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Crank-Nicolson Schemes for Optimal Control Problems with Evolution Equations

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Crank-Nicolson schemes for optimal control problems with evolution equations

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Abstract

Crank-Nicolson methods are often used for the simulation of initial boundary value problems for parabolic partial differential equations. In this paper we present a family of discretizations for parabolic optimal control problems based on Crank-Nicolson schemes with different time discretizations for state y and adjoint state p so that discretization and optimization commute. One of these methods can also be explained as a Störmer-Verlet scheme in the context of geometric numerical integration of Hamiltonian systems. Finally two of the schemes may also be obtained as a Galerkin method with quadrature. Further we investigate the schemes for a variable time step size and prove second order convergence for this case if the time step size is chosen with respect to an arbitrary, sufficiently smooth mesh generating function.

1 Introduction

The novelty of this paper is the derivation of variants of the Crank-Nicolson scheme for a distributed parabolic optimal control problem for which discretization and optimization commute. This commutability is desirable for the following reasons: If we discretize first and optimize afterwards, the discrete gradient is the right direction of descent but it is not clear if the discrete adjoint equation is an appropriate discretization of the continuous adjoint equation. On the other hand, if we optimize first and discretize afterwards, we can choose a good approximation of the adjoint equation but the solution operator may not be symmetric and positive definite. Therefore our goal is to find a scheme which combines the advantages of both approaches. Further we prove that our scheme is of second order in time, both for constant and appropriately chosen variable time step sizes.

In particular we discuss the optimal control problem

$$\min \int_0^T \frac{1}{2}\|y - y_d\|_H^2 + \frac{\nu}{2}\|u\|_H^2 \ \mathrm{d}\,t,$$

$$My_{,t} + Ay = Bu,$$

$$y(0) = 0,$$

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with the control u and the state y. The Hilbert space H is appropriately chosen, the desired state $y_d \in H$ is given, the operator A is self-adjoint, and the operators M and B are regular. Examples contain the following (but are not restricted to these cases):

1. Optimal control problem for parabolic partial differential equations:

$$\min \int_0^T \frac{1}{2}\|y - y_d\|^2_{L^2(\Omega)} + \frac{\nu}{2}\|u\|^2_{L^2(\Omega)} \, \mathrm{d}\, t,$$

$$\begin{aligned} y_{,t} - \Delta y &= u && \text{in } (0,T] \times \Omega, \\ \frac{\partial}{\partial n} y &= 0 && \text{on } (0,T] \times \partial\Omega, \\ y(\cdot, 0) &= 0 && \text{in } \{0\} \times \Omega. \end{aligned}$$

   The problem is well posed if we choose $y_d \in L^2((0,T), L^2(\Omega))$, but to show the second order convergence we need more regularity.

2. Optimal control problem for a system of ordinary differential equations:

$$\min \int_0^T \frac{1}{2}\|y - y_d\|^2_{\mathbb{R}^n} + \frac{\nu}{2}\|u\|^2_{\mathbb{R}^n} \, \mathrm{d}\, t,$$

$$\begin{aligned} My_{,t} + Ay &= Mu, \\ y(0) &= 0, \end{aligned}$$

   We can think of the spatial discretization of a parabolic partial differential equation, where M is the mass matrix and A is the stiffness matrix.

Bonnans and Laurent-Varin [3, 4] have analyzed the application of symplectic partitioned Runge-Kutta schemes (SPRK) to the optimal control problem

$$\begin{aligned} &\min \Phi\left(y(T)\right) \\ &y_{,t} = f\left(u(t), y(t)\right), \qquad y(0) = y_0, \end{aligned} \tag{1}$$

with terminal observation in the target function. With the aim that both approaches (optimize then discretize and discretize then optimize) result in the same scheme, they obtained order conditions up to order six, but no method, which fulfills the conditions. Our schemes can be modified for a cost functional with terminal observation and satisfy the conditions for second order. On the other hand a tracking type cost functional for an ordinary differential equation can be treated as terminal cost functional (1) on additional components of y, see [14, Section 1]: The optimal control problem

$$\begin{aligned} &\min_u \int_0^T \frac{1}{2}\|y - y_d\|^2_H + \frac{\nu}{2}\|u\|^2_H \, \mathrm{d}\, t \\ &y_{,t} = f(u(t), y(t)), \qquad y(0) = y_0 \end{aligned}$$

is equivalent to the following optimal control problem with terminal observation

$$\begin{aligned} &\min \; z(T) \\ &y_{,t} = f(u(t), y(t)), && y(0) = y_0, \\ &z_{,t} = \frac{1}{2}\|y(t) - y_d(t)\|^2_H + \frac{\nu}{2}\|u(t)\|^2_H, && z(0) = 0. \end{aligned}$$

Some of the order conditions of Bonnans and Laurent-Varin can also be found in two papers by Hager [14, 15]. Moreover Chyba, Hairer and Vilmart [9] analyze for what kind of optimal control problem with ordinary differential equations symplectic methods are superior to non-symplectic methods.

For optimal control problems with ordinary differential equations and constraints we mention an article by Dontchev, Hager and Veliov [11]. They develop a second order Runge-Kutta method for control constrained problems and prove an error estimate for the case, when the derivative of the optimal control has bounded variation.

All these articles deal only with ordinary differential equations but not with partial differential equations. We emphasize that our analysis covers also the case of time dependent partial differential equations and we give a numerical example for the optimal control of parabolic partial differential equations in Section 5.2.

In recent papers about the optimal control of parabolic partial differential equations the mentioned results about the interchangeability of discretization and optimization for certain time stepping schemes seem to be unknown, or at least uncited [2, 10, 17, 18, 20, 21, 22, 23, 24, 25, 29].

For the optimal control of parabolic partial differential equations space-time finite element methods are very common. In several papers Vexler and coworkers have developed such methods, based on a continuous or discontinuous Galerkin method for the time discretization [2, 20, 21, 22, 23, 29], see also [24]. They also achieve the interchangeability of discretization and optimization. Both, Meidner and Vexler [22] and Neitzel, Prüfert and Slawig [25], discuss optimal control problems with parabolic partial differential equations with control constraints. The approach of space-time finite elements is also used by Deckelnick and Hinze [10], who consider state constraints. Almost all of these discretizations are first order in time. Only Meidner and Vexler obtain second order in the recent preprint [23] by using a postprocessing technique.

Due to the coupling of the forward in time state equation and the backward in time adjoint equation all these discretizations can not be resolved time step by time step but result in a huge system of equations. Multigrid methods on the space-time grid are particularly efficient for their solution, see the fundamental work by Borzì [5] which extends earlier works by Hackbusch, e.g. [13], and the transfer to flow control problems by Hinze, Köster and Turek [17, 18]. The first order implicit Euler scheme is used for time discretization in all these papers. As the $L^2(\Omega)$-approximation error for linear finite elements is of second order this suggests the choice of $\tau = \mathcal{O}(h^2)$ for balancing the errors. With further refinements this leads to an anisotropic mesh and should influence the smoothing and (semi-)coarsening techniques. With the Crank-Nicolson method, space and time discretization have the same order, and the choice $\tau = \mathcal{O}(h)$ is possible for a well-balanced error distribution. We assume that the isotropic elements simplify the solving techniques.

As indicated above, our contribution is the investigation of variants of the Crank-Nicolson scheme for a parabolic optimal control problem. In the next section we introduce our discretization and prove that optimization and discretization commute. We investigate also Störmer-Verlet and Galerkin discretization schemes and show that these schemes can be interpreted as a Crank-Nicolson method. In Section 3 we analyze the convergence in time for a constant time step size. Afterwards in Section 4 we discuss the method for variable time steps and analyse the convergence. There we use a generating function for the time step size. Finally we give some numerical examples in Section 5.

