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Technische Universität Graz
Institut für Angewandte Mathematik
Steyrergasse 30
A 8010 Graz

WWW: `http://www.applied.math.tugraz.at`

Space–time finite element methods for parabolic evolution equations: Discretization, a posteriori error estimation, adaptivity and solution

Olaf Steinbach[1], Huidong Yang[2]

[1]Institut für Angewandte Mathematik, TU Graz,
Steyrergasse 30, 8010 Graz, Austria

o.steinbach@tugraz.at

[2]Johann Radon Institute for Computational and Applied Mathematics,
Altenberger Strasse 69, 4040 Linz, Austria

huidong.yang@oeaw.ac.at

Abstract

In this work, we present an overview on the development of space–time finite element methods for the numerical solution of some parabolic evolution equations with the heat equation as a model problem. Instead of using more standard semi–discretization approaches such as the method of lines or Rothe's method, our specific focus is on continuous space–time finite element discretizations in space and time simultaneously. While such discretizations bring more flexibility to the space–time finite element error analysis and error control, they usually lead to higher computational complexity and memory consumptions in comparison with standard time–stepping methods. Therefore, progress on a posteriori error estimation and respective adaptive schemes in the space–time domain is reviewed, which aims to save a number of degrees of freedom, and hence reduces complexity, and recovers optimal order error estimates. Further, we provide a summary on recent advances in efficient parallel space–time iterative solution strategies for the related large–scale linear systems of algebraic equations, that are crucial to make such all–at–once approaches competitive with traditional time stepping methods. Finally, some numerical results are given to demonstrate the benefits of a particular adaptive space–time finite element method, the robustness of some space–time algebraic multigrid methods, and the applicability of space–time finite element methods for the solution of some parabolic optimal control problem.

1 Introduction

Throughout this paper, we mainly focus on a space–time finite element solution for the following parabolic model problem:

$$
\begin{aligned}
\partial_t u(x,t) - \Delta_x u(x,t) &= f(x,t) && \text{for } (x,t) \in Q := \Omega \times (0,T], \\
u(x,t) &= g(x,t) && \text{for } (x,t) \in \Sigma := \partial\Omega \times (0,T], \\
u(x,0) &= u_0(x) && \text{for } x \in \Omega,
\end{aligned}
\tag{1}
$$

where $\Omega \subset \mathbb{R}^d$, $d = 2, 3$, is a convex polygonal or polyhedral bounded Lipschitz domain, and T is a given final time. Note that f, g, and u_0 are given data which are specified later. For the ease of presentation, modifications of the model problem (1), e.g. including nonlinear terms, will be stated explicitly in the context.

Classical numerical methods for solving the model problem (1) are the method of lines, i.e., discretize first in space and then in time, see, e.g., [210], or Rothe's method, i.e., discretize first in time and then in space, see, e.g. [139]. However, here we review alternative approaches performing Galerkin–type finite element discretizations simultaneously in space and time.

Galerkin–type finite element methods, continuous in space and possibly discontinuous in time, on unstructured space–time meshes for the solution of general linear parabolic equations in a moving domain have been considered already in the 1970s [120], but without optimal order error estimates. In this approach, time is considered as another variable. Later, related error estimates were further improved when using discontinuous in time Galerkin methods, see [78, 79, 80, 81, 83, 160].

In the 1980s, a time–discontinuous Galerkin least–squares formulation for elastodynamics in mixed displacement–velocity form, along with an optimal convergence rate in a norm stronger than the total energy norm, was derived in [119]. The basis functions were chosen to be piecewise polynomials on each space–time finite element at a time slab, with no separation in spatial and temporal variables. The concept of this method has been recently extended in [202] for continuous space–time finite element discretizations of linear parabolic problems. Therein, a Petrov–Galerkin finite element method has been derived, using continuous and piecewise linear finite elements simultaneously in space and time on arbitrary admissible simplicial meshes, along with optimal error estimates in the respective energy norm. In a similar spirit, discontinuous Galerkin space–time finite element discretizations, also allowing hanging nodes, and related optimal error estimates in the respective DG–norms have been consecutively investigated in [122, 123, 124, 171, 172, 173]. Current interests in space–time finite element methods are, e.g., hp–approximations [72], isogeometric analysis [142, 143], Petrov–Galerkin streamline diffusion and edge average finite elements [21], finite element exterior calculus [11], fractional diffusion equations [177], discontinuous Petrov–Galerkin [102], to name a few.

While the above–mentioned space–time finite element methods are based on variational formulations in the Bochner space $L^2(0,T;H_0^1(\Omega)) \cap H^1(0,T;H^{-1}(\Omega))$, an alternative approach is based on variational formulations in anisotropic Sobolev spaces $H^{1,1/2}(Q)$. This goes back to the pioneering work [155] using Fourier analysis in space and time with $T = \infty$. Related variational formulations were then analyzed in [96], and a corresponding stability and error analysis of wavelet discretizations is given in [71, 72, 147], where the Hilbert transformation is used to construct optimal test functions. This approach can be generalized to the case of a finite time interval $(0, T]$, see [206] for more details.

Meanwhile, a posteriori error estimates and related adaptive schemes for parabolic problems have been considerably studied since the early works [77, 78, 79, 80, 81, 82] in the 1980s–1990s. As it is well known, the general aim of a posteriori error estimates is to obtain computable upper (reliability) and lower (efficiency) bounds for the error with respect to a certain norm in terms of local error indicators that are used to drive a local mesh refinement in order to achieve optimality in the error control. Most of the techniques to obtain a posteriori error estimates for parabolic problems are borrowed and adapted from the ones for elliptic problems. Usually, the full error is split into spatial and temporal contributions, and others, e.g., the error from data approximations, each of which can be bounded separately. Well studied approaches are parabolic duality methods [78, 178], using energy arguments [59, 60, 199], reconstruction techniques [24, 68, 159], functional type estimates [145, 163, 185], residual type estimates [180, 218, 219], flux reconstruction methods [85, 88], and using recovered gradients [138, 151]. However, many of these methods demand adaptive refinements in space and in time separately, which often results in complications of the link between the adaptive mesh refining/coarsening in space and in time. Recently, we have considered a residual type a posteriori error indicator [203, 204, 205] in space and time simultaneously, which shows reliability in our numerical experiments. A posteriori error estimates are also applicable to more involved parabolic type evolution problems, e.g., for parabolic variational inequalities [1, 170, 179], the Allen–Cahn equation [94, 127], the Schrödinger equation [126], the p–Laplacian [56, 132], interface problems [198, 199] with jumping coefficients [35, 36], the Navier–Stokes system [34, 37, 183], and parabolic optimal control problems [157, 167, 181].

With the rapid growth in hardware development, parallel space–time solution methods become more feasible running on high–performance computers [90, 105, 144], since we usually face a large–scale system of algebraic equations arising from space–time finite element discretizations. In comparison with space parallel methods, the time parallel approach has only a relatively short history [104] due to the naturally sequential feature of conventional time stepping methods. Very recent advances in parallel space–time solution methods concern space–time multigrid with concurrency [91, 92, 99, 105] and space–time domain decomposition by constraints [17]. We have recently considered space–time algebraic multigrid (AMG) [204, 205] methods as black box type solvers for the linear system of algebraic equations arising from the space–time finite element discretization [202] of the heat equation. In comparison with space–time geometric multigrid methods [105, 172], coarsening in algebraic multigrid requires special care since the spatial and temporal directions are not easily detected on the pure algebraic level, and the strength of connections may need to be taken into account [48, 50, 190].

The remainder of this paper is organized in the following way. Section 2 mainly deals with Galerkin space–time finite element methods for the discretization of related parabolic problems. In Section 3, we review a posteriori error estimates and space–time adaptive schemes mainly for linear parabolic equations and their variants. In Section 4, we describe recent developments on space–time solution methods. Some numerical results are presented in Section 5. Finally, we draw some conclusions in Section 6.

2 Space–time finite element discretization

In this section, we present an overview on space–time Galerkin finite element methods for an approximate solution of the model problem (1). The main focus is on discontinuous approximations either in time or both in space and time, see Subsection 2.1, and on approximations continuous in space and time, see Subsection 2.2. A Petrov–Galerkin space–time finite element method [202], that we have used in our numerical experiments, will be discussed in Subsection 2.3. Subsection 2.4 provides a short report on recent developments in space–time finite element methods, e.g., for solving the related parabolic evolution equations, the exterior calculus, fractional diffusion equations, and discontinuous Petrov–Galerkin methods.

2.1 Discontinuous space–time finite element methods

A general class of Galerkin–type methods, which are based on a weak formulation similar to the one in [154], for the solution of general linear parabolic equations in a given time dependent domain were discussed in [120]. The used approximations are continuous in space and, possibly, discontinuous in time. Although the method in principle allows using quite flexible space–time finite element meshes, the total space–time domain is decomposed into time slabs, and each time slab is decomposed into simplicial (or prismatic) elements. It is possible to have hanging nodes on the interface between two time slabs. The consideration of time slabs allows in most cases the interpretation of discontinuous finite elements in time as time stepping schemes. The finite element functions restricted to a simplicial element are polynomials of degree k with respect to the spatial and temporal variables, and they are in general discontinuous at a time level t^n. In this method, time is treated as another variable, and the discretization is performed in space and time simultaneously. The convergence of the space–time finite element solution is considered in $L^2(0,T;H^1(\Omega))$, see [120, Theorem 5.1]. Under proper assumptions on the structure of the mesh, improved error estimates were considered in [78, 79, 80, 81, 83, 160].

A time–discontinuous Galerkin least–squares method for a mixed displacement–velocity formulation in elastodynamics and an optimal convergence result with respect to a special norm, which is stronger than the energy norm, were derived in [119]. The finite element mesh for this approach is obtained by a decomposition of tensor–structured time slabs into triangular elements. The finite element basis functions for the displacement and for the velocity are piecewise polynomials on each space–time finite element, where no separation in spatial and temporal variables is considered. Optimal error estimates were numerically confirmed for arbitrary combinations of polynomial basis functions for the displacement and the velocity.

