Space-Time Finite Element Methods for the Initial Temperature Reconstruction

Ulrich Langer, Olaf Steinbach, Fredi Tröltzsch, and Huidong Yang

1 Introduction

In this work, we investigate the applicability of unstructured space-time methods to the numerical solution of inverse problems considering the classical inverse problem of the reconstruction of the initial temperature in the heat equation from an observation of the temperature $u_T^\delta \in L^2(\Omega)$ at a finite time horizon as model problem: Find the initial temperature $u_0^\delta(\cdot) := u(\cdot, 0) \in L^2(\Omega)$ on Σ_0 of the solution u of the backward heat equation

$$\partial_t u - \Delta_x u = 0 \quad \text{in } Q, \quad u = 0 \quad \text{on } \Sigma, \quad u = u_T^\delta \quad \text{on } \Sigma_T, \tag{1}$$

where $Q := \Omega \times (0, T)$ denotes the space-time cylinder with the boundary $\partial Q = \overline{\Sigma} \cup \overline{\Sigma}_0 \cup \overline{\Sigma}_T$, $\Sigma := \partial\Omega \times (0, T)$, $\Sigma_0 := \Omega \times \{0\}$, $\Sigma_T := \Omega \times \{T\}$, the bounded Lipschitz domain $\Omega \subset \mathbb{R}^d$, $d \in \{1, 2, 3\}$, and a finite time horizon $T > 0$. The observed terminal temperature u_T^δ may contain some noise characterized by the noise level $\delta \geq 0$,

$$\|u_T^\delta - u_T\|_{L^2(\Omega)} \leq \delta, \tag{2}$$

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where $u_T = u(\cdot, T) \in L^2(\Omega)$ represents the unpolluted exact data.

In contrast to the forward heat equation with known initial data, the backward heat equation (1) is severely ill-posed; see [2, Example 2.9]. In fact, the solution of (1) does not continuously depend on the data u_T^δ even when the solution exists. Following the notation in [2], the problem (1) may be reformulated as an abstract operator equation in a more general setting: Find $u_0 \in \mathcal{X}$ such that

$$Su_0 = u_T, \qquad (3)$$

where $S : \mathcal{X} \to \mathcal{Y}$ denotes a bounded linear operator between two Hilbert spaces $\mathcal{X}$ and $\mathcal{Y}$. It is clear that there does not exist a continuous inverse operator $S^{-1} : \mathcal{Y} \to \mathcal{X}$ in general. Therefore, we consider a regularized solution, depending on the choice of Tikhonov's regularization parameter $\varrho := \varrho(\delta)$,

$$u_0^{\delta,\varrho} := (S^*S + \varrho I)^{-1} S^* u_T^\delta,$$

as the unique minimizer of the Tikhonov functional [9]

$$\mathcal{J}_\varrho(z) := \frac{1}{2} \|Sz - u_T^\delta\|_{\mathcal{Y}}^2 + \frac{\varrho}{2} \|z\|_{\mathcal{X}}^2. \qquad (4)$$

It is well known that we have the convergence

$$\lim_{\delta \to 0} u_0^{\delta,\varrho} = u_0^\dagger \text{ in } \mathcal{X}, \text{ if the conditions } \quad \lim_{\delta \to 0} \varrho(\delta) = 0 \text{ and } \lim_{\delta \to 0} \frac{\delta^2}{\varrho(\delta)} = 0$$

are satisfied. Here, $u_0^\dagger$ denotes the best-approximated solution to the operator equation (3); see [2, Theorem 5.2] for a more detailed discussion, and also [1, 7].

The main focus of this work is to describe a space-time finite element method (FEM) on fully unstructured simplicial meshes to solve the minimization problem (4) subject to the solution of the backward heat equation (1). Such a space-time method has been studied for the forward heat equation in [8], and for other parabolic optimal control problems in [5, 6].

The remainder of this paper is structured as follows: In Section 2, we discuss the related optimal control problem. Its solution is obtained by the optimality system consisting of the (forward) heat equation, the adjoint heat equation, and the gradient equation. Based on the Banach–Nečas–Babuška theory [3], we establish unique solvability of the resulting coupled system, when eliminating the unknown initial datum. In Section 3, for the numerical solution of the inverse problem (1), we first consider the discrete optimal control problem, which is based on the space-time discretization of the forward problem. The solution is characterized by a discrete gradient equation, which turns out to be the Schur complement system of the discretized coupled variational formulation. First numerical results are reported in Section 4. These results show the potential of the space-time approach proposed. Finally, some conclusions are drawn in Section 5.