For simplicity and shortness of notation we assume in Sections 2 to 4 that $M = B = \mathrm{Id}$. The generalization to another choice of regular operators M and B is straightforward. So we

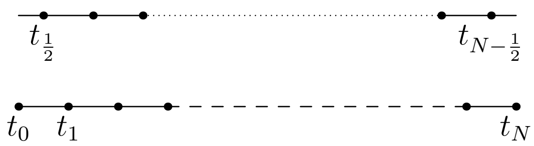


Figure 1: Comparison of the time grids for the discretization of y and p. First line p, second line y.

discuss

$$\min_u \int_0^T \frac{1}{2}\|y - y_d\|_H^2 + \frac{\nu}{2}\|u\|_H^2 \, \mathrm{d}\, t, \tag{2}$$

$$y_{,t} + Ay = u, \tag{3}$$

$$y|_{\partial\Omega} = 0 \text{ or } \left.\frac{\partial y}{\partial n}\right|_{\partial\Omega} = 0, \tag{4}$$

$$y(0) = 0. \tag{5}$$

with $H = L^2(\Omega)$.

2 Time Discretizations

In this section we develop variants of the Crank-Nicolson scheme for which optimization and discretization commute. For clarity of the exposition we consider an equidistant time grid and postpone the generalization to variable time steps to Section 4.

2.1 Crank-Nicolson

Let $0 = t_0 < t_1 < \cdots < t_{N-1} < t_N = T$ be the equidistant time grid with time step size $\tau = t_{k+1} - t_k$ and let $t_{k+\frac{1}{2}} = \frac{1}{2}(t_k + t_{k+1})$. In the following the index k denotes the approximation of a function at the time t_k. The Crank-Nicolson scheme for equation (3) reads

$$\frac{y_{k+1} - y_k}{\tau} + A\frac{y_{k+1} + y_k}{2} = \tilde{u}_{k+\frac{1}{2}} \tag{6}$$

$$\text{where } \tilde{u}_{k+\frac{1}{2}} = u\left(t_{k+\frac{1}{2}}\right) + \mathcal{O}(\tau^2).$$

For the choice of $\tilde{u}_{k+\frac{1}{2}}$ different possibilities exist. Whith $\tilde{u}_{k+\frac{1}{2}} = u(t_{k+\frac{1}{2}})$ we obtain the midpoint rule. The trapezoidal rule $\frac{u_{k+1}+u_k}{2}$ is another popular choice for $\tilde{u}_{k+\frac{1}{2}}$. The less popular choice is $\tilde{u}_{k+\frac{1}{2}} = \frac{1}{6}u_{k-\frac{1}{2}} + \frac{4}{6}u_{k+\frac{1}{2}} + \frac{1}{6}u_{k+\frac{3}{2}}$ is equally well suited and will also be used in Remark 2.4.

For the discretization of the optimal control problem (2)–(5) not only the differential equation but also the cost functional has to be discretized. In view of (6) we discretize y in the grid points t_k and u in the midpoints $t_{k+\frac{1}{2}}$ (see Figure 1). A discretization of (2) is given by

$$\min \frac{1}{2}\left(\frac{\tau}{2}\left(y_0 - y_{d,0}\right)^2 + \tau\sum_{k=1}^{N-1}\left(y_k - y_{d,k}\right)^2 + \frac{\tau}{2}\left(y_n - y_{d,N}\right)^2\right) + \frac{\tau\nu}{2}\sum_{k=0}^{N-1} u_{k+\frac{1}{2}}^2 =$$
$$= \min \ \frac{\tau}{4} y_{d,0}^2 + \frac{\tau}{2}\sum_{k=1}^{N-1}\left(y_k - y_{d,k}\right)^2 + \frac{\tau}{4}\left(y_n - y_{d,N}\right)^2 + \frac{\tau\nu}{2}\sum_{k=0}^{N-1} u_{k+\frac{1}{2}}^2,$$

where the trapezoidal rule is used for the discretization of the first integral and the midpoint rule for the second integral. Together with the differential equation we obtain our first discretization

$$\left.\begin{aligned} &\min \ \frac{\tau}{4} y_{d,0}^2 + \frac{\tau}{2}\sum_{k=1}^{N-1}\left(y_k - y_{d,k}\right)^2 + \frac{\tau}{4}\left(y_N - y_{d,N}\right)^2 + \frac{\tau\nu}{2}\sum_{k=0}^{N-1} u_{k+\frac{1}{2}}^2 \\ &\frac{y_{k+1} - y_k}{\tau} + A\frac{y_{k+1} + y_k}{2} = u_{k+\frac{1}{2}}. \end{aligned}\right\} \qquad \text{(CN1)}$$

To obtain the solution of this linear-quadratic optimization problem we form a Lagrange functional as

$$\begin{aligned} \mathcal{L}\left(\mathbf{y},\mathbf{u},\mathbf{p}\right) &= \frac{\tau}{4} y_{d,0}^2 + \frac{\tau}{2}\sum_{k=1}^{N-1}\left(y_k - y_{d,k}\right)^2 + \frac{\tau}{4}\left(y_N - y_{d,N}\right)^2 + \frac{\tau\nu}{2}\sum_{k=0}^{N-1} u_{k+\frac{1}{2}}^2 \\ &+ \tau\sum_{k=0}^{N-1}\left(\frac{y_{k+1} - y_k}{\tau} + A\frac{y_{k+1} + y_k}{2} - u_{k+\frac{1}{2}}\right)\cdot p_{k+\frac{1}{2}} \\ &\text{with } \mathbf{y} = \left(y_1, \cdots, y_N\right)^T, \ \mathbf{u} = \left(u_{\frac{1}{2}}, \cdots, u_{N-\frac{1}{2}}\right)^T \text{ and } \mathbf{p} = \left(p_{\frac{1}{2}}, \cdots, p_{N-\frac{1}{2}}\right)^T, \end{aligned}$$

with the Lagrange multipliers $\mathbf{p}$ and solve the first order necessary conditions for the optimal solution $(\bar{y},\ \bar{u},\ \bar{p})$

$$\begin{aligned} \frac{\partial\mathcal{L}\left(\bar{\mathbf{y}},\bar{\mathbf{u}},\bar{\mathbf{p}}\right)}{\partial y_i} &= 0 && \text{for } i = 1,\cdots,N, \\ \frac{\partial\mathcal{L}\left(\bar{\mathbf{y}},\bar{\mathbf{u}},\bar{\mathbf{p}}\right)}{\partial p_{i+\frac{1}{2}}} &= 0 && \text{for } i = 0,\cdots,N-1, \\ \frac{\partial\mathcal{L}\left(\bar{\mathbf{y}},\bar{\mathbf{u}},\bar{\mathbf{p}}\right)}{\partial u_{i+\frac{1}{2}}} &= 0 && \text{for } i = 0,\cdots,N-1. \end{aligned}$$

We do not need to compute $\frac{\partial\mathcal{L}(\bar{\mathbf{y}},\bar{\mathbf{u}},\bar{\mathbf{p}})}{\partial y_0}$ as y_0 is not a variable but a given initial value. Note further that we discuss a convex cost functional such that the necessary first order optimality conditions are sufficient, too. The resulting system is

$$\left.\begin{aligned} \frac{\bar{y}_{i+1} - \bar{y}_i}{\tau} + A\frac{\bar{y}_{i+1} + \bar{y}_i}{2} &= \bar{u}_{i+\frac{1}{2}} && \text{for } i = 1,\cdots,N, \\ \nu\bar{u}_{i+\frac{1}{2}} &= \bar{p}_{i+\frac{1}{2}} && \text{for } i = 0,\cdots,N-1, \\ \frac{\bar{p}_{i+\frac{1}{2}} - \bar{p}_{i-\frac{1}{2}}}{\tau} - A\frac{\bar{p}_{i+\frac{1}{2}} + \bar{p}_{i-\frac{1}{2}}}{2} &= \bar{y}_i - y_{d,i} && \text{for } i = 0,\cdots,N-2, \\ -\frac{\bar{p}_{N-\frac{1}{2}}}{\tau} - A\frac{\bar{p}_{N-\frac{1}{2}}}{2} &= \frac{1}{2}\left(\bar{y}_N - y_{d,N}\right). \end{aligned}\right\} \qquad \text{(OC CN1)}$$

