^2(\Omega)}^2 + \nu \|u_\perp\|_{L^2 H_0^1}^2 &\le \frac{C_\Omega(h)^2}{\nu} \left(2\|\triangle_t u\|_{L^2 L^2}^2 + \left\|\frac{\partial P_h u}{\partial t}\right\|_{L^2 L^2}^2 + \left\|\frac{\partial u}{\partial t}\right\|_{L^2 L^2}^2\right) \\
&\le \frac{4}{\nu} C_\Omega(h)^2 \|\triangle_t u\|_{L^2\left(J;L^2(\Omega)\right)}^2,
\end{aligned}$$

which implies

$$\|u_\perp\|_{L^2\left(J;H_0^1(\Omega)\right)} \leq \frac{2}{\nu} C_\Omega(h) \|\triangle_t u\|_{L^2\left(J;L^2(\Omega)\right)}.$$

This completes the proof. □

Finally, we conclude this section by showing the L^2L^2 error estimates for P_h.

THEOREM 4.7 ([15, Theorem 5]). *Under Assumption 4.5, we have the following constructive a priori error estimates:*

$$\|u - P_h u\|_{L^2\left(J;L^2(\Omega)\right)} \leq 4C_\Omega(h) \|u - P_h u\|_{L^2\left(J;H_0^1(\Omega)\right)}, \quad \forall u \in V. \tag{4.9}$$

The proof of this theorem is given in [15].

5. Constructive estimates for full discretization. We introduced, in Section 3, a full discrete projection $P_h^k u$ for the solution u of the heat equation (1.1) and explained that it is computable by using the fundamental matrix for an ODE system generated by the semidiscretization. We now derive the constructive a priori error estimates for the full discrete projection $P_h^k u$ and the approximation u_h^k. As described in Section 2, this full discretization operator is composed of the semidiscretization in space and interpolation in time, i.e., $P_h^k = \Pi_k P_h$. Therefore, in the discussion below, we will use the approximation properties for the semidiscrete projection P_h derived in the previous section as well as the interpolation Π_k to obtain the desired estimates.

First of all, we assume the inverse estimates on $S_h(\Omega)$.

ASSUMPTION 5.1. *There exists a constant $C_{inv}(h) > 0$ satisfying*

$$\|u_h\|_{H_0^1(\Omega)} \leq C_{inv}(h) \|u_h\|_{L^2(\Omega)}, \quad \forall u_h \in S_h(\Omega). \tag{5.1}$$

For example, if Ω is a bounded open interval in $\mathbb{R}$, and $S_h(\Omega)$ is the P1 finite element space, then Assumption 5.1 is satisfied with $C_{\mathrm{inv}}(h) = \frac{\sqrt{12}}{h_{\min}}$, where $h_{\min}$ is the minimum mesh size for Ω (see, e.g., [17, Theorem 1.5]).

For the interpolation operator, we make the following assumption.

ASSUMPTION 5.2. *There exists a constant $C_J(k) > 0$ satisfying*

$$\|u - \Pi_k u\|_{L^2(J)} \leq C_J(k) \|u\|_{V^1(J)}, \quad \forall u \in V^1(J). \tag{5.2}$$

For example, if $V_k^1(J)$ is the P1 finite element space, then Assumption 5.2 is satisfied by $C_J(k) = \frac{k}{\pi}$ (see, e.g., [17, Theorem 2.4]).

The following theorem shows $L^2H_0^1$ stability for the full discretization operator P_h^k.