For the heat equation the stability for a class of discontinuous Galerkin methods on tensor–structured meshes, which are constructed as a product of separate partitions in space and time, was analyzed in [160]. The finite element spaces consist of piecewise polynomial functions on each tensor–structured space–time slab, which are the product of continuous piecewise polynomial functions in space and piecewise polynomial and possible discontinuous functions in time. The methods were shown to be stable with respect to a mesh dependent norm, a discrete analogue to the L^2 norm in space and time. An optimal error estimate in $L^2(0,T;L^2(\Omega))$ was derived, see [160, Theorem 1.2]. The main tools for proving the error estimates are the well known finite element interpolation properties in space [61], the approximation property of the interpolation operator on the time slab [83], and the stability properties of the L^2 projection in time.

Recently, in a series of recent papers [123, 171, 172, 173], discontinuous Galerkin discretizations in the space–time domain have been analyzed for parabolic problems. There, the jumping operator in spatial and in the temporal directions and the upwinding operator in time have been exploited. In fact, time is considered as another spatial coordinate, and the discrete finite element spaces of piecewise polynomials are designed accordingly on each space–time finite element. Optimal error estimates in the respective DG–norms were derived. The method allows to use arbitrary admissible simplex meshes in the space–time domain, also allowing hanging nodes. For an application in coupled cardiac electro–mechanics, see [122, 124].

In [149], a global best approximation and an interior best approximation of fully discrete Galerkin finite element solutions of second order parabolic problems on convex polygonal and polyhedral domains were shown with respect to the L^∞–norm, see [149, Theorems 1,2]. The space–time finite element space for the discrete approximation consists of a product of continuous piecewise polynomial functions in space and discontinuous piecewise polynomial functions in time on each space–time slab. The main tools for proving the best approximation results are corresponding elliptic estimates in weighted norms, weighted resolvent estimates, and maximal parabolic [150] and smoothing estimates.

2.2 Continuous space–time finite element methods

A novel variational method for approximating the heat equation using continuous spatial and temporal finite element functions was analyzed in [16]. The tensor–product based finite element space consists of continuous piecewise polynomials of order p on the spatial mesh, and continuous piecewise polynomials of order q on the temporal partition. In the discrete variational formulation, the test function has been differentiated with respect to the time variable. The solution of the proposed discrete variational formulation can be computed by successively marching through the time partition while the test function is of one order less in temporal direction. This explains that the proposed method can be viewed as a Petrov–Galerkin method with trial functions continuous in space and time, and test functions continuous in space, but discontinuous in time. Error estimates in different norms have been derived using the properties of the constructed spatial elliptic projection and the one–dimensional temporal projection from the continuous to discrete spaces.

The stability of space–time Petrov–Galerkin discretizations applied to parabolic evolution problems was discussed in [168]. In order to obtain a mesh independent positive lower bound in the discrete inf–sup condition, different discretization levels for the trial and test spaces have to be chosen. In particular, this requirement can be fulfilled by using suitable hierarchical families of discrete spaces. The method is applicable to both finite element and wavelet discretizations in space and time [169]. The analysis of the method is based on some regularity assumption on the spatial partial differential operator involved, and on the so–called Jackson– and Bernstein estimates and a reverse Cauchy–Schwarz inequality with respect to the discrete trial and test spaces, that can be easily fulfilled with properly chosen spaces.

Recently, a new stable single patch space–time isogeometric analysis method [118] for the numerical solution of parabolic evolution equations in both spatially fixed and moving computational domains were derived in [143]. Starting from the standard weak space–time variational formulation [134, 135], a stable discrete weak formulation is achieved by using a time–upwind test function. The space–time finite element spaces consist of the tensor–product multivariate B–spline basis functions. Optimal a priori error estimates for such a stable discretization were shown with respect to a corresponding mesh dependent norm. This approach has been extended to (time–) multipatch space–time isogemetric analysis [113, 144]. Further, the stabilization term has been localized in [192, 193]. In [211], the approach has been extended to stabilized space–time finite element methods using bubble spaces.

Two stable space–time variational formulations in weighted Bochner spaces for the heat equation on the unbounded temporal interval were devised in [8]. The discrete weak formulations were shown to be stable with respect to suitable weighted space–time norms. The space–time finite element spaces were taken as space–time tensor–product spaces of Laguerre polynomials in time and arbitrary nontrivial finite–dimensional subspaces in space.

In [21], a standard Petrov–Galerkin streamline diffusion method [51] and the edge average finite element [229] were applied to a time–dependent partial differential equation, that is embedded into a convection–diffusion type equation with singularity. These schemes provide proper discretizations for convection–diffusion problems with suitable stability and approximation properties. The methods allow using arbitrary simplex meshes in high dimensions, which usually demand extensive memory usage in space–time simulations. To cure this drawback, accurate dimension reduction algorithms on tetrahedral space–time meshes have been proposed in, e.g., [148].

2.3 A Petrov–Galerkin space–time finite element method

In [202], a Petrov–Galerkin finite element method for the approximate solution of parabolic evolution equations was proposed, in which stability conditions and a priori error estimates were derived for the space–time finite element approximations. Since we have used this approach in our numerical experiments, we will discuss this method in more detail. Note that similar weak formulations have been considered in [6, 7, 196, 216], but using wavelet discretization techniques. Since time is considered as another spatial coordinate, we employ piecewise linear finite elements in both space and time simultaneously where arbitrary admissible simplex meshes are allowed.

Since the initial condition is, as the Dirichlet boundary condition, considered as an essential boundary condition, we introduce a suitable $\overline{u}_0 \in L^2(0,T;H^1(\Omega)) \cap H^1(0,T;H^{-1}(\Omega))$ as an arbitrary but fixed extension of the given Dirichlet and initial data. Then the Petrov–Galerkin variational formulation for the heat equation (1) is to find $\overline{u} \in X := \{v \in L^2(0,T;H_0^1(\Omega)) \cap H^1(0,T;H^{-1}(\Omega)),\ v(x,0) = 0 \text{ for } x \in \Omega\}$ such that

$$a(\overline{u}, v) = \langle f, v \rangle - a(\overline{u}_0, v) \tag{2}$$

is satisfied for all $v \in Y := L^2(0,T;H_0^1(\Omega))$, where

$$\begin{aligned} a(u,v) &:= \int_0^T \int_\Omega \Big[\partial_t u(x,t) v(x,t) + \nabla_x u(x,t) \cdot \nabla_x v(x,t) \Big] \, dx \, dt, \\ \langle f, v \rangle &:= \int_0^T \int_\Omega f(x,t) v(x,t) \, dx \, dt. \end{aligned}$$

Under proper assumptions, the uniqueness of the solution to the varitional problem (2) can be shown, see also [155, 196, 216].

Theorem 2.1 ([202]) *Let $\overline{u}_0 \in L^2(0,T;H^1(\Omega)) \cap H^1(0,T;H^{-1}(\Omega))$ be an extension of the initial datum $u_0 \in L^2(\Omega)$ and of the Dirichlet datum $g \in H^{1/2,1/4}(\Sigma)$, and assume $f \in L^2(0,T;H^{-1}(\Omega))$. The bilinear form $a(\cdot,\cdot)$ is bounded,*

$$a(u,v) \le \sqrt{2}\, \|u\|_{L^2(0,T;H_0^1(\Omega)) \cap H^1(0,T;H^{-1}(\Omega))} \|v\|_{0,T;H_0^1(\Omega)} \tag{3}$$

for all $u \in L^2(0,T;H_0^1(\Omega)) \cap H^1(0,T;H^{-1}(\Omega))$ and $v \in L^2(0,T;H_0^1(\Omega))$. In addition, it satisfies the stability condition

$$\frac{1}{2\sqrt{2}} \|u\|_{L^2(0,T;H_0^1(\Omega)) \cap H^1(0,T;H^{-1}(\Omega))} \le \sup_{0 \ne v \in L^2(0,T;H_0^1(\Omega))} \frac{a(u,v)}{\|v\|_{L^2(0,T;H_0^1(\Omega))}}. \tag{4}$$

Then there exists a unique solution $\overline{u} \in X$ of the variational formulation (2) satisfying

$$\begin{aligned} &\|\overline{u}\|_{L^2(0,T;H_0^1(\Omega)) \cap H^1(0,T;H^{-1}(\Omega))} \le \\ &\qquad \le 2\sqrt{2}\, \|f\|_{L^2(0,T;H^{-1}(\Omega))} + 4\, \|\overline{u}_0\|_{L^2(0,T;H^1(\Omega)) \cap H^1(0,T;H^{-1}(\Omega))}. \end{aligned} \tag{5}$$

Proof. See the proof for Theorem 2.1 and Corollary 2.3 in [202]. ■

The related discrete Galerkin–Petrov problem is to find $\overline{u}_h \in X_h \subset X$ such that

$$a(\overline{u}_h, v_h) = \langle f, v_h \rangle - a(\overline{u}_0, v_h) \tag{6}$$

is satisfied for all $v_h \in Y_h \subset Y$, where we assume $X_h \subset Y_h$. The discrete stability condition is shown in the following theorem, where we use a discrete norm for $H^1(0,T;H^{-1}(\Omega))$,

$$\|u\|_{X_h}^2 := \|w_h\|_{L^2(0,T;H_0^1(\Omega))}^2 + \|u\|_{L^2(0,T;H_0^1(\Omega))}^2$$

with $w_h \in Y_h$ being the unique finite element solution of the quasi–static variational formulation

$$\int_0^T \int_\Omega \nabla_x w_h(x,t) \cdot \nabla_x v_h(x,t)\, dx\, dt = \int_0^T \int_\Omega \alpha \partial_t u(x,t) v_h(x,t)\, dx\, dt$$

for all $v_h \in Y_h$.

Theorem 2.2 ([202]) *Assuming $X_h \subset X$, $Y_h \subset Y$, and $X_h \subset Y_h$, there holds the stability condition*

$$\frac{1}{2\sqrt{2}} \|u_h\|_{X_h} \leq \sup_{0 \neq v_h \in Y_h} \frac{a(u_h, v_h)}{\|v_h\|_{L^2(0,T;H_0^1(\Omega))}} \tag{7}$$

for all $u_h \in X_h$.