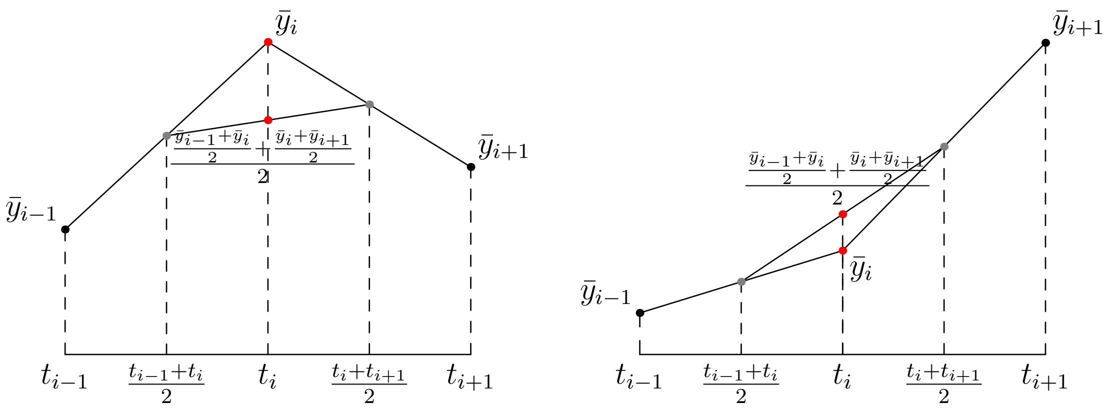


Figure 2: $\frac{\frac{\bar{y}_{i-1}+\bar{y}_i}{2}+\frac{\bar{y}_i+\bar{y}_{i+1}}{2}}{2}$ vs $\bar{y}_i$

Remark 2.1. At the beginning we had to choose a discretization of the cost functional. Another possible choice is the midpoint rule for both integrals in the cost functional. This gives the optimization problem

$$\left.\begin{aligned} \min\ \frac{\tau}{2}\sum_{k=0}^{N-1}\left(\frac{y_k+y_{k+1}}{2}-\frac{y_{d,k+1}+y_{d,k}}{2}\right)^2+\frac{\tau\nu}{2}\sum_{k=0}^{N-1}u_{k+\frac{1}{2}}^2 \\ \frac{y_{i+1}-y_i}{\tau}+A\frac{y_{i+1}+y_i}{2}=u_{i+\frac{1}{2}} \end{aligned}\right\} \tag{CN2}$$

The corresponding first order conditions are

$$\left.\begin{aligned} \frac{\bar{y}_{i+1}-\bar{y}_i}{\tau}+A\frac{\bar{y}_{i+1}+\bar{y}_i}{2} &= \bar{u}_{i+\frac{1}{2}} \\ &\text{for } i=1,\cdots,N, \\ \nu\bar{u}_{i+\frac{1}{2}} &= \bar{p}_{i+\frac{1}{2}} \\ &\text{for } i=0,\cdots,N-1, \\ \frac{\bar{p}_{i+\frac{1}{2}}-\bar{p}_{i-\frac{1}{2}}}{\tau}-A\frac{\bar{p}_{i+\frac{1}{2}}+\bar{p}_{i-\frac{1}{2}}}{2} &= \\ =\frac{\frac{\bar{y}_i+\bar{y}_{i-1}}{2}-\frac{y_{d,i-1}+y_{d,i}}{2}}{2}&+\frac{\frac{\bar{y}_i+\bar{y}_{i+1}}{2}-\frac{y_{d,i+1}+y_{d,i}}{2}}{2} \\ &\text{for } i=0,\cdots,N-2, \\ -\frac{\bar{p}_{N-\frac{1}{2}}}{\tau}-A\frac{\bar{p}_{N-\frac{1}{2}}}{2} &= \frac{\frac{\bar{y}_{N-1}+\bar{y}_N}{2}-\frac{y_{d,N}+y_{d,N-1}}{2}}{2}. \end{aligned}\right\} \tag{OC CN2}$$

The right hand side of the adjoint state equation, $\frac{\frac{\bar{y}_i+\bar{y}_{i-1}}{2}-\frac{y_{d,i+1}+y_{d,i}}{2}}{2}+\frac{\frac{\bar{y}_i+\bar{y}_{i+1}}{2}-\frac{y_{d,i+1}+y_{d,i}}{2}}{2}$, can be interpreted as averaged approximation of $\bar{y}_i-y_{d,i}$ (see Figure 2).

Remark 2.2. The approach used till now is called discretize than optimize. The other way, optimize than discretize, can also be used. We form a continuous Lagrange functional, compute the first order optimality conditions and get the system

$$\left.\begin{aligned} \bar{y}_{,t} + A\bar{y} &= \bar{u}, & \bar{y}(0) &= 0, \\ \bar{p}_{,t} - A\bar{p} &= \bar{y} - y_d, & \bar{p}(T) &= 0, \\ \nu\bar{u} &= \bar{p} & & \end{aligned}\right\} \tag{7}$$

These equations are discretized afterwards. In order to use the shifted time grid $\{t_{\frac{1}{2}}, \cdots, t_{N-\frac{1}{2}}\}$ for the discretization of the adjoint state $\bar{p}$ we consider the modified adjoint problem

$$\begin{aligned} \tilde{p}_{,t} - A\tilde{p} &= \begin{cases} \bar{y} - y_d & \text{in } (0,T), \\ 0 & \text{in } (T, T+\frac{\tau}{2}), \end{cases} \\ \tilde{p}(T + \frac{\tau}{2}) &= 0. \end{aligned} \tag{8}$$

It is easy to see that $\tilde{p} \equiv \bar{p}$ in the time interval $(0, T]$. Application of the midpoint rule to the state equation and a kind of the trapezoidal rule to the adjoint equation yields discretization (OC CN2). Thus we have explained that optimization and discretization commute in the scheme (OC CN2).

The discretization (OC CN1) can also be obtained by the optimize then discretize approach, for details see the next section about the Störmer-Verlet scheme.

2.2 Störmer-Verlet

Hairer, Lubich and Wanner propose in [16, Chapter II.2] an extension of the Störmer-Verlet scheme to general partitioned problems

$$\dot{y} = g(y,p), \qquad\qquad \dot{p} = f(y,p).$$

They prove in [16, Theorem VI.3.4 or Theorem III.2.5] that this scheme applied to a Hamiltonian system, is a method of second order.

Our optimal control problem is a Hamiltonian system because the function

$$H(y,p) = \frac{1}{2}\langle y, y\rangle - \langle y_d, y\rangle + \langle Ay, p\rangle - \frac{1}{2\nu}\langle p, p\rangle + C$$

is a Hamiltonian as

$$\begin{aligned} y_{,t} &= -H_{,p} = -Ay + \frac{1}{\nu}p, \\ p_{,t} &= H_{,y} = Ap + y - y_d, \end{aligned}$$

where we have used that A is self adjoint. If we apply the Störmer-Verlet scheme to this Hamiltonian system we obtain the discrete optimization problem (OC CN1), which shows that optimization and discretization commute also for (CN1). Thus we have immediately that this system is of order two in time [16, Theorem VI.3.4 or Theorem III.2.5].

Remark 2.3. The Störmer-Verlet scheme is a symplectic partitioned Runge-Kutta scheme. In [3, 4] Bonnans and Laurent-Varin discuss the application of such schemes to optimal control problems with ordinary differential equations. They use a slightly different Hamiltonian and prove order conditions.

Order conditions for third and higher order symplectic partitioned Runge-Kutta scheme are also given in [3, 4, 14, 15, 16], but we do not discuss such schemes as they need a high regularity of the solution. For a solution of a parabolic partial differential equation this regularity can only be obtained if further conditions are fulfilled, e.g. the initial and boundary conditions must be compatible (for y and p) and the right hand sides must be smooth.