2 The related optimal control problem

In our case, the Hilbert spaces $\mathcal{X}$ and $\mathcal{Y}$ are specified as $\mathcal{X} = \mathcal{Y} = L^2(\Omega)$, and the image Sz of the operator $S : L^2(\Omega) \to L^2(\Omega)$ in the Tikhonov functional (4) is defined by the solution $u \in X := L^2(0, T; H_0^1(\Omega)) \cap H^1(0, T; H^{-1}(\Omega))$ of the forward heat conduction problem

$$\partial_t u - \Delta_x u = 0 \quad \text{in } Q, \quad u = 0 \quad \text{on } \Sigma, \quad u = z \quad \text{on } \Sigma_0, \tag{5}$$

and its evaluation on Σ_T, i.e., $(Sz)(x) = u(x, T), x \in \Omega$. Here, the control $z \in L^2(\Omega)$ represents the initial data in (5). Rewriting the minimization of the functional (4) in terms of z, we obtain the *optimal control problem*

$$\mathcal{J}_\varrho(z) := \frac{1}{2} \|u(x, T) - u_T^\delta\|_{L^2(\Omega)}^2 + \frac{\varrho}{2} \|z\|_{L^2(\Omega)}^2 \to \min_{z \in L^2(\Omega)}, \tag{6}$$

where the *state* $u \in X$ is associated to the *control* z subject to (5).

To set up the necessary and sufficient optimality conditions for the optimal control z with associated state u, we introduce the adjoint equation

$$-\partial_t p - \Delta_x p = 0 \quad \text{in } Q, \quad p = 0 \quad \text{on } \Sigma, \quad p = u - u_T^\delta \quad \text{on } \Sigma_T. \tag{7}$$

It has a unique solution $p \in X$, the *adjoint state*. The adjoint equation can be derived by a formal Lagrangian technique as in [10]. If z is the optimal control with associated state $u \in X$, then a unique adjoint state $p \in X$ solving (7) exists such that the *gradient equation*

$$p + \varrho z = 0 \quad \text{on } \Sigma_0 \tag{8}$$

is satisfied. Using this equation, we can eliminate the unknown initial datum z in the state equation (5) to conclude

$$\partial_t u - \Delta_x u = 0 \quad \text{in } Q, \quad u = 0 \quad \text{on } \Sigma, \quad u = -\frac{1}{\varrho} p \quad \text{on } \Sigma_0 \tag{9}$$

for the optimal state u. The *reduced optimality system* (7),(9) is necessary and sufficient for optimality of u with associated adjoint state p. In what follows, we will describe a space-time finite element approximation of this system.

The space-time variational formulation of the heat equation in (9) (without initial condition) is to find $u \in X$ such that

$$b(u, v) := \int_0^T \int_\Omega \left[\partial_t u(x, t) v(x, t) + \nabla_x u(x, t) \cdot \nabla_x v(x, t) \right] dx \, dt = 0 \tag{10}$$

is satisfied for all $v \in Y := L^2(0, T; H_0^1(\Omega))$. The spaces X and Y are equipped with the norms

$$\|v\|_Y = \|\nabla_x v\|_{L^2(Q)} \quad \text{and} \quad \|u\|_X = \sqrt{\|\partial_t u\|_{Y^*}^2 + \|u\|_Y^2} = \sqrt{\|w_u\|_Y^2 + \|u\|_Y^2},$$

with $w_u \in Y$ being the unique solution of the variational problem

$$\int_0^T \int_\Omega \nabla_x w_u(x,t) \cdot \nabla_x v(x,t)\, dx\, dt = \int_0^T \int_\Omega \partial_t u(x,t)\, v(x,t)\, dx\, dt \quad \forall\, v \in Y.$$

We multiply the adjoint heat equation (7) by a test function $q \in X$, integrate over Q, and apply integration by parts both in space and time. Then we insert the terminal data $u(T) - u_T^\delta$ of p in the arising term $p(T)$, and substitute the term $p(0)$ by $-\rho z = -\rho u(0)$ in view of (8). In this way, we arrive at the weak form of the adjoint problem (7)

$$\begin{aligned}
0 &= \int_0^T \int_\Omega \Big[-\partial_t p(x,t)\, q(x,t) - \Delta_x p(x,t)\, q(x,t) \Big] dx\, dt \\
&= -\int_\Omega [u(x,T) - u_T^\delta(x)]\, q(x,T)\, dx - \varrho \int_\Omega u(x,0)\, q(x,0)\, dx \\
&\quad + \int_0^T \int_\Omega \Big[p(x,t)\, \partial_t q(x,t) + \nabla_x p(x,t) \cdot \nabla_x q(x,t) \Big] dx\, dt\,.
\end{aligned}$$