Proof. See the proof of Theorem 3.1 in [202]. ■

We then have the following a priori error estimate.

Theorem 2.3 ([202]) *Let $\overline{u} \in X$ and $\overline{u}_h \in X_h$ be the unique solutions of the variational problems (2) and (7), respectively. Then there holds the a priori error estimate*

$$\|\overline{u} - \overline{u}_h\|_{X_h} \leq 5 \inf_{z_h \in X_h} \|\overline{u} - z_h\|_X. \tag{8}$$

Proof. See the proof of Theorem 3.3 in [202]. ■

In particular, the space–time cylinder $Q = \Omega \times (0,T)$ is decomposed into admissible and shape regular finite elements q_ℓ, i.e. $Q_h = \cup_{\ell=1}^N \overline{q}_\ell$. For simplicity, we assume that Ω is polygonal or polyhedral bounded, i.e., $\overline{Q} = Q_h$. The finite element spaces are given by $X_h = S_h^1(Q_h) \cap X$ and $Y_h = X_h$ with $S_h^1(Q_h) = \mathrm{span}\{\varphi_i\}_{i=1}^M$ being the span of piecewise linear and continuous basis functions φ_i. The following energy error estimate is shown in [202].

Theorem 2.4 ([202]) *Let $\overline{u} \in X$ and $\overline{u}_h \in X_h$ be the unique solutions of the variational problem (2) and (6), respectively. Assuming $\overline{u} \in H^2(Q)$, then there holds the energy error estimate*

$$\|\overline{u} - \overline{u}_h\|_{L^2(0,T;H_0^1(\Omega))} \leq c\, h\, \|\overline{u}\|_{H^2(Q)}, \tag{9}$$

Proof. See the proof of Theorem 3.3 in [202]. ■

We mention that on the discrete level we obtain a non–symmetric but positive definite linear system of algebraic equations, that will be solved by algebraic multigrid (AMG) methods as discussed in Subsection 5.2. The adaptivity related to this method will be discussed in Subsection 3.8, and corresponding numerical experiments are presented in Section 5.

2.4 Some other space–time finite element methods

As an extension of the finite element exterior calculus for linear elliptic problems in mixed variational formulations [12, 13] to parabolic problems, a Galerkin method for a model Hodge heat equation was considered in [11]. Both semi–discrete and fully–discrete numerical schemes, which are based on a mixed formulation, were analyzed therein. The well–posedness of the mixed variational formulation was shown using the Hille–Yosida–Phillips theory. Error estimates for the finite element approximation to the evolution equation were obtained by a comparison with a corresponding elliptic projection of the exact solution into the finite element space. In a special case, this mixed form reduces to the standard weak formulation for the heat equation, that has been considered in [73, 227].

Recently, another extension of the finite element exterior calculus has been considered in [107], namely to parabolic and hyperbolic problems. A priori error estimates for Galerkin finite element approximations in the natural Bochner space norms were derived therein by combining recent results on the finite element exterior calculus for elliptic problems with a classical approach in [210]. The method has been recently extended to parabolic evolution problems on Riemannian manifolds [116] by using the framework developed in [115].

Numerical solution techniques for parabolic equations with fractional diffusion and the Caputo fractional time derivative were studied in [177]. Therein, the evolution problem was written as a quasi–stationary elliptic problem with a dynamic boundary condition. The spatial fractional diffusion is treated as the Caffarelli–Silvestre extension problem on a semi–infinite cylinder in one more spatial dimension [54]. The finite difference scheme proposed in [153] was employed to discretize the fractional time derivative. First–degree tensor product finite elements for the truncation problem with exponential decay adapted from [176] were used for the spatial discretization. Unconditional stability and error estimates for the fully discrete scheme were shown therein. Using a similar discretization scheme, a convergence analysis for the discretization of a space–time fractional optimal control problem has been discussed in the recent work [9].

A time–stepping discontinuous Petrov–Galerkin method with optimal test functions for the heat equation was discussed in [102]. The stability for the semi–discrete and fully–discrete schemes based on a backward Euler time stepping and an ultra–weak variational formulation [66] at each time step was shown. We mention that a more detailed discussion on discontinuous Petrov–Galerkin methods with optimal test functions for elliptic and fluid problems can be found in, e.g., [65, 66, 67, 75, 76].

3 A posteriori error estimates and adaptivity

In this section, we discuss a posteriori error estimates and corresponding adaptive schemes for parabolic problems. Well established methods for deriving a posteriori error estimates and devising respective adaptive refinement strategies are reviewed, namely,

1. parabolic duality – Subsection 3.1,
2. energy arguments – Subsection 3.2,

3. reconstruction – Subsection 3.3,
4. functional type – Subsection 3.4,
5. residual type – Subsection 3.5,
6. flux reconstruction – Subsection 3.6, and
7. recovered gradient – Subsection 3.7.

Further, we provide some details on our space–time adaptive method relying on a residual type error indicator with conforming local mesh refinements, see Subsection 3.8, that has been recently developed [204, 205], and which drives the adaptive refinement in space and time simultaneously.

A posteriori error estimates in different applications are reported in Subsection 3.9. We mention that the given overview is not restricted to a posteriori error estimates using space–time finite element approximations, i.e., time–stepping methods may also be considered.

3.1 Parabolic duality

Adaptive finite element methods for linear parabolic problems using a discontinuous Galerkin approach in time, and on each time interval a continuous finite element approximation in space were considered in [78]. The discrete space is a tensor–product space of polynomials in space and time. This separation offers some flexibility on the spatial and temporal mesh adaptivity. The a posteriori error estimates in $L^\infty(0,T;L^2(\Omega))$ were derived using duality techniques involving both continuous and discrete dual problems, and strong stability properties of the dual problems. In [79], error estimates have been extended to $L^\infty(0,T;L^\infty(\Omega))$ and $L^\infty(0,T;L^2(\Omega))$. The a posteriori estimates have been further generalized to nonlinear parabolic problems in [80], for the error control in $L^\infty(0,T;L^2(\Omega))$. Using similar techniques from [78], adaptive finite element methods for long–time integration of parabolic problems have been discussed in [81] for time discontinuous Galerkin methods.

The duality technique has been applied to a posteriori error estimates for a degenerate parabolic problem in [178], where the related dual problem corresponds to a nonstrictly parabolic equation in non–divergence form with a vanishing rough diffusion coefficient [101, 175]. Moreover, goal oriented a posteriori error estimates for space–time discretizations based on dual weighted residual apperoaches are considered, e.g. in [195].

3.2 Energy arguments

Using so the so–called direct energy estimate argument [60], i.e. a coupled system of one parabolic equation with one variational inequality, the error indicator, which consists of the time and space error indicators, which are designed for linear parabolic problems discretized by backward Euler in time and continuous finite elements in space, has been shown to be an upper bound of the error in the respective norm, see [59, Theorem 2.1]. A new refinement/coarsening strategy based on a bisection algorithm, see, e.g., [23], has been proposed. In addition, a coarsening error indicator was also provided therein. The time and space adaptive algorithms were further developed, see Algorithm 3.2 in [59]. The algorithm includes time and space refining, and space and time coarsening with respect to a prescribed spatial and temporal tolerance. The adaptive algorithm has been further improved in [133] so that it always reaches the final time for a given tolerance.

3.3 Reconstruction methods

Using the so–called elliptic reconstruction of the finite element solution of a spatially semi–discretized equation, which is considered as an "a posteriori dual" to the elliptic projection in the classical a priori error analysis for semidiscrete linear parabolic problems [106, 111, 112, 210, 227], a posteriori error estimates for parabolic problems in $L^\infty(0,T;L^2(\Omega))$ were derived in [159]. A similar idea, the so–called postprocessed Galerkin approximation has been used to derive a posteriori error estimates for nonlinear parabolic problems [63, 64, 106]. A posteriori analysis of evolution problems based on both spatial and temporal reconstructions can be found in [58].

As an extension of [159], and using a combination of the elliptic reconstruction and other properly related techniques, e.g., main parabolic error estimates, heat kernel estmates [15], pointwise boundedness of the spatial derivatives of the Green's function for the parabolic problem [74], a posteriori error estimates for fully discrete linear parabolic problems were derived in various norms. In particular, the following spaces were considered: $L^\infty(0,T;L^2(\Omega))$, see [24, 136, 137], $L^\infty(0,T;H_0^1(\Omega))$, see [136], $L^\infty(0,T;H^1(\Omega))$ and $H^1(0,T;L_2(\Omega))$, see [136], $L^\infty(0,T;L^\infty(\Omega))$, see [41, 68, 129, 130], and $L^\infty(D\subset Q)$ [69].

3.4 Functional type estimates

As an extension of functional type a posteriori error estimates derived for elliptic problems in [161, 184, 186], error bounds for the heat equation were derived in [185]. These functional estimates are upper bounds (majorants) for the difference in a certain norm between the exact solution of the heat equation and any admissible approximation from the associated function space. Error majorants have been further derived for evolutionary convection–diffusion problems in [187]. In [164], both the error majorant and error minorant (lower bound) were derived for evolutionary reaction–diffusion problems with mixed Dirichlet–Neumann boundary conditions.

Functional type a posteriori error estimates for time–periodic parabolic boundary value problems have been derived in [145], which provide guaranteed and fully computable upper bounds (majorants) for the error in $H^{1,1/2}(Q)$. As an extension, functional type a posteriori error estimates for the state and adjoint errors in distributed time–periodic parabolic optimal control problems were derived in [146]. Further, guaranteed and computable upper bounds for the cost functionals, and their sharpness, were derived therein, using a posteriori estimates for the state equation. Similar results for elliptic optimal control problems can be found in [103, 186].

Recently, following the approaches [164, 185], error majorants for the stabilized space–time weak formulation of the parabolic problem using isogeometric analysis [143] have been derived in [140, 141]. A comparison of efficiency of the functional type a posteriori error estimates applied to a class of parabolic problems, using both the time–marching and space–time approaches, was discussed in [114].