An example for a forth order symplectic partitioned Runge Kutta scheme which fulfills the condition for commutability of optimization and discretization of [3, 4] is the three stage Lobatto IIIA-IIIB pair given in [16, Chapter II.2.2].

2.3 Galerkin method

Galerkin methods are also popular discretizations of evolution equations. Therefore we introduce the Gelfand triplet $V \subseteq H \cong H^* \subseteq V^*$ and the function spaces

$$\begin{aligned}\mathcal{Y} &= \left\{y \in L^2\left((0,T),V\right) \cap H^1\left((0,T),V^*\right)\right\}\\ \mathcal{P} &= \left\{p \in L^2\left((0,T),V\right)\right\}\end{aligned}$$

and the corresponding discretized function spaces

$$\begin{aligned}\mathbb{P}_n &= \operatorname{span}\left\{t^0,\ t^1, \cdots,\ t^n\right\},\\ \mathcal{Y}_1 &= \Big\{y \in \mathcal{C}\left([0,T],V\right),\ y|_{(t_i,t_{i+1})} \in \mathbb{P}_1\left((t_i,t_{i+1}),V\right)\ \forall i \in \{0,1,\cdots,N\}\Big\},\\ \mathcal{P}_0 &= \Big\{p \in L^2\left((0,T),V\right),\ p|_{(t_i,t_{i+1}]} \in \mathbb{P}_0\left((t_i,t_{i+1}),V\right)\ \forall i \in \{0,1,\cdots,N\}\Big\},\end{aligned}$$

where V and H are $\mathbb{R}^n$ in the case of ordinary differential equations or appropriate function spaces in the case of partial differential equations (e. g. $V = H^1(\Omega)$ or $V = H_0^1(\Omega)$, depending on the boundary conditions, and $H = L^2(\Omega)$). We interpret the degrees of freedom so that they are located in the time discretization points for functions of the space $\mathcal{Y}_1$ and in the midpoint of the time discretization intervals for functions of the space $\mathcal{P}_0$.

We start with the continuous Lagrange functional

$$\mathcal{L}(y,u,p) = \int_0^T \frac{1}{2}\|y - y_d\|_H^2 + \frac{\nu}{2}\|u\|_H^2 + \langle y_{,t} + Ay - u, p\rangle_{V^\star \times V}\,\mathrm{d}\,t.$$

The functional is well defined for $y \in \mathcal{Y}$ and $u,\ p \in \mathcal{P}$. The optimality conditions are obtained by setting the first variations of the Lagrange functional zo zero,

$$\begin{aligned}\left.\frac{\partial \mathcal{L}(\bar{y} + \varepsilon\varphi, \bar{u}, \bar{p})}{\partial \varepsilon}\right|_{\varepsilon=0} &= \int_0^T \langle \bar{y} - y_d, \varphi\rangle_{V^*\times V} + \langle \varphi_{,t} + A\varphi, \bar{p}\rangle_{V^*\times V}\,\mathrm{d}\,t = 0 && \forall \varphi \in \mathcal{Y},\\ \left.\frac{\partial \mathcal{L}(\bar{y}, \bar{u} + \varepsilon\psi, \bar{p})}{\partial \varepsilon}\right|_{\varepsilon=0} &= \int_0^T \langle \nu\bar{u} - \bar{p}, \psi\rangle_{V^*\times V} = 0 && \forall \psi \in \mathcal{P},\\ \left.\frac{\partial \mathcal{L}(\bar{y}, \bar{u}, \bar{p} + \varepsilon\phi)}{\partial \varepsilon}\right|_{\varepsilon=0} &= \int_0^T \langle \bar{y}_{,t} + A\bar{y} - \bar{u}, \phi\rangle_{V^*\times V}\,\mathrm{d}\,t = 0 && \forall \phi \in \mathcal{P}.\end{aligned}$$

Note that $\langle y, \varphi \rangle_{V^* \times V} = \langle y, \varphi \rangle_{H \times H}$ for $\varphi \in V \subset H$ and $y \in H \subset V^*$. For the discretization we choose test functions $\varphi_i \in \mathcal{Y}_1$ and $\psi_{i+\frac{1}{2}},\ \phi_{i+\frac{1}{2}} \in \mathcal{P}_0$, so that

$$\varphi_i(t_j) = \delta_{ij}, \qquad \varphi_i \text{ linear in } [t_j, t_{j+1}] \quad \forall i, j \in \{0, 1, 2, \dots, N\},$$
$$\phi_{i+\frac{1}{2}} = \psi_{i+\frac{1}{2}}(t) = \begin{cases} 1 & \text{if } t \in (t_i, t_{i+1}], \\ 0 & \text{if } t \notin (t_i, t_{i+1}]. \end{cases}$$

Using that A is self-adjoint in the sense $\langle A\varphi, p \rangle_{V^* \times V} = \langle Ap, \varphi \rangle_{V^* \times V}\ \forall p, \varphi \in V$ the integrals simplify to

$$\left.\begin{aligned} \int_{t_{i-1}}^{t_{i+1}} -\langle \varphi_{i,t}, \bar{p} \rangle_{V^* \times V} - \langle A\bar{p}, \varphi_i \rangle_{V^* \times V} \,\mathrm{d}\,t &= \int_{t_{i-1}}^{t_{i+1}} \langle \bar{y} - y_d, \varphi_i \rangle_{V^* \times V} \,\mathrm{d}\,t \\ &\text{for } i = 1, \cdots, N-2, \\ \int_{t_{N-1}}^{t_N} -\langle \varphi_{N,t}, \bar{p} \rangle_{V^* \times V} - \langle A\bar{p}, \varphi_N \rangle_{V^* \times V} \,\mathrm{d}\,t &= \int_{t_{N-1}}^{t_N} \langle \bar{y} - y_d, \varphi_N \rangle_{V^* \times V} \,\mathrm{d}\,t, \\ \int_{t_i}^{t_{i+1}} \langle \bar{y}_{,t}, \phi_{i+\frac{1}{2}} \rangle_{V^* \times V} + \langle A\bar{y}, \phi_{i+\frac{1}{2}} \rangle_{V^* \times V} \,\mathrm{d}\,t &= \int_{t_i}^{t_{i+1}} \langle \bar{u}, \phi_{i+\frac{1}{2}} \rangle_{V^* \times V} \,\mathrm{d}\,t \\ &\text{for } i = 0, \cdots, N-1, \\ \int_{t_i}^{t_{i+1}} \nu \langle \bar{u}, \psi_{i+\frac{1}{2}} \rangle_{V^* \times V} \,\mathrm{d}\,t &= \int_{t_i}^{t_{i+1}} \langle \bar{p}, \psi_{i+\frac{1}{2}} \rangle_{V^* \times V} \,\mathrm{d}\,t \\ &\text{for } i = 0, \cdots, N-1. \end{aligned}\right\} \tag{9}$$

There are different possibilities to treat these equations.

The first possibility is a discretization with $y \in \mathcal{Y}_1,\ u,\ p \in \mathcal{P}_0$ and calculation of the integrals. This yields

$$\left.\begin{aligned} \frac{\bar{y}_{i+1} - \bar{y}_i}{\tau} + A\frac{\bar{y}_{i+1} + \bar{y}_i}{2} &= \bar{u}_{i+\frac{1}{2}} \\ &\text{for } i = 1, \cdots, N-1, \\ \frac{\bar{p}_{i+\frac{1}{2}} - \bar{p}_{i-\frac{1}{2}}}{\tau} - A\frac{\bar{p}_{i+\frac{1}{2}} + \bar{p}_{i-\frac{1}{2}}}{2} &= \frac{\bar{y}_{i-1} - y_{d,i-1}}{6} + \frac{4}{6}\left(\bar{y}_i - y_{d,i}\right) + \frac{\bar{y}_{i+1} - y_{d,i+1}}{6} \\ &\text{for } i = 1, \cdots, N-2, \\ -\frac{\bar{p}_{N-\frac{1}{2}}}{\tau} - A\frac{\bar{p}_{N-\frac{1}{2}}}{2} &= \frac{1}{6}\left(\bar{y}_{N-1} - y_{d,N-1}\right) + \frac{2}{6}\left(\bar{y}_N - y_{d,N}\right), \\ \bar{p}_{i+\frac{1}{2}} &= \nu \bar{u}_{i+\frac{1}{2}}, \\ &\text{for } i = 1, \cdots, N-1. \end{aligned}\right\} \tag{OC G1}$$

Remark 2.4. This scheme (OC G1) can also be obtained by the optimize then discretize approach when we apply the midpoint rule to the state equation (7) and the second order rule

$$\frac{\bar{p}_{i+\frac{1}{2}} - \bar{p}_{i-\frac{1}{2}}}{\tau} - A\frac{\bar{p}_{i+\frac{1}{2}} + \bar{p}_{i-\frac{1}{2}}}{2} = \frac{\bar{y}_{i-1} - y_{d,i-1}}{6} + \frac{4}{6}\left(\bar{y}_i - y_{d,i}\right) + \frac{\bar{y}_{i+1} - y_{d,i+1}}{6}$$

to the modified adjoint state $\tilde{p}$ of (8). Finally, for the last half step of $\tilde{p}$ we use again the modified equation (8) for $\tilde{p}$.