LEMMA 5.3. *Under assumptions 5.1 and 5.2, we have the estimates:*

$$\left\|P_h^k u\right\|_{L^2\left(J;H_0^1(\Omega)\right)} \leq \left(\frac{C_p}{\nu} + C_{inv}(h)C_J(k)\right) \|\triangle_t u\|_{L^2\left(J;L^2(\Omega)\right)}, \quad \forall u \in V \cap L^2\big(J;X(\Omega)\big). \tag{5.3}$$

Proof. For arbitrary $u \in V \cap L^2\big(J; X(\Omega)\big)$, from (5.1), (5.2), (4.3), and (4.4), we have

$$\begin{aligned}
\left\|P_h^k u\right\|_{L^2\left(J;H_0^1(\Omega)\right)} &\le \left\|\Pi_k P_h u - P_h u\right\|_{L^2\left(J;H_0^1(\Omega)\right)} + \left\|P_h u\right\|_{L^2\left(J;H_0^1(\Omega)\right)} \\
&\le C_{\mathrm{inv}}(h) \left\|\Pi_k P_h u - P_h u\right\|_{L^2\left(J;L^2(\Omega)\right)} + \left\|P_h u\right\|_{L^2\left(J;H_0^1(\Omega)\right)} \\
&\le C_{\mathrm{inv}}(h) C_J(k) \left\|P_h u\right\|_{V^1\left(J;L^2(\Omega)\right)} + \left\|P_h u\right\|_{L^2\left(J;H_0^1(\Omega)\right)} \\
&\le \left(C_{\mathrm{inv}}(h) C_J(k) + \frac{C_p}{\nu}\right) \left\|\triangle_t u\right\|_{L^2\left(J;L^2(\Omega)\right)}.
\end{aligned}$$

This completes the proof. □

We obtain the following V^1L^2 stability.

THEOREM 5.4. *Let $V_k^1(J)$ be the P1 finite element space. Under assumptions 5.1 and 5.2, we have the estimates:*

$$\left\|P_h^k u\right\|_{V^1\left(J;L^2(\Omega)\right)} \le 2 \left\|\triangle_t u\right\|_{L^2\left(J;L^2(\Omega)\right)}, \quad \forall u \in V \cap L^2\big(J; X(\Omega)\big). \tag{5.4}$$

Proof. Since, for the P1 finite element space, it is seen that the V^1-projection P_1^k coincides with the interpolation, e.g., [2, Theorem 2.2], we have $P_h^k = P_1^k P_h$. Therefore, for an arbitrary $u \in V \cap L^2\big(J; X(\Omega)\big)$, we have

$$\left\|P_1^k P_h u(x,\cdot) - P_h u(x,\cdot)\right\|_{V^1(J)} \le \left\|P_h u(x,\cdot)\right\|_{V^1(J)}, \quad \forall x \in \Omega.$$

Integrating this on Ω, we get

$$\left\|P_1^k P_h u - P_h u\right\|_{V^1\left(J;L^2(\Omega)\right)} \le \left\|P_h u\right\|_{V^1\left(J;L^2(\Omega)\right)}.$$

On the other hand, from (4.3), we obtain

$$\begin{aligned}
\left\|P_h^k u\right\|_{V^1\left(J;L^2(\Omega)\right)} &\le \left\|P_1^k P_h u - P_h u\right\|_{V^1\left(J;L^2(\Omega)\right)} + \left\|P_h u\right\|_{V^1\left(J;L^2(\Omega)\right)} \\
&\le 2 \left\|\triangle_t u\right\|_{L^2\left(J;L^2(\Omega)\right)},
\end{aligned}$$

which proves the desired estimates. □

The above V^1L^2 stability was obtained in neither [12] nor [14]. Moreover, we believe there are no existing estimates of the form (5.4) for any full discrete approximations.

Next, we describe the constructive a priori $L^2H_0^1$ error estimates for P_h^k.

THEOREM 5.5. *Under assumptions 4.5, 5.1, and 5.2, we have the following constructive a priori error estimates:*

$$\left\|u - P_h^k u\right\|_{L^2\left(J;H_0^1(\Omega)\right)} \le C_1(h,k) \left\|\triangle_t u\right\|_{L^2\left(J;L^2(\Omega)\right)}, \quad \forall u \in V \cap L^2\big(J; X(\Omega)\big), \tag{5.5}$$

where $C_1(h,k) := \frac{2}{\nu} C_\Omega(h) + C_{inv}(h) C_J(k)$.