We end up with the variational problem to find $(u,p) \in X \times Y$ such that

$$\mathcal{B}(u,p;v,q) = \langle u_T^\delta, q(T) \rangle_{L^2(\Omega)} \quad \forall\, (v,q) \in Y \times X, \tag{11}$$

where the bilinear form $\mathcal{B}(\cdot,\cdot;\cdot,\cdot)$ is given as

$$\mathcal{B}(u,p;v,q) := b(u,v) - b(q,p) + \langle u(T), q(T) \rangle_{L^2(\Omega)} + \varrho\, \langle u(0), q(0) \rangle_{L^2(\Omega)}\,.$$

We note that the bilinear form $b(\cdot,\cdot)$, as defined by (10), is bounded:

$$|b(u,v)| \leq \sqrt{2}\, \|u\|_X \|v\|_Y \quad \forall\, u \in X, v \in Y.$$

Since X is continuously embedded in $C([0,T]; L^2(\Omega))$, there is a positive constant μ such that $\|u(0)\|_{L^2(\Omega)} \leq \mu\, \|u\|_X$ and $\|u(T)\|_{L^2(\Omega)} \leq \mu\, \|u\|_X$,

$$\mu = \left(1 + \frac{1}{2} \left[\frac{c_F}{T} \right]^2 + \sqrt{\frac{1}{4} \left[\frac{c_F}{T} \right]^4 + \left[\frac{c_F}{T} \right]^2} \right)^{1/2},$$

where c_F is the constant in Friedrichs' inequality in $H_0^1(\Omega)$. With these ingredients, we are in the position to prove that the bilinear form $\mathcal{B}(\cdot,\cdot;\cdot,\cdot)$ is bounded, i.e., for all $(u,p), (q,v) \in X \times Y$, there holds

$$|\mathcal{B}(u,p;v,q)| \leq 2\,(1+\varrho)\,\mu^2\, \sqrt{\|u\|_X^2 + \|p\|_Y^2}\, \sqrt{\|q\|_X^2 + \|v\|_Y^2}\,.$$

Moreover, we can establish the following inf-sup stability condition which can be proved similarly to [5, Lemma 3.2].

Lemma 1 *For simplicity, let us assume $\varrho \in (0, 1]$. Then there holds the inf-sup stability condition*

$$\frac{3}{10} \varrho \sqrt{\|u\|_X^2 + \|p\|_Y^2} \leq \sup_{0 \neq (v,q) \in Y \times X} \frac{\mathcal{B}(u, p; v, q)}{\sqrt{\|q\|_X^2 + \|v\|_Y^2}} \quad \forall (u, p) \in X \times Y.$$

Moreover, for any $(0, 0) \neq (v, q) \in Y \times X$, there exist $(\overline{u}, \overline{p}) \in X \times Y$ satisfying

$$\mathcal{B}(\overline{u}, \overline{p}; v, q) > 0.$$

Now, using the Banach–Nečas–Babuška theorem (see, e.g., [3]), we can ensure well-posedness of the variational optimality problem (11) for any fixed positive regularization parameter ϱ.

3 Space-time finite element methods

For the space-time finite element discretization of the variational formulation (11), we first introduce conforming finite element spaces $X_h \subset X$ and $Y_h \subset Y$. In particular, we consider $X_h = Y_h$ spanned by piecewise linear continuous basis functions which are defined with respect to some admissible decomposition of the space-time domain Q into shape regular simplicial finite elements. In addition, we will use the subspace $Y_{0,h} \subset Y_h$ of basis functions with zero initial values. Moreover, $Z_h \subset L^2(\Omega)$ is a finite element space to discretize the control z. The space-time finite element discretization of the forward problem (5) reads to find $u_h \in X_h$ such that

$$b(u_h, v_h) = 0 \quad \forall v_h \in Y_{0,h}, \quad \langle u_h - z_h, v_h \rangle_{L^2(\Sigma_0)} = 0 \quad \forall v_h \in Y_h \backslash Y_{0,h}. \quad (12)$$