Another possible discretization of the equations (9) is obtained by again using $y \in \mathcal{Y}_1$, $u,\ p \in \mathcal{P}_0$ but the approximate evaluation of the integral with the midpoint rule for the intervals $[t_{i-1}, t_i]$ and $[t_i, t_{i+1}]$. This yields

$$\left.\begin{aligned}
\frac{\bar{y}_{i+1}-\bar{y}_i}{\tau} + A\frac{\bar{y}_{i+1}-\bar{y}_i}{2} &= \bar{u}_{i+\frac{1}{2}} \\
&\text{for } i = 1, \cdots, N-1, \\
\frac{\bar{p}_{i+\frac{1}{2}}-\bar{p}_{i-\frac{1}{2}}}{\tau} - A\frac{\bar{p}_{i-\frac{1}{2}}+\bar{p}_{i+\frac{1}{2}}}{2} &= \frac{\frac{\bar{y}_{i-1}+\bar{y}_i}{2} - \frac{y_{d;i-1}+y_{d;i}}{2}}{2} + \frac{\frac{\bar{y}_i+\bar{y}_{i+1}}{2} - \frac{y_{d;i}+y_{d;i+1}}{2}}{2} \\
&\text{for } i = 1, \cdots, N-2, \\
-\frac{\bar{p}_{N-\frac{1}{2}}}{\tau} - A\frac{\bar{p}_{N-\frac{1}{2}}}{2} &= \frac{\frac{\bar{y}_N+\bar{y}_{N-1}}{2} - \frac{y_{d,N}+y_{d,N}}{2}}{2}, \\
\nu\bar{u}_{i+\frac{1}{2}} &= \bar{p}_{i+\frac{1}{2}} \\
&\text{for } i = 1, \cdots, N-1,
\end{aligned}\right\} \qquad \text{(OC G2)}$$

which is (OC CN2).

As a third variant, let us discuss discretization and exact calculation of the integrals but projection of $(y - y_d) \in \mathcal{Y}_1$ on the right hand side to $z \in \mathcal{P}_0$. This corresponds to the Lagrange functional

$$\mathcal{L}(y, z, u, p, q) = \int_0^T \frac{1}{2}\|z\|_H^2 + \frac{\nu}{2}\|u\|_H^2 + \langle y_{,t} + Ay - u, p\rangle_{V^\star \times V} + \langle y - y_d - z, q\rangle_{V^\star \times V} \,\mathrm{d}\,t$$

with an additional Lagrange multiplier q. This functional is well defined for $y \in \mathcal{Y}$ and $u,\ p,\ q,\ z \in \mathcal{P}$. The first order optimality conditions are

$$\begin{aligned}
\left.\frac{\partial\mathcal{L}(\bar{y}+\varepsilon\varphi, \bar{z}, \bar{u}, \bar{p}, \bar{q})}{\partial\varepsilon}\right|_{\varepsilon=0} &= \int_0^T \langle \varphi_t + A\varphi, \bar{p}\rangle_{V^\star\times V} + \langle\varphi, \bar{q}\rangle_{V^\star\times V} \,\mathrm{d}\,t = 0 && \forall\varphi \in \mathcal{Y}, \\
\left.\frac{\partial\mathcal{L}(\bar{y}, \bar{z}+\varepsilon\vartheta, \bar{u}, \bar{p}, \bar{q})}{\partial\varepsilon}\right|_{\varepsilon=0} &= \int_0^T \langle\vartheta, \bar{z} - \bar{q}\rangle_{V^\star\times V} \,\mathrm{d}\,t = 0 && \forall\vartheta \in \mathcal{P}, \\
\left.\frac{\partial\mathcal{L}(\bar{y}, \bar{z}, \bar{u}+\varepsilon\psi, \bar{p}, \bar{q})}{\partial\varepsilon}\right|_{\varepsilon=0} &= \int_0^T \langle\nu\bar{u} - \bar{p}, \psi\rangle_{V^\star\times V} \,\mathrm{d}\,t = 0 && \forall\psi \in \mathcal{P}, \\
\left.\frac{\partial\mathcal{L}(\bar{y}, \bar{z}, \bar{u}, \bar{p}+\varepsilon\phi, \bar{q})}{\partial\varepsilon}\right|_{\varepsilon=0} &= \int_0^T \langle\bar{y}_t + A\bar{y} - \bar{u}, \phi\rangle_{V^\star\times V} \,\mathrm{d}\,t = 0 && \forall\phi \in \mathcal{P}, \\
\left.\frac{\partial\mathcal{L}(\bar{y}, \bar{z}, \bar{u}, \bar{p}, \bar{q}+\varepsilon\eta)}{\partial\varepsilon}\right|_{\varepsilon=0} &= \int_0^T \langle\bar{y} - y_d - \bar{z}, \eta\rangle_{V^\star\times V} \,\mathrm{d}\,t = 0 && \forall\eta \in \mathcal{P}.
\end{aligned}$$

If we choose for the discretization $\varphi,\ y \in \mathcal{Y}_1$ and for all other functions the discretization space

$\mathcal{P}_0$ we have to solve, after elimination of the additional variables z and q

$$\frac{\bar{y}_{i+1} - \bar{y}_i}{\tau} + A\frac{\bar{y}_{i+1} - \bar{y}_i}{2} = \bar{u}_{i+\frac{1}{2}}$$
$$\text{for } i = 1, \cdots, N-1,$$
$$\frac{\bar{p}_{i+\frac{1}{2}} - \bar{p}_{i-\frac{1}{2}}}{\tau} - A\frac{\bar{p}_{i-\frac{1}{2}} + \bar{p}_{i+\frac{1}{2}}}{2} = \frac{\frac{\bar{y}_{i-1}+\bar{y}_i}{2} - \frac{y_{d;i-1}+y_{d;i}}{2}}{2} + \frac{\frac{\bar{y}_i+\bar{y}_{i+1}}{2} - \frac{y_{d;i}+y_{d;i+1}}{2}}{2}$$
$$\text{for } i = 1, \cdots, N-2,$$
$$-\frac{\bar{p}_{N-\frac{1}{2}}}{\tau} - A\frac{\bar{p}_{N-\frac{1}{2}}}{2} = \frac{\frac{\bar{y}_N+\bar{y}_{N-1}}{2} - \frac{y_{d,N}+y_{d,N-1}}{2}}{2},$$
$$\nu\bar{u}_{i+\frac{1}{2}} = \bar{p}_{i+\frac{1}{2}}$$
$$\text{for } i = 1, \cdots, N-1.$$

Hence, this approach is equivalent to (OC CN2), too.

In summary, the Galerkin method with exact integration led to a new scheme which can be interpreted as another variant of the Crank-Nicolson scheme. The Galerkin method with quadrature or projection reproduced scheme (OC CN2). For the scheme (OC CN1) we did not find a quadrature rule with which it is a Galerkin scheme.