Proof. For an arbitrary $u \in V \cap L^2\big(J; X(\Omega)\big)$, from (4.7), (5.1), (5.2), and (4.3), we have

$$\begin{aligned}\left\|u - P_h^k u\right\|_{L^2\left(J;H_0^1(\Omega)\right)} &\le \left\|u - P_h u\right\|_{L^2\left(J;H_0^1(\Omega)\right)} + \left\|P_h u - \Pi_k P_h u\right\|_{L^2\left(J;H_0^1(\Omega)\right)} \\ &\le \frac{2}{\nu} C_\Omega(h) \left\|\triangle_t u\right\|_{L^2\left(J;L^2(\Omega)\right)} + C_{\mathrm{inv}}(h) C_J(k) \left\|\frac{\partial P_h u}{\partial t}\right\|_{L^2\left(J;L^2(\Omega)\right)} \\ &\le \left(\frac{2}{\nu} C_\Omega(h) + C_{\mathrm{inv}}(h) C_J(k)\right) \left\|\triangle_t u\right\|_{L^2\left(J;L^2(\Omega)\right)},\end{aligned}$$

which concludes the proof. □

Finally in this section, we describe the constructive a priori L^2L^2 error estimates for P_h^k.

THEOREM 5.6. *Under assumptions 4.5 and 5.2, we have the following constructive a priori error estimates:*

$$\left\|u - P_h^k u\right\|_{L^2\left(J;L^2(\Omega)\right)} \le C_0(h,k) \left\|\triangle_t u\right\|_{L^2\left(J;L^2(\Omega)\right)}, \quad \forall u \in V \cap L^2\big(J; X(\Omega)\big), \tag{5.6}$$

where $C_0(h,k) = \frac{8}{\nu} C_\Omega(h)^2 + C_J(k)$.

Proof. For an arbitrary $u \in V \cap L^2\big(J; X(\Omega)\big)$, from (4.9), (5.2), (4.7), and (4.3), we have

$$\begin{aligned}\left\|u - P_h^k u\right\|_{L^2\left(J;L^2(\Omega)\right)} &\le \left\|u - P_h u\right\|_{L^2\left(J;L^2(\Omega)\right)} + \left\|P_h u - \Pi_k P_h u\right\|_{L^2\left(J;L^2(\Omega)\right)} \\ &\le 4C_\Omega(h) \left\|u - P_h u\right\|_{L^2\left(J;H_0^1(\Omega)\right)} + C_J(k) \left\|\frac{\partial P_h u}{\partial t}\right\|_{L^2\left(J;L^2(\Omega)\right)} \\ &\le 4C_\Omega(h) \frac{2C_\Omega(h)}{\nu} \left\|\triangle_t u\right\|_{L^2\left(J;L^2(\Omega)\right)} + C_J(k) \left\|\triangle_t u\right\|_{L^2\left(J;L^2(\Omega)\right)}.\end{aligned}$$

Therefore, this completes the proof. □

REMARK 5.7. *Since $C_{inv}(h)$ generally has the order $O(h^{-1})$, if we take $k = h^2$, then the estimates in Theorem 5.5 give an $O(h)$ error estimate. On the other hand, if we use the higher-order derivative of u, e.g., $\left\|\nabla u_t\right\|_{L^2\left(J;L^2(\Omega)\right)}$ on the right-hand side of* (5.5)*, then, from the argument in the proof, we can easily obtain the constructive estimates with order $O(h+k)$. Therefore, we could say that our estimates, i.e., the order of the constants $C_1(h,k)$ in Theorem 5.5, should be optimal. Moreover, the estimates in Theorem 5.6 are $O(h^2+k)$, which is clearly an optimal error bound in the sense of a concerned norm. And if we choose $k = h^2$, then it yields $O(h^2)$ estimates. But, of course, the value of the constant may not be the best possible, and there is some possibility to improve the magnitude, which is desirable in order to realize an efficient numerical verification method(cf. [13]).*

6. Conclusions. We presented constructive a priori error estimates for the full discrete approximation for the heat equation. In particular, it should be emphasized that the time derivative of this full discretization scheme has stability for an external force with L^2L^2 regularity, and our error estimate has an optimal order of convergence. These results should greatly contribute to the efficient implementation of the numerical verification method for solutions of nonlinear evolutional problems.