3.5 Residual type methods

Based on a general framework [218], the work [219] derives a residual type posteriori error estimate in $L^r(0,T;W^{1,\rho}(\Omega))$ for a space–time finite element discretization of a nonlinear parabolic boundary value problem and non–stationary incompressible Navier–Stokes equations. With additional regularity assumptions, a residual type posteriori error in the weaker space $L^r(0,T;L^\rho(\Omega))$ with $1 < r, \rho < \infty$ has been shown in [220].

Under the assumption that the triangulations are nested, residual a posteriori error indicators with respect to $L^2(0,T;H_0^1(\Omega))$ for a standard discretization of the heat equation has been reported in [180].

Residual a posteriori error indicators with respect to a certain norm were derived in [221] for a discretization of the heat equation by A–stable θ–schemes ($\theta \in [0.5, 1]$) in time and conforming finite elements in space.

Residual a posteriori error indicators in $L^\infty(0,T;L^2(\Omega))$ for a discretization of the heat equation using Euler's implicit scheme in time and continuous, piecewise polynomial finite elements in space were constructed in [32].

3.6 Flux reconstruction methods

A posteriori error estimates in a broken norm for an approximate solution of the heat equation were derived in [88]. The estimates are based on H^1–conforming reconstructions of the potential, which is continuous and piecewise affine in time, and a locally conservative $H(div)$–conforming reconstruction of the flux, which is piecewise constant in time. Such a method is inspired by a posteriori error estimates for elliptic problems in [84, 87, 224, 225]. Further, the $H(div)$–conforming flux reconstruction can be found in [2, 32, 43, 125]. Whereas the potential reconstruction is discussed in [53, 125, 221].

In [85], a posteriori error estimates in $L^2(0,T;H^1(\Omega)) \cap H^1(0,T;H^{-1}(\Omega))$ for the error and for the temporal jumps of the numerical solution of parabolic problems were considered. This technique can be viewed as a natural extension of flux reconstructions for elliptic problems [43, 44, 70, 89]. Such estimators have been shown to be unconditionally locally space–time efficient with respect to local errors, with constants independent of both the spatial and temporal approximation orders. They also allow very general refinement and coarsening strategies between the time steps.

The equilibrated flux reconstruction has been used in [86] to obtain a posteriori estimates in $L^2(0,T;H^1(\Omega))$ of the error and of the temporal jumps. Under the so–called one–side parabolic condition $h^2 \lesssim \tau$, it was shown that the constants in the bounds are robust with respect to the mesh and time step sizes h and τ, respectively, the spatial polynomial degrees, and the refinement and coarsening strategies between time steps.

3.7 Recovered gradient approach

In [151], gradient recovery a posteriori error estimators [4, 22, 55, 95, 152] have been extended from elliptic equations to the linear heat equation, under the condition that the time–stepping error must be strictly smaller than the space discretization error. As improvement, in [138], a posteriori error estimates in the energy norm using gradient recovery approaches have been investigated for the full discretization of the linear heat equation, without such restrictive assumptions on the time step size. Here, gradient recovery is a local weighted averaging with gradient sampled from neighbouring elements.

3.8 A residual type error indicator with conforming space–time local mesh refinements

3.8.1 A space–time local error indicator

In our recent work [204, 205], a residual based a posteriori error indicator for the space–time Petrov–Galerkin finite element method [202] has been proposed.

Let $u_h \in X_h$ be the space–time finite element solution of the variational problem (6), where X_h is a properly defined finite element space, see Subsection 2.3. Then we can define the local residuals

$$R_{q_\ell}(u_h) := f + \Delta_x u_h - \partial_t u_h$$

on each space–time finite element q_ℓ, and the jumps

$$J_\gamma(u_h) := [n_x \cdot \nabla_x u_h]_{|\gamma}$$

of the normal flux in the spatial direction across the inner boundaries γ between q_ℓ and its neighbouring elements. Then, the local error indicator on each element q_ℓ is given as

$$\eta_{q_\ell} = \left\{ c_1 h_{q_\ell}^2 \|R_{q_\ell}\|^2_{L^2(q_\ell)} + c_2 h_{q_\ell} \|J_\gamma\|^2_{L^2(\partial q_\ell)} \right\}^{\frac{1}{2}}, \tag{10}$$

with suitably chosen positive constants c_1, c_2, which may depend on the model problem and the shape of the considered domain. In all our numerical examples we have used $c_1 = c_2 = 1$ for simplicity. For more details, we refer to our recent work [203]. It is obvious that this method allows performing spatial and temporal adaptivity simultaneously.

3.8.2 An adaptive space–time finite element loop

The adaptive loop in the space–time finite element method follows the standard adaptive finite element approach, see, e.g., [223], which consists of the following four main steps: Given a conforming decomposition Q_0 at the initial mesh level $k = 0$,

1. SOLVE: Solve the discrete problem (6) on the adaptive mesh level k,
2. ESTIMATE: Compute the local error indicators (10) on each element q_ℓ and the global error indicator, stop if the solution is accurate enough,
3. MARK: Mark the elements for refinement using a proper marking strategy,

4. REFINE: Perform the local mesh refinement using octasection or bisection (see the following description), increase the level $k := k+1$, obtain the conforming decomposition Q_k, and go to Step 1.

For the module MARK, we use the maximal marking strategy: For a given parameter $\vartheta \in [0,1]$, mark all elements q_k that fulfill

$$\eta_{q_k} \geq \vartheta \max_{\ell=1\ldots,N_k} \eta_{q_\ell}, \tag{11}$$

where N_k denotes the total number of space–time finite elements on the current level k. Those marked and the affected neighbouring elements will be refined on the next level $k+1$. In our numerical experiments, we use $\vartheta = 0.5$ for the adaptive mesh refinement.

3.8.3 An octasection based adaptive mesh refinement method

For the adaptive local mesh refinement, we first adopt a method mainly following the idea in [38], i.e., the so–called octasection, which is strongly connected to the *Red–Green* refinement in two dimensions [19, 20, 201]. In the software package UG [27], a similar method has been implemented, while in [109], a parallel version of this method has been developed. Here, we have only considered a refining procedure without coarsening. While in the following the focus is to discuss a Galerkin–Petrov space–time finite element method on simplicial meshes, space–time adaptivity can be considered for more general situations as well, e.g., for higher order tensor product spaces, or hexahedral meshes.

Starting from an initial mesh with shape regular tetrahedral elements, we mark the tetrahedra that shall be refined on the next level. Each of these marked tetrahedra is divided into four congruent tetrahedra and one octahedron by connecting middle edge points on each face of the tetrahedron. Following the shortest–interior–edge strategy [231], we further divide the remaining octahedron into four tetrahedra.

During the regular refining procedure, hanging nodes appear, i.e., some edges of the tetrahedron are divided but the tetrahedron itself is not yet divided, which has to be closed by a combined regular and irregular refinement strategy. According to how many, i.e., maximal five, and which edges of a tetrahedron are divided, there exist 62 possible cases for the irregular refinement. Due to a symmetry argument, the number of cases is reduced to nine. In [38, 42], only four types of irregular refinement are considered for simplicity.

By building proper connections among the tetrahedral vertex and the middle edge points on the face of a tetrahedron locally, we obtain a hybrid mesh without hanging nodes, but with a mixture of different elements: tetrahedra, pyramids and triangular prisms; see Figure 1 for an illustration.

The remaining task is to further divide the pyramids and triangular prisms into tetrahedra in a conformal way, which does not introduce any additional nodes in the mesh and at the same time subdivide each rectangular face shared by two elements into two triangles in a conforming way. This is realized in the same manner as detailed in [230].

It is important that on the next refinement levels, the tetrahedra from the irregular refinement will never be refined again. If such an element is marked for further refinement,

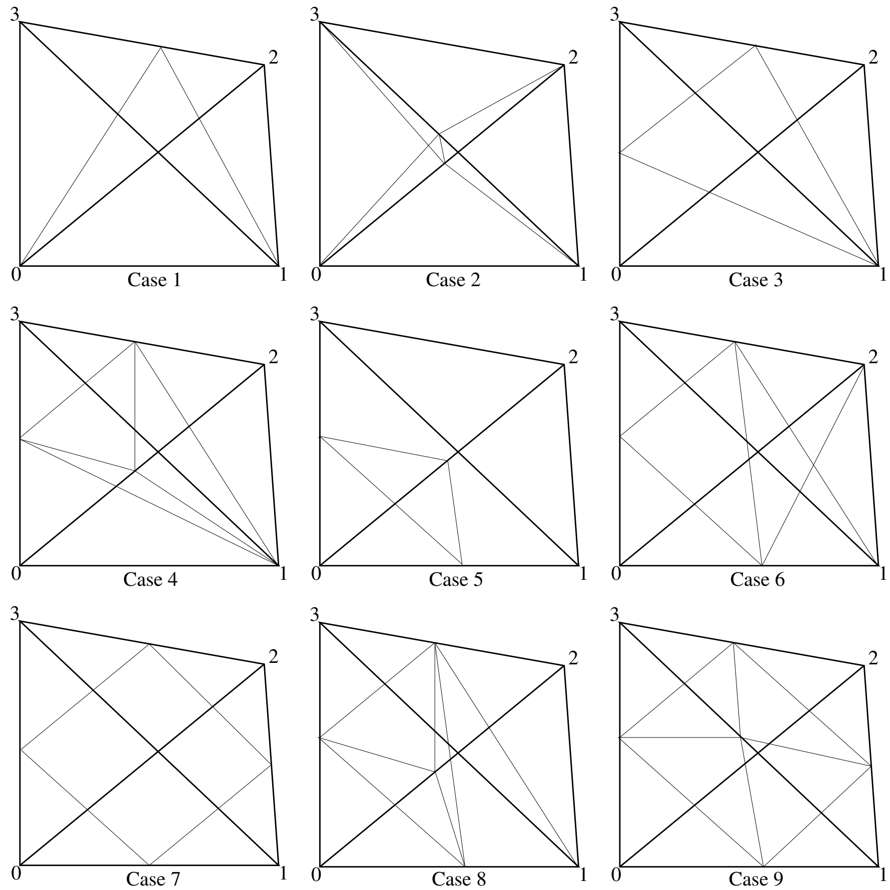

Figure 1: Irregular refinements of a tetrahedron with local vertex numbering $0, ..., 3$ into hybrid elements: tetrahedra, pyramids and triangular prisms: Case 1 (two tetrahedra), Case 2 (four tetrahedra), Case 3 (one tetrahedron and one pyramid), Case 4 (four tetrahedra), Case 5 (one tetrahedron and one triangular prism), Case 6 (one tetrahedron and two triangular prisms), Case 7 (two triangular prisms), Case 8 (two tetrahedra and two pyramids), Case 9 (two tetrahedra, one triangular prism and one pyramid).

we will return to its "parent", which is regular, and make a regular refinement for this element and meanwhile remark all neighboring elements that are affected. In this way, we avoid a mesh degeneration during the adaptive refinement procedure.