3 Error analysis for optimal control with parabolic partial differential equations and constant time step size

We prove that the error is of order 2 for the case of optimal control with parabolic partial differential equations. The case of ordinary differential equations is also covered by the analysis of this section if one replaces $L^2(\Omega)$ and $H^2(\Omega)$ by $\mathbb{R}^n$ and discusses the time discretization error only. Further we restrict ourself to the case of the Laplace operator and homogenous Dirichlet or homogenous Neumann boundary conditions.

In our analysis we need $\bar{y},\ \bar{p} \in H^3((0,T), L^2(\Omega)) \cap H^2((0,T), H^2(\Omega))$. For such a regularity in a problem with parabolic partial differential equations we need a smooth right hand side and further compatibility conditions on initial and boundary conditions. These are discussed e.g. in [12, Theorem 7.1.5, 7.1.6 and 7.1.7] or [32, Theorem 27.2 and 27.3]. In the example of a smooth domain Ω, e.g. if the domain is one dimensional, one obtains from Theorem 7.1.6 of [12]

$$\bar{y} \in L^2((0,T), H^2(\Omega)) \cap L^\infty((0,T), H^1_0(\Omega)) \cap H^1((0,T), L^2(\Omega))$$

and hence

$$\bar{p} \in H^2((0,T), L^2(\Omega)) \cap H^1((0,T), H^2(\Omega)) \cap L^2((0,T), H^4(\Omega))$$

and with a bootstrapping argument

$$\bar{y},\ \bar{p} \in H^3((0,T), L^2(\Omega)) \cap H^2((0,T), H^2(\Omega)) \cap H^1((0,T), H^4(\Omega)) \cap L^2((0,T), H^6(\Omega))$$

under the assumption

$$y_d \in H^2((0,T), L^2(\Omega)) \cap H^1((0,T), H^2(\Omega)) \cap L^2((0,T), H^4(\Omega)).$$

The space V_h is the space of piecewise linear, continuous functions to a given triangulation with mesh size parameter h. For the convergence of the time discretization scheme for parabolic partial differential equations we use an error splitting technique. Let $\bar{y}$ and $\bar{p}$ be the solution of the continuous problem, $I_h\bar{y}_h$ and $I_h\bar{p}_h$ the solution of the problem after discretization in space with linear finite elements corresponding to the vectors $\bar{y}_h(t)$ and $\bar{p}_h(t)$ of coefficients with respect to the Lagrangian basis functions and the interpolation operator $I_h : \mathbb{R}^n \to V_h$. So the functions $\bar{y}_h$ and $\bar{p}_h$ are functions $\mathbb{R}^+ \to \mathbb{R}^n$. Finally let $\bar{y}_{h,i}$ and $\bar{p}_{h,i-\frac{1}{2}}$ be the approximation of $\bar{y}_h$ and $\bar{p}_h$ with the scheme (OC CN1) at the time t_i and $t_{i-\frac{1}{2}}$, respectively.

We introduce the projection $R_h y(\cdot, t_i) \in V_h$ as

$$(\nabla R_h y(\cdot, t_i), \nabla\chi) = (\nabla y(\cdot, t_i), \nabla\chi) \qquad \forall\chi \in V_h, \tag{10}$$

$$\text{and} \int_\Omega R_h y(\cdot, t_i)\,\mathrm{d}\,\omega = \int_\Omega y(\cdot, t_i)\,\mathrm{d}\,\omega. \tag{11}$$

Lemma 3.1. *The projection $R_h y(\cdot, t_i)$ is well-defined and if the domain Ω is convex we have the estimate*

$$\|R_h y(\cdot, t_i) - y(\cdot, t_i)\|_{L^2(\Omega)} \le h^2 \|y(\cdot, t_i)\|_{H^2(\Omega)}.$$

Proof. Consider the function

$$\tilde{y}(\cdot) = y(\cdot, t_i) - \frac{1}{\mathrm{meas}(\Omega)} \int_\Omega y(\cdot, t_i)\,\mathrm{d}\,\omega \in H^\star(\Omega) = \left\{ v \in H^1(\Omega) : \int_\Omega v\,\mathrm{d}\,\omega = 0 \right\}$$

for any t_i and its projection $\tilde{y}_h \in V_h^\star = \left\{ v \in V_h : \int_\Omega v_h\,\mathrm{d}\,\omega = 0 \right\}$ defined by

$$(\nabla\tilde{y}_h, \nabla\chi) = (\nabla\tilde{y}, \nabla\chi) \qquad \forall\chi \in V_h. \tag{12}$$

It is well known that this projection is unique [7, Chapter 5.2] and it is well known that

$$\|\tilde{y} - \tilde{y}_h\|_{H^1(\Omega)} \lesssim h|\tilde{y}|_{H^2(\Omega)}.$$

As the domain Ω is convex we get second order convergence in $L^2(\Omega)$ with the usual duality argument [7, Chapter 5.4 and 5.5]. We compute the projection $R_h y(\cdot, t_i)$ as

$$R_h y(\cdot, t_i) = \tilde{y}_h + \int_\Omega y(\cdot, t_i)\,\mathrm{d}\,\omega. \tag{13}$$

It is easy to see that this $R_h y$ fullfills (10) and (11).

The projection is unique as (12) has a unique solution and any function $y \in H^1(\Omega)$ can be written as $y = y_0 + c$ with $y_0 \in H^\star(\Omega)$ and a constant c. □

Then we can split the errors into the differences between the exact solution and its projection

$$\rho_i^y(\cdot) = R_h y(\cdot, t_i) - y(\cdot, t_i), \qquad \rho_{i-\frac{1}{2}}^p(\cdot) = R_h p(\cdot, t_{i-\frac{1}{2}}) - p(\cdot, t_{i-\frac{1}{2}}),$$

and the difference between the projection and the numerical approximation

$$\theta_i^y(\cdot) = I_h y_{h,i}(\cdot) - R_h y(\cdot, t_i), \qquad \theta_{i-\frac{1}{2}}^p(\cdot) = I_h p_{h,i}(\cdot) - R_h p(\cdot, t_{i-\frac{1}{2}}).$$

With these nomenclature we can prove the convergence for the case of optimal control of parabolic partial differential equations:

Theorem 3.2. *If*

- *the scheme (OC CN1) is applied to the optimal control problem (2)–(5) with parabolic partial differential equation and*
- $A = -\Delta$ *and homogeneous Dirichlet or homogeneous Neumann boundary conditions,* $V = H_0^1(\Omega)$ *or* $V = H^1(\Omega)$*, respectively,*
- *linear finite elements are used for space discretization,*
- *for the exact solution* $\bar{y}, \bar{p}, \bar{u} \in H^3((0,T), L^2(\Omega)) \cap H^2((0,T), H^2(\Omega))$ *holds,*

then the error can be estimated by

$$\|I_h\bar{y}_{h,i}(\cdot) - \bar{y}(\cdot,t_i)\|_{L^2(\Omega)} + \|I_h\bar{p}_{h,i-\frac{1}{2}}(\cdot) - \bar{p}(\cdot,t_{i-\frac{1}{2}})\|_{L^2(\Omega)} \lesssim C_1(\bar{y},\bar{p})h^2 + C_2(\bar{y},\bar{p})\tau^2, \quad i = 1,\cdots,N$$

$$\text{with } C_1(\bar{y},\bar{p}) = \int_0^T \|\bar{y}_{,t}(\cdot,s)\|_{H^2(\Omega)} + \|\bar{p}_{,t}(\cdot,s)\|_{H^2(\Omega)}\,\mathrm{d}\,s \tag{14}$$

$$\left.\begin{aligned} C_2(\bar{y},\bar{p}) = &\int_0^T \|\bar{y}_{,ttt}(\cdot,s)\|_{L^2(\Omega)} + \|\Delta\bar{y}_{,tt}(\cdot,s)\|_{L^2(\Omega)}\,\mathrm{d}\,s \\ &+ \int_0^T \|\bar{p}_{,ttt}(\cdot,s)\|_{L^2(\Omega)} + \|\Delta\bar{p}_{,tt}(\cdot,s)\|_{L^2(\Omega)} + \|\bar{u}_{,tt}(\cdot,s)\|\,\mathrm{d}\,s \\ &+ \|\bar{p}_{,tt}(\cdot,T)\|_{L^2(\Omega)} + \|\Delta\bar{p}_{,t}(\cdot,T)\|_{L^2(\Omega)}, \end{aligned}\right\} \tag{15}$$

i.e. we have a scheme of second order in h *and* τ*.*

Remark 3.3. The smoothness assumption of Theorem 3.2 is the same as needed in Thomée's book, [31, Theorem 1.6], for the proof of second order convergence of the Crank-Nicolson scheme for the uncontrolled heat equation with inhomogeneous right hand side.