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Appendix A. Symmetricity of $L_\phi^{-1}D_\phi$ for Q1 element.

In general, the matrix $L_\phi^{-1}D_\phi$ introduced in Section 3 is not symmetric, but we can show it is symmetric for the Q1 finite element space on a rectangular domain Ω with uniform mesh.

First we consider the one-dimensional case. If the basis consists of so called '*hat functions*' with uniform mesh size h, then it is readily seen that matrices L_ϕ and D_ϕ

can be represented as the following tri-diagonal form:

$$L_\phi = \frac{h}{6}\begin{pmatrix} 4 & 1 & & & \\ 1 & 4 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & 1 & 4 & 1 \\ & & & 1 & 4 \end{pmatrix}, \quad D_\phi = \frac{1}{h}\begin{pmatrix} 2 & -1 & & & \\ -1 & 2 & -1 & & \\ & \ddots & \ddots & \ddots & \\ & & -1 & 2 & -1 \\ & & & -1 & 2 \end{pmatrix}. \tag{A.1}$$

THEOREM A.1. *For the matrices in* (A.1)*, $L_\phi^{-1}D_\phi$ is symmetric positive definite.*

Proof. Note that, from the symmetricity of L_ϕ and D_ϕ, the following equivalence relation holds:

$$L_\phi^{-1}D_\phi = \left(L_\phi^{-1}D_\phi\right)^T \Longleftrightarrow L_\phi^{-1}D_\phi = D_\phi L_\phi^{-1} \Longleftrightarrow D_\phi L_\phi = L_\phi^T D_\phi^T.$$

Therefore, it suffices to show the symmetricity of $D_\phi L_\phi$. By using the representation (A.1), some simple calculations yield the explicit form

$$D_\phi L_\phi = \frac{1}{6}\begin{pmatrix} 7 & -2 & -1 & & & \\ -2 & 6 & -2 & -1 & & \\ -1 & -2 & 6 & -2 & -1 & \\ & \ddots & \ddots & \ddots & \ddots & \\ & -1 & -2 & 6 & -2 & -1 \\ & & -1 & -2 & 6 & -2 \\ & & & -1 & -2 & 7 \end{pmatrix}.$$

Thus the symmetricity of the above matrix is clear. The positive definiteness was already given by the proposition in Section 3. □

For the two-dimensional case, the basis of the Q1 finite element space is constituted by the tensor product of the one-dimensional case. Therefore, the corresponding matrices can be represented as

$$L_\phi = L_{\phi_x} \otimes L_{\phi_y}, \quad D_\phi = D_{\phi_x} \otimes L_{\phi_y} + L_{\phi_x} \otimes D_{\phi_y},$$

where $\otimes$ is the Kronecker product, and ϕ_x and ϕ_y correspond to the bases for x and y directions, respectively. Then observe that

$$\begin{aligned} L_\phi^{-1}D_\phi &= \left(L_{\phi_x}^{-1} \otimes L_{\phi_y}^{-1}\right)\left(D_{\phi_x} \otimes L_{\phi_y} + L_{\phi_x} \otimes D_{\phi_y}\right) \\ &= \left(L_{\phi_x}^{-1}D_{\phi_x}\right) \otimes I_{\phi_y} + I_{\phi_x} \otimes \left(L_{\phi_y}^{-1}D_{\phi_y}\right), \end{aligned}$$

where I_{ϕ_x} and I_{ϕ_y} are the identity matrices. The matrices $L_{\phi_x}^{-1}D_{\phi_x}$ and $L_{\phi_y}^{-1}D_{\phi_y}$ are symmetric positive definite by Theorem A.1. Therefore, by the fact that the Kronecker product of the symmetric positive definite matrix and the identity matrix is also symmetric positive definite, $L_\phi^{-1}D_\phi$ has this same property.

For the three-dimensional case, we obtain the same conclusion using similar arguments.