For high dimensions, the regular (*Red*) refinement has been considered in [39] using Freudenthal's algorithm [100]. The conforming *Red–Green* refinement of simplicial meshes in arbitrary dimensions has been recently investigated in [108] using the placing triangulation technique. A special refinement strategy to decompose pentatopes into smaller ones for the four–dimensional space–time cylinder has been introduced in [173].

3.8.4 A bisection based adaptive mesh refinement method

We further consider a bisection–based mesh refinement method [14] in three dimensions, which is strongly related to the newest vertex bisection method proposed and developed in [23, 131, 156]. The local mesh refinement is summarized as follows: For each marked tetrahedron we choose one edge as the so–called refinement edge, and the two faces intersecting at this edge as the refinement faces. For the other two nonrefinement faces, we choose a particular edge on each face as the so–called marked edge. Once a tetrahedron is marked for refinement, we will divide this tetrahedron into two smaller ones by connecting the middle point on the refinement edge with the other two tetrahedral vertices that are not lying on the refinement edge. This simplifies the local refinement patterns.

In fact, according to the relative position between the marked and refinement edges, the marked tetrahedra can be grouped into four types: Type P (planar, where the marked edges and the refinement edge are coplanar), Type A (adjacent, where each marked edge shares a common vertex with the refinement edge, but they are not coplanar), Type O (opposite, where the marked edges have no intersection with the refinement edge), and Type M (mixed, one marked edge does not intersect the refinement edge, and the other does), see Figure 2 for an illustration.

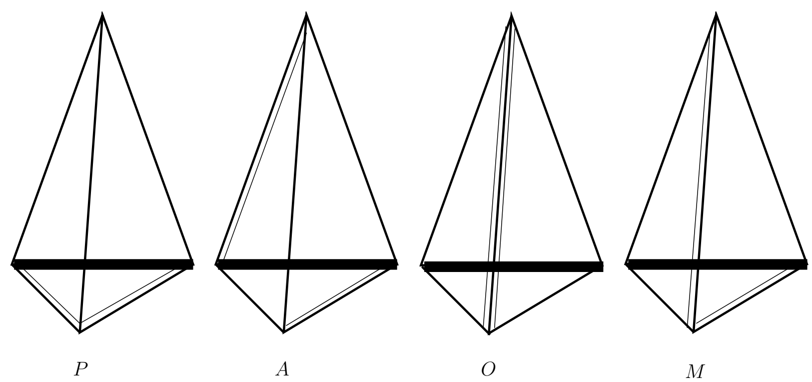

Figure 2: The four types of marked tetrahedra (from left to right): P, A, O and M. The refinement edge is indicated by the thick solid line, and the marked edge is highlighted by a double line. The two faces sharing the refinement edge are the refinement faces, and the other remaining two faces the nonrefinement faces.

In addition, a flag $f_\tau \in \{0, 1\}$ is attached to the type P so that P is classified as type P_f ($f_\tau = 1$) or P_u ($f_\tau = 0$). The local refinement follows the rules:

$$P_u \longrightarrow P_f,\ A \longrightarrow P_u,\ M \longrightarrow P_u,\ O \longrightarrow P_u,\ P_f \longrightarrow A. \tag{12}$$

It is sufficient and necessary to obtain conforming refinements in three dimensions provided that the refinement edges of two neighboring elements have to coincide, when they are on the common sharing face [174]. This condition is easily fulfilled for any initial conforming triangulation by, e.g., choosing the longest edge of each tetrahedral element as the refinement edge [14]. A conforming mesh is obtained by a recursive calling of the local mesh refinement until no hanging nodes exist, see [14, Theorem 3.1].

We mention that bisection methods have been extended to any dimension in [165, 207, 212], which is very useful for the space–time adaptivity in four dimensions. In addition, it has been shown in [207] that the newest vertex bisection refinement stays local for any dimension, which is extended from the result [40] in two dimensions.

Compared with the octasection–based method, the refinement pattern for each tetrahedron has been fixed from the very beginning in the bisection–based approach. During the adaptive refinement procedure, the tetrahedron chosen for refinement will be continuously refined according to the strict rules (12) specified above. Some related numerical results concerning adaptive space–time finite element methods for both linear and nonlinear parabolic problems are shown in Subsection 5.1.

3.9 Some other topics of a posteriori error estimates in space–time FEM

In [170], a residual type a posteriori error analysis was derived for a fully discrete method using piecewise linear finite elements in space and backward Euler discretization in time of parabolic variational inequalities in the pricing of American options for baskets. A posteriori error estimators were derived for the error in $L^2(0,T;H^1(\Omega))$. Two residual type error indicators have been considered in [1] for a posteriori error estimates for parabolic variational inequalities. In [179], an a posteriori error analysis was investigated for a class of integral equations and variational inequalities in the pricing of European or American options under Lévy processes, discretized by piecewise linear finite elements in space and the implicit Euler method in time. A residual type a posteriori error estimator was derived for the error in H^s, $s \in (0,2]$.

A posteriori error estimates for space–time discretizations with discontinuous finite elements in time for a parabolic obstacle problem were derived in [25].

Using the so–called energy argument and a topological continuation argument, a posteriori error control in $L^\infty(0,T;L^2(\Omega))$ for the Allen–Cahn's problem was derived in [127], which only has a low order polynomial dependence in ε^{-1} with ε being the interface thickness parameter. A similar result has been also achieved in [94]. These results have been improved from the old results which have an exponential dependence on ε^{-2}. Similarly, in [26], quasi–optimal a posteriori error estimates in $L^\infty(0,T;L^2(\Omega))$ for the finite element approximation of Allen–Cahn equations were derived, with a low order polynomial dependence in ε^{-1}.

In [126], optimal order residual type a posteriori error estimates for the fully discrete linear Schrödinger–type equations in $L^\infty(0,T;L^2(\Omega))$ were derived, using a Crank–Nicolson method in time, and a finite element method in space which may change in time. In addition, a practical space–time adaptive algorithm was realized, which guarantees rigorously that the total error remains below a given tolerance as long as the algorithm converges.

As an extension of the a posteriori estimates for the linear heat equation considered in [221], a reliable and efficient a posteriori estimate for the fully discrete implicit Euler Galerkin finite element scheme of the nonlinear p–Laplacian problem was derived in [132]. In an earlier work [56], a posteriori error estimates for the finite element approximation of the nonlinear p–Laplacian have been derived, too.

Following the reconstruction approaches studied in [5, 24, 136], residual type a posteriori error estimates for the linear parabolic problems with two transmission conditions on the common space–time interface were derived in [198]. In [199], using an energy argument, residual–based a posteriori error estimates for linear parabolic interface problems were derived with optimal order convergence in $L^2(0,T;H^1(\Omega))$, and with an almost optimal order in $L^\infty(0,T;L^2(\Omega))$.

Following the approach in [180, 221], residual type a posteriori error estimates were derived in [35] for the heat equation with a diffusion coefficient which is constant in time and piecewise constant within the subdomains. In [36], as an extension of the results in [35], a residual based a posteriori error estimator was further derived for a new discretization method, i.e. Crank–Nicolson in time and a conforming finite element method in space, of the heat equation with jumping diffusion coefficients. This method allows varying time step sizes on different elements at the same time.

A fully combined spatial and temporal adaptive scheme was applied to the unsteady Navier–Stokes equations in [37], using the results of a posteriori error estimates and adaptive algorithms for the steady Navier–Stokes system [34, 183], the heat equation [32, 35, 180, 221], an unsteady reaction–convection–diffusion equation [222], and the unsteady Stokes system [33]. In particular, local–in–space error indicators [34] and local–in–time error indicators [32, 33, 35, 180, 221] were adopted in the adaptive algorithm in space and in time.

Following the approach in [28], an anisotropic a posteriori error estimate for controlling the error between the true and the computed cost functional in an optimal control problem governed by a parabolic equation was derived in [181], which is discretized by a Crank–Nicolson scheme in time, and continuous piecewise linear finite elements in space. In the error analysis, a space–time interpolation operator was built as a combination of a Clément [62] or Scott–Zhang [197] type quasi–interpolation operator on strongly anisotropic meshes [10, 97, 98] in space, and the standard Lagrange interpolation in time. With the help of the simple Zienkiewicz–Zhu type error estimator [3, 189], and assuming that the time step size is small enough, an anisotropic a posteriori error estimate for the cost functional was designed.

In [157], a posteriori error estimates for both the state and the control approximation of a quadratic optimal control problem governed by a linear parabolic equation were derived. In [200], equivalent a posteriori error estimators of residual type with lower and upper bounds for both the state and control approximations of a constrained optimal control problem governed by a parabolic integro–differential equation on multi–meshes were considered.

As an extension of the work [29, 30, 31], a posteriori error estimates were derived for a cost functional of parabolic optimization problems in [167]. In [195], as an extension of an optimal control approach to a posteriori error estimation in finite element methods proposed in [18, 29], an a posteriori error estimator and an adaptive space–time algorithm for parabolic equations have been considered, that allow dynamic locally refined meshes and nonuniform time discetizations.

4 Solution methods

For a general discussion on parallel solution methods for time dependent problems we refer to the recent review work [104] and the references therein, where four main types of space–time solution methods have been discussed in detail: Shooting type time parallel methods, space–time domain decomposition methods, geometric multigrid methods in space and time, and direct solvers. Here, we are mainly concerned with very recent developments of space–time geometric multigrid methods, algebraic multigrid methods, and space–time domain decomposition by constraints as discussed in Subsections 4.1–4.3, respectively.