In preparation of the proof of Theorem 3.2 we will prove some lemmas. We begin with some variations of the proof of [31, Theorem 1.6] as the right hand side of the continuous and the discrete equations do not coincide in the case of optimal control problems.

Lemma 3.4. *The error between the state, adjoint state and the corresponding projections can be estimated by*

$$\|\rho_i^y\|_{L^2(\Omega)} = \|R_h y(\cdot,t_i) - y(\cdot,t_i)\|_{L^2(\Omega)} \lesssim h^2 \int_0^{t_i} \|y_{,t}(\cdot,s)\|_{H^2(\Omega)}\,\mathrm{d}\,s,$$

$$\|\rho^p_{i-\frac{1}{2}}\|_{L^2(\Omega)} = \|R_h p(\cdot,t_{i-\frac{1}{2}}) - p(\cdot,t_{i-\frac{1}{2}})\|_{L^2(\Omega)} \lesssim h^2 \int_{t_{i-\frac{1}{2}}}^T \|p_{,t}(\cdot,s)\|_{H^2(\Omega)}\,\mathrm{d}\,s.$$

Proof. For the projection the estimate

$$\|R_h y(\cdot,t_i) - y(\cdot,t_i)\|_{L^2(\Omega)} \lesssim h^2 \|y(\cdot,t_i)\|_{H^2(\Omega)} \tag{16}$$

is well known (see Lemma 3.1). With the fundamental theorem of calculus we have

$$\|y(\cdot,t_i)\|_{H^2(\Omega)} = \|y(\cdot,0) + \int_0^{t_i} y_t(\cdot,s)\|_{H^2(\Omega)}\,\mathrm{d}\,s \le \|y(\cdot,0)\|_{H^2(\Omega)} + \int_0^{t_i} \|y_{,t}(\cdot,s)\|_{H^2(\Omega)}\,\mathrm{d}\,s.$$

For the adjoint state we integrate backward in time from $t = T$ to $t = t_{i-\frac{1}{2}}$. As $y(\cdot,0) = p(\cdot,T) = 0$ the proof of the lemma is finished. □

We prove now two lemmata where we show that the state and the adjoint state are $\mathcal{O}(h^2+\tau^2)$ close to the optimal ones, if the control is $\mathcal{O}(h^2+\tau^2)$ close to the optimal control.

Lemma 3.5. *For a given control $I_h u_{h,i+\frac{1}{2}}$ with $\|I_h u_{h,i+\frac{1}{2}} - \bar{u}(\cdot, t_{i+\frac{1}{2}})\|_{L^2(\Omega)} \leq C_1 h^2 + C_2\tau^2$ with C_1 and C_2 specified in (14) and (15), the error in the state variable is bounded by*

$$\|I_h y_{h,i}(\cdot) - y(\cdot, t_i)\|_{L^2(\Omega)} \lesssim C_1 h^2 + C_2 \tau^2.$$

Proof. With the error splitting and Lemma 3.4 it is sufficient to discuss the difference θ_i^y between the projection and the numerical approximation. For this estimate we follow the proof of [31, Theorem 1.6]. Therefore we insert $\theta^{\bar{y}}$ into the weak form of the discrete scheme

$$\begin{aligned}
&\left(\frac{\theta_i^{\bar{y}} - \theta_{i-1}^{\bar{y}}}{\tau}, \chi\right) + \left(\frac{\nabla\theta_i^{\bar{y}} + \nabla\theta_{i-1}^{\bar{y}}}{2}, \nabla\chi\right) = \\
&= \left(I_h u_{h,i-\frac{1}{2}}(\cdot), \chi\right) - \left(\frac{\nabla R_h \bar{y}(\cdot, t_i) + \nabla R_h \bar{y}(\cdot, t_{i-1})}{2}, \nabla\chi\right) - \left(\frac{R_h\bar{y}_i(\cdot) - R_h\bar{y}_{i-1}(\cdot)}{\tau}, \chi\right) \\
&= \left(\bar{y}_{,t}(\cdot, t_{i+\frac{1}{2}}), \chi\right) + \left(\nabla\bar{y}(\cdot, t_{i+\frac{1}{2}}), \nabla\chi\right) + \left(I_h u_{h,i-\frac{1}{2}}(\cdot) - \bar{u}(\cdot, t_{i-\frac{1}{2}}), \chi\right) \\
&- \left(\frac{\nabla\bar{y}(\cdot, t_i) + \nabla\bar{y}(\cdot, t_{i-1})}{2}, \nabla\chi\right) - \left(\frac{R_h\bar{y}_i(\cdot) - R_h\bar{y}_{i-1}(\cdot)}{\tau}, \chi\right) \\
&= -\left((R_h - I)\frac{\bar{y}(\cdot, t_i) - \bar{y}(\cdot, t_{i-1})}{\tau} + \frac{\bar{y}(\cdot, t_i) - \bar{y}(\cdot, t_{i-1})}{\tau} - \bar{y}_{,t}(\cdot, t_{i+\frac{1}{2}})\right. \\
&\qquad \left. + \Delta\bar{y}(\cdot, t_{i+\frac{1}{2}}) - \Delta\left(\frac{\bar{y}(\cdot, t_{i+1}) + \bar{y}(\cdot, t_i)}{2}\right), \chi\right) + \left(I_h u_{h,i-\frac{1}{2}}(\cdot) - \bar{u}(\cdot, t_{i-\frac{1}{2}}), \chi\right) \\
&=: -(\omega_i, \chi) + \left(I_h u_{h,i-\frac{1}{2}}(\cdot) - \bar{u}(\cdot, t_{i-\frac{1}{2}}), \chi\right).
\end{aligned}$$

Using $\frac{\theta_i^{\bar{y}} + \theta_{i-1}^{\bar{y}}}{2}$ as test function yields

$$\begin{aligned}
\|\theta_i^{\bar{y}}\|_{L^2(\Omega)} &\leq \|\theta_{i-1}^{\bar{y}}\|_{L^2(\Omega)} + \tau\|\omega_i\|_{L^2(\Omega)} + \tau\|I_h u_{h,i-\frac{1}{2}} - \bar{u}(\cdot, t_{i-\frac{1}{2}})\|_{L^2(\Omega)} \\
&\leq \|\theta_0^{\bar{y}}\|_{L^2(\Omega)} + \sum_{j=1}^{i} \tau\|\omega_j\|_{L^2(\Omega)} + \tau\sum_{j=1}^{i}\left(C_1 h^2 + C_2\tau^2\right) \\
&\leq \|\theta_0^{\bar{y}}\|_{L^2(\Omega)} + \sum_{j=1}^{i} \tau\|\omega_j\|_{L^2(\Omega)} + \left(C_1 h^2 + C_2\tau^2\right).
\end{aligned}$$

As $\|\theta_0^{\bar{y}}\|_{L^2(\Omega)} = 0$ and $\sum_{j=1}^{i} \tau\|\omega_j\|_{L^2(\Omega)}$ can be bounded by standard estimates and by using (16), see [31, Theorem 1.6], the proof is done. □