When denoting the degrees of freedom of u_h at Σ_0, at Σ_T, and in Q by $\underline{u}_0$, $\underline{u}_T$, and $\underline{u}_I$, respectively, the variational formulation (12) is equivalent to the linear system

$$\begin{pmatrix} M_{00} & & \\ K_{0I} & K_{II} & K_{TI} \\ & K_{IT} & K_{TT} \end{pmatrix} \begin{pmatrix} \underline{u}_0 \\ \underline{u}_I \\ \underline{u}_T \end{pmatrix} = \begin{pmatrix} M_h^\top \underline{z} \\ \underline{0} \\ \underline{0} \end{pmatrix},$$

where the block entries of the stiffness matrix K_h and the mass matrices M_{00} and M_h are defined accordingly. After eliminating $\underline{u}_0$, the resulting system corresponds to the space-time finite element approach as considered in [8]. In particular, we can compute $\underline{u}_T = A_h \underline{z}$ to determine $u_h(T)$ in dependency on the initial datum z_h, where

$$A_h = \left(K_{TT} - K_{IT} K_{II}^{-1} K_{TI} \right)^{-1} K_{IT} K_{II}^{-1} K_{0I} M_{00}^{-1} M_h^\top = \widetilde{A}_h M_h^\top.$$

Instead of the cost functional (6), we now consider the discrete cost functional

$$\mathcal{J}_{\varrho,h}(z_h) = \frac{1}{2} \|u_h(x,T) - u_T^\delta\|_{L^2(\Omega)}^2 + \frac{\varrho}{2} \|z_h\|_{L^2(\Omega)}^2$$
$$= \frac{1}{2} (A_h^\top M_{TT} A_h \underline{z}, \underline{z}) - (A_h^\top \underline{f}, \underline{z}) + \frac{1}{2} \|u_T^\delta\|_{L^2(\Omega)}^2 + \frac{\varrho}{2} (\overline{M}_h \underline{z}, \underline{z}),$$

whose minimizer is given as the solution of the linear system

$$A_h^\top (M_{TT} A_h \underline{z} - \underline{f}) + \varrho \overline{M}_h \underline{z} = \underline{0}. \tag{13}$$

Note that M_{TT} is the mass matrix formed by the basis functions of X_h at Σ_T, $\overline{M}_h$ is the mass matrix related to the control space Z_h, and $\underline{f}$ is the load vector of the target u_T^δ tested with basis functions from X_h at Σ_T. When inserting $\underline{u}_T = A_h \underline{z}$ and introducing $\underline{p}_0 := \widetilde{A}_h^\top (M_{TT} \underline{u}_T - \underline{f})$, $\underline{p}_T := (K_{TT} - K_{IT} K_{II}^{-1} K_{TI})^{-\top} (M_{TT} \underline{u}_T - \underline{f})$, $\underline{p}_I := -K_{II}^{-\top} K_{IT}^\top \underline{p}_T$, this finally results in the linear system to be solved:

$$\begin{pmatrix} & & & & -M_{00} & -K_{0I}^\top & \\ & & & & & -K_{II}^\top & -K_{IT}^\top \\ & M_{TT} & & & & -K_{TI}^\top & -K_{TT}^\top \\ & & \varrho\overline{M}_h & M_h & & & \\ M_{00} & & -M_h^\top & & & & \\ K_{0I} & K_{II} & K_{TI} & & & & \\ & K_{IT} & K_{TT} & & & & \end{pmatrix} \begin{pmatrix} \underline{u}_0 \\ \underline{u}_I \\ \underline{u}_T \\ \underline{z} \\ \underline{p}_0 \\ \underline{p}_I \\ \underline{p}_T \end{pmatrix} = \begin{pmatrix} \underline{0} \\ \underline{0} \\ \underline{f} \\ \underline{0} \\ \underline{0} \\ \underline{0} \\ \underline{0} \end{pmatrix}. \tag{14}$$

In the particular case, when $Z_h = Y_{h|\Sigma_0} \subset H_0^1(\Omega)$ is the space of piecewise linear basis functions as well, the mass matrices $M_{00} = \overline{M}_h = M_h$ coincide, and therefore we can eliminate $\underline{z} = \underline{u}_0$ and $\underline{p}_0 = -\varrho\underline{z} = -\varrho\underline{u}_0$ to obtain

$$\begin{pmatrix} \varrho M_{00} & & & -K_{0I}^\top & \\ & & & -K_{II}^\top & -K_{IT}^\top \\ & & M_{TT} & -K_{TI}^\top & -K_{TT}^\top \\ K_{0I} & K_{II} & K_{TI} & & \\ & K_{IT} & K_{TT} & & \end{pmatrix} \begin{pmatrix} \underline{u}_0 \\ \underline{u}_I \\ \underline{u}_T \\ \underline{p}_I \\ \underline{p}_T \end{pmatrix} = \begin{pmatrix} \underline{0} \\ \underline{0} \\ \underline{f} \\ \underline{0} \\ \underline{0} \end{pmatrix}. \tag{15}$$

Note that (15) is nothing but the Galerkin discretization of the variational formulation (11) when using $X_h \subset X$ and $Y_{0,h} \subset Y$ as finite element ansatz and test spaces. Obviously, the linear system (13) and, therefore, (15) are uniquely solvable.