We mention that there are many other techniques for designing parallel space–time solvers. For example, in [90, 91, 92], optimal–scaling parallel multigrid–reduction–in–time and multigrid methods with space–time concurrency were developed for solving linear and nonlinear parabolic model problems with both implicit and explicit time discretizations, which are mainly based on multigrid reduction [188]. In [110], so–called semi–geometric multigrid methods for a new continuous space–time finite element discretization of transient problems in continuum mechanics have been developed.

4.1 Space–time geometric multigrid

In [105, 172], a new space–time parallel geometric multigrid method was developed for solving fully discrete parabolic equations, i.e., using an arbitrarily high order discontinuous Galerkin discretization in time and a finite element method in space. Using exponential local Fourier mode analysis [45, 47, 117, 226], block Jacobi smoothing factors and two–grid convergence factors for arbitrary discontinuous Galerkin time discretization schemes were investigated, which lead to a precise criterion, i.e. a restriction on the discretization parameter $\mu = \tau h^{-2}$ with respect to the polynomial degree in time, for determining semi–coarsening in time or full coarsening in space and time. It is concluded that semi–coarsening in time within the two–grid cycle always converges to the exact solution, while full space–time coarsening can be applied when the discretization parameter μ is large enough in comparison with the critical value.

Instead of an adaptive coarsening as proposed in, e.g., [105, 117], a space–time multigrid method using an adaptive smoothing strategy in combination with standard coarsening in both temporal and spatial domains was developed in [99]. According to a critical value, the adaptive strategy determines a choice of smoothers between zebra line–in–time relaxation/read–black line–in–time relaxation and zebra line–in–space relaxation/zebra plane–in–space relaxation in one/two space dimensions, respectively. This critical value is obtained by performing a local Fourier analysis [45, 47, 209, 214, 226, 228]. The proposed multigrid method is robust for both first–order Euler and second–order Crank–Nicolson temporal discretization schemes.

4.2 Space–time algebraic multigrid

In our recent work [204, 205], considering local mesh refinement and using arbitrary simplex meshes in three and four space–time dimensions in a space–time finite element discretization method [202] for the heat equation, we have compared algebraic multigrid methods [48, 50, 190, 208] using different coarsening for solving the arising linear system of algebraic equations:

$$Ax = b. \tag{13}$$

It is clear from [202] that the matrix A is non–symmetric but positive definite. The linear system (13) is solved by a preconditioned GMRES method with different algebraic multigrid preconditioners. In particular, we use two V(1,1)–cycles with one pre– and post–smoothing step as a preconditioner in the GMRES method. We have considered a pure matrix–graph [128], a greedy coarse–grid selection [158], compatible relaxation [49, 93], and Petrov–Galerkin smoothed aggregation [217].

The simple pure matrix–graph coarsening strategy yields a very aggressive coarsening method, and a rather low operator and grid complexities. It treats all connection equally without taking into account the strength of a connection in the classical Ruge–Stüben algebraic multigrid [50, 190], that is actually important in our space–time algebraic multigrid methods.

In the greedy strategy, the strength of a connection has been taken into account and only strong connections are to be considered in the definition of the interpolation operator, by using a dynamic measure to determine the diagonal dominance of a row among those rows already selected as fine degrees of freedom or undesignated.

In the compatible relaxation algebraic multigrid, the coarse grid set is selected by performing compatible relaxation restricted to the fine degrees of freedom only.

In the smoothed aggregation algebraic multigrid method, the interpolation operator is constructed by smoothing a tentative interpolation operator, e.g., using piecewise constant basis functions, on the decomposition of degrees of freedom into small disjoint subsets. More details are reported in our recent work [205] and the related references therein.

Further, we employ one sweep of the Kaczmarz relaxation scheme [121] as pre– and postsmoother for the non–symmetric and positive definite system on multigrid levels: Let x^0 be a given initial guess, for $i = 1, ..., n$, compute

$$x^i = x^{i-1} + \frac{b_i - \langle A_i, x^{i-1} \rangle}{\|A_i\|_{l_2}^2} A_i, \tag{14}$$

with A_i being the ith row of A presented as a column vector, and b_i the ith component of b. The algebraic multigrid smoothing property of the Kaczmarz relaxation scheme for even more general non–symmetric matrices has been discussed in [46, 182].

All methods have shown relative robustness with respect to the mesh discretization parameters in space and time, the heat capacity constant, and local mesh adaptivity.

Some numerical results concerning algebraic multigrid performance will be demonstrated in Subsection 5.2.

4.3 Space–time balancing domain decomposition by constraints

In [17], weakly scalable space–time preconditioners based on non–overlapping multilevel balancing domain decomposition by constraints (BDDC) methods have been developed for solving both linear and nonlinear parabolic problems discretized using finite elements in space and backward Euler schemes in time. The essential components in the space–parallel BDDC method [162, 215], namely, sub–assembled spaces and operators, coarse degrees of freedom, and transfer operators, have been extended to space–time. In this method, the space domain is decomposed into fine space elements, and coarse space subdomains partitions, and the time domain is decomposed into a fine–time interval and coarse time subdomain partitions. The space–time subdomain partition is then defined as Cartesian product of the space and time subdomains. A sub–assembled problem involving independent subdomain corrections within the sub–assembled space is then defined on the space–time subdomain partition, with introduced perturbation terms on inner time interfaces, i.e. the first and last time steps of the time subinterval. The coarse degrees of freedom are associated with the geometrical objects, namely, vertices, edges, and faces, among space–time subdomains. Every coarse degree of freedom is enforced to be continuous among subdomains by respective constraints. The space–time transfer operator is then constructed as a combination of the so–called space–time weighting operator and space–time "harmonic" extension operator. Finally, using all these components, the space time BDDC preconditioner is built as in the additive Schwarz method.

5 Numerical experiments

5.1 Space–time finite element adaptivity

5.1.1 A linear model problem

We first consider some numerical results for the adaptive solution of the linear model equation (1). For this purpose, we consider the exact solution

$$u(x_1, x_2, t) = (x_1^2 - x_1)(x_2^2 - x_2)(t^2 - t)e^{-100((x_1-t)^2+(x_2-t)^2)} \tag{15}$$

for $(x_1, x_2) \in (0,1)^2$ and $t \in (0,1]$, i.e. $Q = (0,1)^3$, and the given data are defined accordingly. The mesh information is prescribed in Table 1: number of degrees of freedom (#Dofs), number of tetrahedral elements (#Tets), and spatial and temporal mesh size (h/τ). The estimated order of convergence (eoc) for the absolute errors in $L^2(0,T;H_0^1(\Omega))$ on five mesh levels L_1–L_5 are given in Table 2.

A comparison of the convergence history using uniform and adaptive refinements is shown in Figure 3. We mention that, for the adaptive mesh refinements, the octasection

Level	#Dofs	#Tets	h/τ
L_1	125	384	0.25
L_2	729	3072	0.125
L_3	4913	24586	0.0625
L_4	35937	196608	0.03125
L_5	274625	1572864	0.015625

Table 1: Mesh information on five uniformly refined levels: L_1–L_5.

[38] and bisection [14] methods have been used. We use the a posteriori error estimators and the adaptive method as discussed in Subsection 3.8. From the results, we observe a linear order of convergence with both the uniform and two adaptive mesh refinements. The adaptive methods show more efficiency than the uniform one, in particular in saving a number of degrees of freedom.

Level	$\|e\|_{L_2(0,T;H_0^1(\Omega))}$	eoc
L_1	$1.64 \cdot 10^{-2}$	–
L_2	$1.49 \cdot 10^{-2}$	0.13
L_3	$1.08 \cdot 10^{-2}$	0.46
L_4	$6.14 \cdot 10^{-3}$	0.82
L_5	$3.17 \cdot 10^{-3}$	0.96

Table 2: The estimated order of convergence (eoc) for the linear model problem on the mesh levels L_1-L_5.

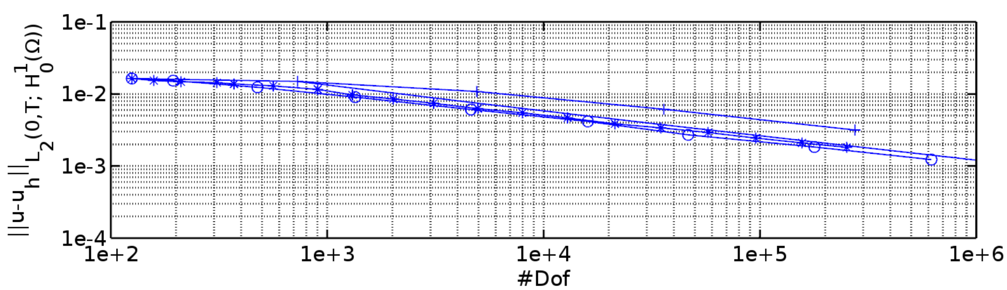

Figure 3: Convergence history of the space–time finite element methods for the linear model problem: uniform $(-+-)$, octasection $(-\circ-)$, bisection $(-*-)$ and linear $(-)$.

In Figure 4, we visualize the adaptive meshes using the octasection and bisection at the time levels $t = 0.25k$, $k = 0, ..., 4$. In Figure 5, we show the numerical solution and adaptive space–time meshes on three planes: $x_1 = 0.5$, $x_2 = 0.5$, $t = 0.5$. Our adaptive methods can effectively capture the moving interface in the space–time domain and make the corresponding adaptive mesh refinements in space–time. More results concerning space–time adaptivity can be found in [203, 205].

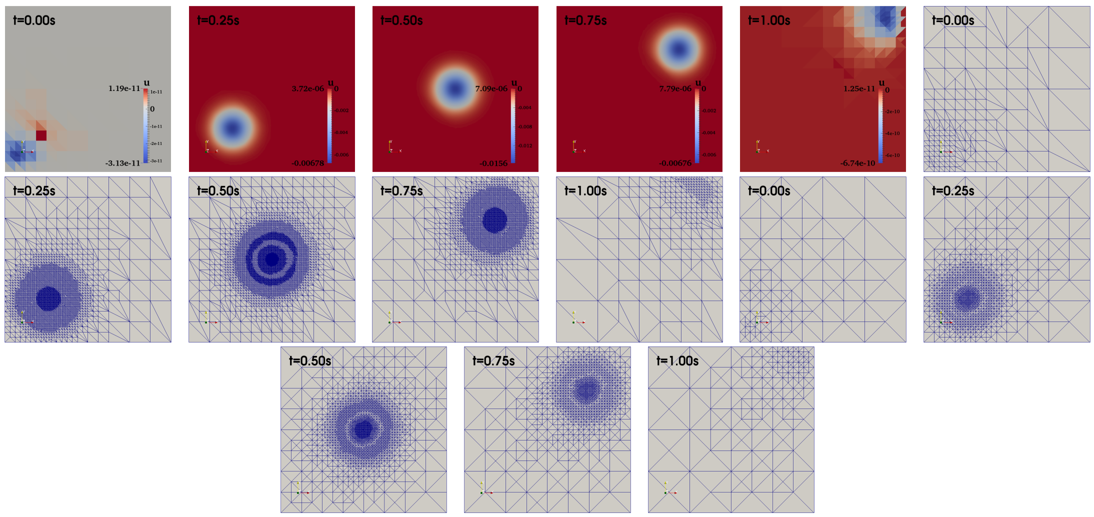

Figure 4: Visualization of numerical solutions and adaptive meshes at time levels $t = 0.25k$, $k = 0, ..., 4$, for the linear model problem: Numerical solution (top), adaptive meshes using octasection at the 9th refinement level (middle) and bisection at the 19th refinement level (bottom).

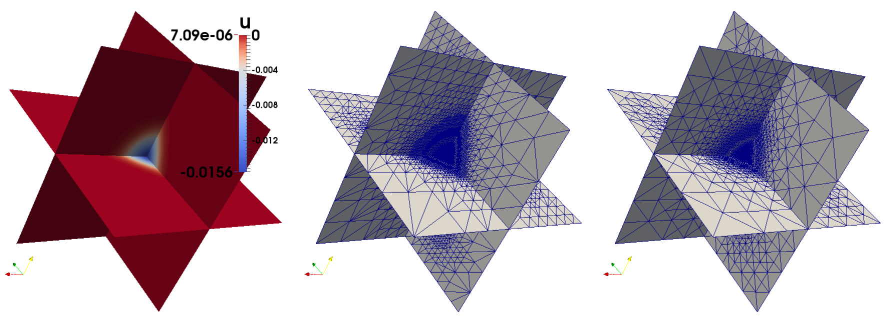

Figure 5: Visualization of the numerical solution and adaptive space-time meshes at $x_1 = 0.5$, $x_2 = 0.5$, $t = 0.5$ for the linear model problem: Numerical solution (left), adaptive meshes using octasection at the 9th refinement level (middle) and bisection at the 19th refinement level (right).

5.1.2 A nonlinear model problem

As an extension of the linear heat equation (1) we also consider the following nonlinear parabolic equation with a third order reaction term and a positive constant ε,

$$\partial_t u(x, t) - \Delta_x u(x, t) + \frac{1}{\varepsilon^2} \left(u^3(x, t) - u(x, t) \right) = 0, \tag{16}$$

which is the so–called Schlögl model [194] or the Nagumo equation [166], with applications in optimal control [52, 57]. We now consider an example with the exact solution

$$u(x_1, x_2, t) = \frac{1}{2}\left(1 - \tanh \frac{x_1 - st}{2\sqrt{2}\varepsilon}\right), \tag{17}$$

in the space–time domain $Q := (17,19)^2 \times (0,5]$, and with $\varepsilon = 0.38$, $s = \frac{3}{\sqrt{2}\varepsilon}$. Note that the spatial domain $\Omega = (17,19)^2$ is chosen such that we can observe the moving interface in the space–time domain Q. The solution and uniform meshes on level 1 are plotted in Figure 6. It is easy to see that the solution changes from 0 to 1 smoothly within a narrow time interval.

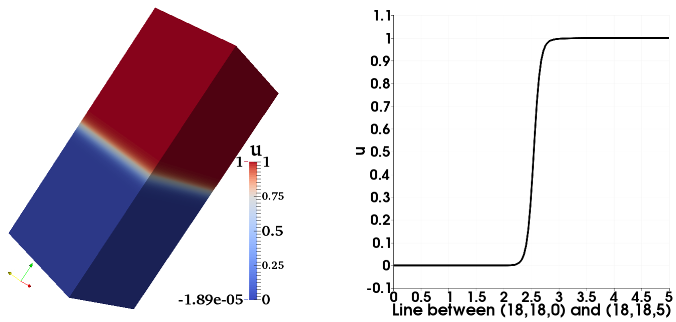

Figure 6: Visualization of the solution (left) for the nonlinear problem, the plot of the solution along the line (time) with the starting point $(18, 18, 0)$ and end point $(18, 18, 5)$ (right).

For this nonlinear model problem, we observe a linear order of convergence of the numerical solution as shown in Table 3. A comparison of adaptive and uniform refinements is demonstrated in Figure 7, where the adaptive ones show a better efficiency. As for the linear model problem, we use the residual based local error indicator (10) on each element to drive the adaptive mesh refinements, where the local residual is replaced by the residual for the nonlinear problem. Note that we observe a better efficiency of the bisection method than the octasection one in this particular example.

Level	#Dofs	$h(\tau)$	$\|e\|_{L_2(0,T;H_0^1(\Omega))}$	eoc
1	225	0.5	$1.35 \cdot 10^{-0}$	–
2	1377	0.25	$8.23 \cdot 10^{-1}$	0.71
3	9537	0.125	$4.78 \cdot 10^{-1}$	0.78
4	70785	0.0625	$2.48 \cdot 10^{-1}$	0.95
5	545025	0.03125	$1.19 \cdot 10^{-1}$	1.06

Table 3: The estimated order of convergence (eoc) for the nonlinear model problem on five mesh levels.

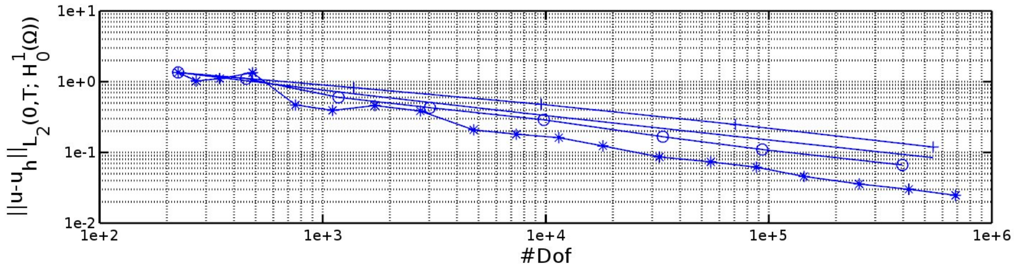

Figure 7: Convergence history of the space-time finite element for the nonlinear model problem: uniform ($-+-$), octasection ($-\circ-$) , bisection ($-*-$) and linear ($-$).

We visualize the numerical solution on the planes $x_1 = 18$, $x_2 = 18$ and $t = 3.0$, and the adaptive space–time meshes on the boundary and on the plane $x_2 = 18$ as given in Figure 8. From the results, we see that the transient interface of the solution in the space–time domain can be captured by the two adaptive methods for this nonlinear model problem.

5.2 Space–time algebraic multigrid methods

To study the performance of the algebraic multigrid methods, we focus on a comparison of algebraic multigrid preconditioned GMRES methods for solving the linear model problem (1), using the greedy (AMG_Greedy) and smoothed aggregation (AMG_SA) coarsening, as discussed in Subsection 4.2. That is because of the pure matrix–graph coarsening leads to a poor performance, and the compatible relaxation scheme leads to a similar performance as the greedy scheme. More numerical results in three and four dimensions are reported in [205].

We use the relative residual reduction tol $= 10^{-8}$ as a stopping criterion for the GMRES method with one V(1,1)–cycle as a preconditioner. The number of AMG_Greedy and AMG_SA preconditioned GMRES iterations and costs in seconds (s) with one V(1,1)–cycle are compared in Table 4. We mention that for this example we use uniform refinements from a bisection method [207]. The preconditioners show relatively good robustness and performance with respect to mesh refinements.

	AMG_Greedy		AMG_SA	
#Dofs	It	sec	It	sec
961	8	0.01	15	0.04
2881	10	0.06	18	0.1
11457	11	0.3	16	0.5
53569	17	2.4	43	7.6
168577	27	13.6	53	27.8

Table 4: Comparison of GMRES iterations and costs in seconds using one V(1,1)–cycle preconditioner on the uniform meshes.

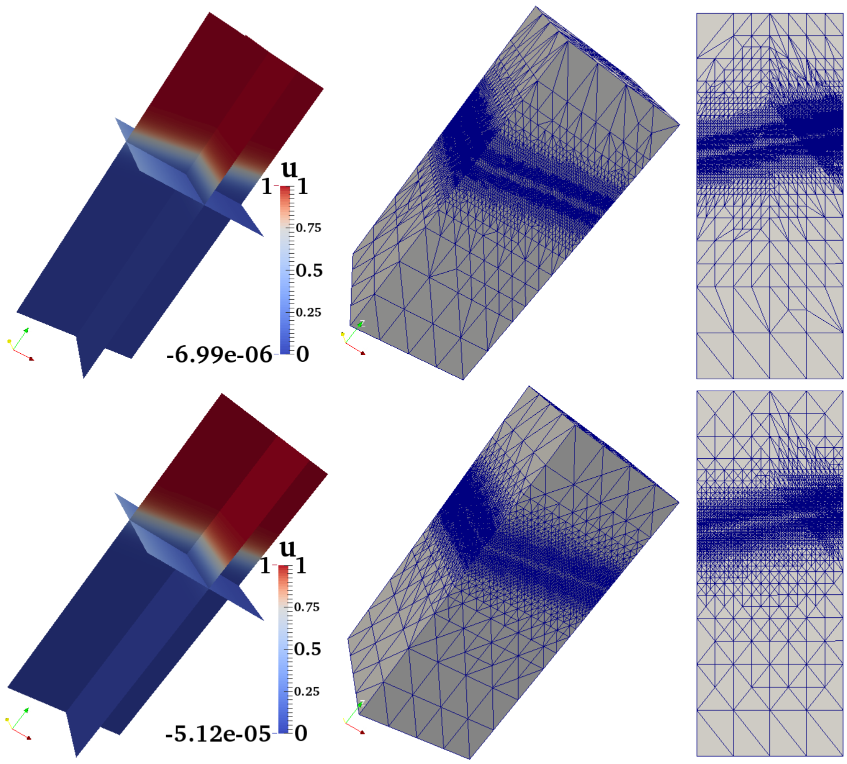

Figure 8: Visualization of the numerical solution on the planes $x_1 = 18$, $x_2 = 18$ and $t = 3.0$ (left), adaptive space-time meshes on the boundary (middle) and on the plane $x_2 = 18$ (right) using octasection at the 8th refinement level (top) and bisection at the 18th refinement level (bottom), for the nonlinear model problem.