In practice, the noise level $\delta \geq 0$ is usually given by the measurement environment, and one has to choose suitable discretization and regularization parameters h and ρ. This is well investigated for linear inverse problems; see, e.g., the classical book by Tikhonov and Arsenin [9] and the more recent publications [2, 4]. In our numerical experiments presented in the next section, we only play with the parmeters δ and h for a fixed small ϱ.

4 Numerical results

We take $\Omega = (0, 1)$ and $T = 1$, i.e., $Q = (0, 1)^2$, and consider the manufactured observation data $u_T^\delta(x) := e^{-\pi^2} \sin(\pi x) + \delta \sin(10\pi x)$ with some noise represented by the second term; see exact and noisy data with $\delta \in \{0, 10^{-5}, 5 \cdot 10^{-6}, 2.5 \cdot 10^{-6}\}$ in Fig. 1. To study the convergence of the space-time finite element solution to the exact
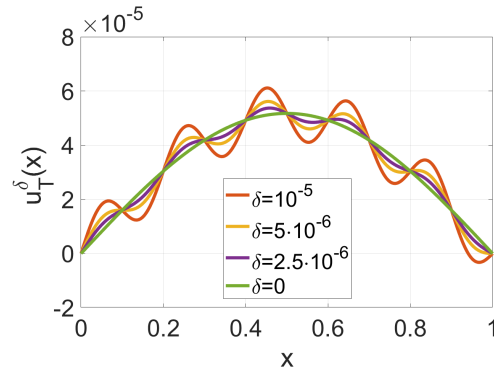

Fig. 1: Comparison of the exact ($\delta = 0$) and noisy ($\delta > 0$) observation data.

initial datum $\sin(\pi x)$, we use the target $u_T(x) = e^{-\pi^2} \sin(\pi x)$ without any noise. The reconstructed initial data with respect to a varying mesh size are illustrated in the left plot of Fig. 2, where $\varrho = 10^{-14}$. We clearly see the convergence of the approximations to the exact initial datum with respect to the mesh refinement. The right plot of Fig. 2 shows the reconstructed initial approximation with different noise levels δ. For a decreasing δ, we observe an improved reconstruction.

5 Conclusions

We have applied the space-time FEM from [8] to the numerical solution of the classical inverse heat conduction problem to determine the initial datum from measured observation data at some time horizon T. The numerical results show the potential of this approach for more interesting inverse problems. The space-time FEM is very much suited for designing smart adaptive algorithms along the line proposed in [4] determining the optimal choice of ϱ and h for a given noise level δ in a multilevel (nested iteration) setting.
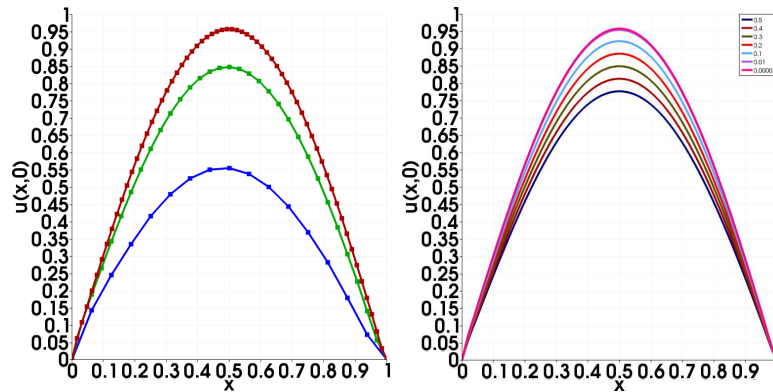
Fig. 2: Convergence of the reconstructed initial data with respect to the mesh refinement $h \in \{1/16, 1/32, 1/64\}$, $\delta = 0$, $\varrho = 10^{-14}$ (left), and convergence with respect to the noise level $\delta \in \{0.5, 0.4, 0.3, 0.2, 10^{-1}, 10^{-3}, 10^{-5}\}$, $h = 1/64$, $\varrho = 10^{-14}$ (right).

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