5.3 An application to a parabolic optimal control problem

In this example, we apply the Petrov–Galerkin space–time finite element method [202] to a parabolic optimal control problem. We consider the following model problem: Minimize the cost functional

$$\mathcal{J}(u, z) := \frac{1}{2} \int_\Omega [u(x, T) - \bar{u}(x)]^2 dx + \frac{1}{2}\rho \|z\|^2_{L^2(Q)} \tag{18}$$

with respect to the state u and control z subject to the following parabolic problem

$$\begin{aligned} \partial_t u(x,t) - \Delta_x u(x,t) &= z(x,t) \quad &&\text{for } (x,t) \in Q := \Omega \times (0,T), \\ u(x,t) &= g(x,t) \quad &&\text{for } (x,t) \in \Sigma := \Gamma \times (0,T), \\ u(x,0) &= u_0(x) \quad &&\text{for } x \in \Omega, \end{aligned} \tag{19}$$

where $\bar{u}(x)$ denotes a desired final temperature distribution, $z = z(x,t)$ is a control acting on the space–time cylinder Q, and $\rho > 0$ is a regularization parameter; see similar problems considered in [213].

The related optimality system consists of the following three parts:

The primal problem

$$\begin{aligned} \partial_t u(x,t) - \Delta_x u(x,t) &= z(x,t) \quad \text{for } (x,t) \in Q := \Omega \times (0,T), \\ u(x,t) &= g(x,t) \quad \text{for } (x,t) \in \Sigma := \Gamma \times (0,T), \\ u(x,0) &= u_0(x) \quad \text{for } x \in \Omega, \end{aligned} \tag{20}$$

the adjoint problem

$$\begin{aligned} -\partial_t p(x,t) - \Delta_x p(x,t) &= 0 && \text{for } (x,t) \in Q, \\ p(x,t) &= 0 && \text{for } (x,t) \in \Sigma, \\ p(x,T) &= u(x,T) - \bar{u}(x) && \text{for } x \in \Omega, \end{aligned} \tag{21}$$

and the optimality condition

$$p(x,t) + \rho z(x,t) = 0 \text{ for } (x,t) \in Q. \tag{22}$$

We apply the space–time finite element discretization method [202] to this optimality system. We consider $\Omega = (0,1)^2$, $T = 1$, i.e. $Q = (0,1)^3$, and the exact solutions

$$\begin{aligned} u(x,t) &= \frac{3}{4}\zeta e^{2\pi^2 t} \sin(\pi x_1)\sin(\pi x_2), \\ p(x,t) &= -3\rho\pi^2\zeta e^{2\pi^2 t} \sin(\pi x_1)\sin(\pi x_2), \\ z(x,t) &= 3\pi^2\zeta e^{2\pi^2 t} \sin(\pi x_1)\sin(\pi x_2) \end{aligned}$$

with $\zeta = 10^{-9}$. The initial condition for the primal variable is then given by

$$u_0(x) = \frac{3}{4}\zeta \sin(\pi x_1)\sin(\pi x_2),$$

and the target is

$$\bar{u}(x) = (\frac{3}{4} + 3\rho\pi^2)\zeta e^{2\pi^2} \sin(\pi x_1)\sin(\pi x_2).$$

We run simulations on the five mesh levels as provided for the linear model problem in Section 5.1. The estimated order of convergence (eoc) for u, p, and z in $L^2(0,T;H_0^1(\Omega))$ are given in Table 5 and Table 6 for $\rho = 1$ and $\rho = 0.001$, respectively. We observe a linear convergence rate as expected. Moreover, in $L^2(Q)$ we observe a quadratic order of convergence, see Table 7 and Table 8 for $\rho = 1$ and $\rho = 0.001$, respectively.
To solve the discrete optimality system, we utilize a monolithic AMG method using a blockwise ILU smoother [191], and a simple blockwise coarsening strategy [128]. We observe a quite robust AMG performance with respect to the mesh refinements and the regularization parameter; see Table 9. However, due to the high cost of the ILU smoother, the computation is rather expensive, which needs further investigations on finding more robust and efficient smoothers for the solution of such an optimality system.

#Dofs	$\|e_u\|_{0,1}$	eoc	$\|e_p\|_{0,1}$	eoc	$\|e_z\|_{0,1}$	eoc
375	$2.3e-1$	–	$7.7e-0$	–	$7.7e-0$	–
2187	$1.4e-1$	0.68	$4.5e-0$	0.79	$4.5e-0$	0.79
14739	$7.1e-2$	1.00	$2.4e-0$	0.92	$2.4e-0$	0.92
107811	$3.2e-2$	1.13	$1.2e-0$	0.98	$1.2e-0$	0.98
823875	$1.5e-2$	1.09	$6.0e-1$	1.01	$6.0e-1$	1.01

Table 5: The estimated order of convergence (eoc) in $L^2(0,T;H_0^1(\Omega))$ for u, p and z, $\rho = 1$. $\|e_v\|_{0,1} := \|v - v_h\|_{L^2(0,T;H_0^1(\Omega))}$, $v = u, p, z$.

#Dofs	$\|e_u\|_{0,1}$	eoc	$\|e_p\|_{0,1}$	eoc	$\|e_z\|_{0,1}$	eoc
375	$2.2e-1$	–	$7.6e-2$	–	$7.6e-0$	–
2187	$1.3e-1$	0.76	$4.4e-2$	0.79	$4.4e-0$	0.79
14739	$6.6e-2$	0.98	$2.5e-2$	0.82	$2.5e-0$	0.82
107811	$3.1e-2$	1.09	$1.3e-2$	0.94	$1.3e-0$	0.94
823875	$1.5e-2$	1.04	$6.6e-3$	1.01	$6.6e-1$	1.01

Table 6: The estimated order of convergence (eoc) for the optimal control problem in $L^2(0,T;H_0^1(\Omega))$ for u, p and z, $\rho = 0.001$. $\|e_v\|_{0,1} := \|v - v_h\|_{L^2(0,T;H_0^1(\Omega))}$, $v = u, p, z$.

6 Conclusions

This work has reviewed space–time finite element methods for the approximate solution of related parabolic type evolution equations. In particular, the following issues have been addressed: space–time finite element discretization, a posteriori error estimates and corresponding space–time adaptive schemes, and modern parallel space–time solution methods.

Some numerical examples using the Petrov–Galerkin space–time finite element method proposed in [202] have been performed for both linear and nonlinear parabolic problems, which show advantages using simultaneous space–time adaptivity. We have provided numerical tests on algebraic multigrid methods for solving the large–scale linear systems of space–time finite element equations, which show the relative robustness of the solution methods with respect to the mesh refinements. Applicability of the proposed space–time finite element method [202] to the parabolic optimal control problems is confirmed by our numerical examples as well.

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#Dofs	$\|e_u\|_{0,0}$	eoc	$\|e_p\|_{0,0}$	eoc	$\|e_z\|_{0,0}$	eoc
375	$4.0e-2$	–	$1.1e-0$	–	$1.1e-0$	–
2187	$2.5e-2$	0.7	$5.6e-1$	0.9	$5.6e-1$	0.9
14739	$1.1e-2$	1.2	$2.3e-1$	1.3	$2.3e-1$	1.3
107811	$3.5e-3$	1.6	$7.3e-2$	1.6	$7.3e-2$	1.6
823875	$9.6e-4$	1.9	$2.0e-2$	1.8	$2.0e-2$	1.8

Table 7: The estimated order of convergence (eoc) for the optimal control problem in $L^2(Q)$ for u, p and z, $\rho = 1$. $\|e_v\|_{0,0} := \|v - v_h\|_{L^2(Q)}$, $v = u, p, z$.

#Dofs	$\|e_u\|_{0,0}$	eoc	$\|e_p\|_{0,0}$	eoc	$\|e_z\|_{0,0}$	eoc
375	$3.8e-2$	–	$1.0e-2$	–	$1.0e-0$	–
2187	$2.3e-2$	0.7	$5.0e-3$	1.0	$5.0e-1$	1.0
14739	$9.9e-3$	1.2	$2.0e-3$	1.3	$2.0e-1$	1.3
107811	$3.2e-3$	1.6	$6.4e-4$	1.6	$6.4e-2$	1.6
823875	$8.7e-4$	1.9	$1.8e-4$	1.9	$1.8e-2$	1.9

Table 8: The estimated order of convergence (eoc) for the optimal control problem in $L^2(Q)$ for u, p and z on five mesh levels, $\rho = 0.001$. $\|e_v\|_{0,0} := \|v - v_h\|_{L^2(Q)}$, $v = u, p, z$.

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#Dofs	$\rho = 10^2$		$\rho = 10^1$		$\rho = 10^0$		$\rho = 10^{-1}$		$\rho = 10^{-2}$	
#Dofs	It	sec	It	sec	It	sec	It	sec	It	sec
375	2	0.03	2	0.03	2	0.02	2	0.03	2	0.03
2187	3	0.09	3	0.10	3	0.09	3	0.10	3	0.10
14739	3	0.98	3	1.21	3	1.03	3	1.04	3	1.01
107811	3	19.6	3	18.9	4	24.3	4	23.3	4	25.3
823875	4	509	4	522	4	500	4	518	4	585

Table 9: AMG iterations and computational costs for solving the optimality system

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