Lemma 3.6. *For a given discretized state $I_h y_{h,i}$ with $\|I_h y_{h,i} - \bar{y}(\cdot, t_i)\|_{L^2(\Omega)} \leq C_1 h^2 + C_2\tau^2$ with C_1 and C_2 specified in (14) and (15), the error of the numerical approximation of the adjoint state is bounded by*

$$\|I_h p_{h,i-\frac{1}{2}}(\cdot) - p(\cdot, t_{i-\frac{1}{2}})\|_{L^2(\Omega)} \lesssim C_1 h^2 + C_2\tau^2.$$

Proof. Again it is sufficient to discuss the error between the projection of the adjoint state and the numerical approximation. With an analogous argument as in the previous proof we get the estimate

$$\begin{aligned}\|\theta^{\bar{p}}_{i-\frac{1}{2}}\|_{L^2(\Omega)} &\leq \|\theta^{\bar{p}}_{i+\frac{1}{2}}\|_{L^2(\Omega)} + \tau\|\omega_{i-\frac{1}{2}}\|_{L^2(\Omega)} + \tau C(h^2+\tau^2)\\ &\leq \tau\|\omega_{N-\frac{1}{2}}\|_{L^2(\Omega)} + \tau\sum_{j=i}^{N-1}\|\omega_{i-\frac{1}{2}}\|_{L^2(\Omega)} + \tau\sum_{j=i}^{N-\frac{1}{2}} C(h^2+\tau^2) \qquad (17)\end{aligned}$$

$$\begin{aligned}\text{with } \omega_{i-\frac{1}{2}} &= (I-R_h)\frac{\bar{p}(t_{i-\frac{1}{2}})-\bar{p}(t_{i+\frac{1}{2}})}{\tau} + \frac{\bar{p}(t_{i+\frac{1}{2}})-\bar{p}(t_{i-\frac{1}{2}})}{\tau} - \bar{p}_t(t_i) +\\ &+ \frac{\Delta\bar{p}(t_{i-\frac{1}{2}})+\Delta\bar{p}(t_{i+\frac{1}{2}})}{2} - \Delta\bar{p}(t_i)\\ \text{and } \omega_{N-\frac{1}{2}} &= (I-R_h)\frac{\bar{p}(t_{N-\frac{1}{2}})}{\tau} - \frac{\bar{p}(t_{N-\frac{1}{2}})}{\tau} - \frac{1}{2}\bar{p}_{,t}(t_N) + \frac{\Delta\bar{p}(t_{N-\frac{1}{2}})}{2} - \frac{1}{2}\Delta\bar{p}(t_N)\end{aligned}$$

As in the previous lemma we can bound $\tau\sum_{j=i}^{N-1}\|\omega_{i-\frac{1}{2}}\|_{L^2(\Omega)}$ as in [31, Theorem 1.6]. So we only need to bound the error $\omega_{N-\frac{1}{2}}$ in the last step.

The first term of $\omega_{N-\frac{1}{2}}$ is the error of a projection and therefore of order h^2, where we used also $-\bar{p}(\cdot,t_{N-\frac{1}{2}}) = \int_{t_{N-\frac{1}{2}}}^{t_N}\bar{p}_{,t}(\cdot,s)\,\mathrm{d}\,s$ and the cancelation of the factor $\frac{1}{\tau}$ with the factor τ in (17). The other terms are of order τ^2 as

$$\begin{aligned}-\frac{\tau}{2}\bar{p}_{,t}(\cdot,t_N) - \bar{p}(\cdot,t_{N-\frac{1}{2}}) &= -\frac{\tau^2}{8}\bar{p}_{,tt}(\cdot,t_N) + \frac{1}{2}\int_{t_{N-\frac{1}{2}}}^{T}(s-t_{N-\frac{1}{2}})^2\bar{p}_{,ttt}(\cdot,s)\,\mathrm{d}\,s,\\ \tau\frac{\Delta\bar{p}(\cdot,t_{N-\frac{1}{2}})}{2} - \tau\frac{1}{2}\Delta\bar{p}(\cdot,t_N) &= -\frac{\tau^2}{4}\Delta\bar{p}_{,t}(\cdot,t_N) + \frac{\tau}{2}\int_{t_{N-\frac{1}{2}}}^{T}(s-t_{N-\frac{1}{2}})\Delta\bar{p}_{,tt}(\cdot,s)\,\mathrm{d}\,s\end{aligned}$$

holds. For the last equality we used $\bar{p}(\cdot,t_N)=0$ and therefore also $\Delta\bar{p}(\cdot,t_N)=0$. □

The last two lemmas may be also used as approximation result for the state and adjoint equation for a given right hand side.

So finally we need to assure that the control approximation is of second order. Therefore we introduce some further notation. The space $L^2(Q)$ has the norm

$$\|u\|^2_{L^2(Q)} = \int_0^T\int_\Omega u^2(\cdot,\cdot)\,\mathrm{d}\,\omega\,\mathrm{d}\,t.$$

The interpolation operator J_τ is defined by

$$\begin{aligned}J_\tau u(\cdot,\cdot)(T) &= u(\cdot,T),\\ J_\tau u(\cdot,\cdot)(t_{k+\frac{1}{2}}) &= u(\cdot,t_{k+\frac{1}{2}}), && \forall k=0,\cdots,N-1\\ J_\tau u(\cdot,\cdot) &\text{ linear in } (t_k,t_{k+1}), && \forall k=0,\cdots,N-1\\ J_\tau u(\cdot,\cdot) &\text{ continuous in } [0,T].\end{aligned}$$

We write $u_{h,k-\frac{1}{2}}$ for the numerical approximation of u with space discretization parameter h at $t = t_{k-\frac{1}{2}}$ and $J_\tau I_h u_{h,\tau}$ as the interpolation of the numerical solution in space and time. The optimal control is denoted by $\bar{u}$ and $\bar{u}_{h,\tau}$ at the discrete level. Finially we recall the estimate

$$\|u(\cdot,\cdot) - J_\tau u(\cdot,\cdot)\|_{L^2(Q)} \leq C\tau^2 \|u_{,tt}(\cdot,\cdot)\|_{L^2(Q)} \forall u \in H^2((=,T), H^2(\Omega)). \tag{18}$$

Lemma 3.7. *If for the optimal control* $\bar{u} \in H^3((0,T), L^2(\Omega)) \cap H^2((0,T), H^2(\Omega))$ *holds, then the error of the control approximation can be bounded by*

$$\|J_\tau I_h \bar{u}_{h,\tau}(\cdot,\cdot) - \bar{u}(\cdot,\cdot)\|_{L^2(Q)} \lesssim C_1 h^2 + C_2 \tau^2.$$

Proof. We follow the proof of [21, Theorem 6.1] and start with the weak form of the optimality condition

$$\int_0^T (\nu \bar{u}(\cdot,t) - \bar{p}(\cdot,t), \varphi) \,\mathrm{d}\,t = 0 \qquad\qquad \forall \varphi \in L^2(\Omega),$$

and its discretization

$$\tau(\nu I_h \bar{u}_{h,k+\frac{1}{2}}(\cdot) - I_h \bar{p}_{h,k+\frac{1}{2}}(\cdot), \varphi) = 0 \qquad \forall \varphi \in V_h(\Omega), \text{ for } k = 0, \cdots, N-1.$$

This form of the optimality condition is equivalent to the optimality condition $\nu u_{k+\frac{1}{2}} = p_{k+\frac{1}{2}}$of (OC CN1). The optimality conditions (OC CN1) are fulfilled for the optimal control $\bar{u}$ together with its corresponding adjoint state $\bar{p}$, but clearly not for any other function $u(\cdot,\cdot) \in H^3((0,T), L^2(\Omega)) \cap H^2((0,T), H^2(\Omega))$ (or respectively $J_\tau I_h u_{h,\tau}(\cdot,\cdot)$) together with the corresponding adjoint state ($p(\cdot,\cdot;u)$ or respectively $J_\tau I_h p_{h,\tau}(\cdot,\cdot; I_h u)$), which is induced by the solution of the state and adjoint equation with the control $u(\cdot,\cdot)$ (or respectively $J_\tau I_h u_{h,\tau}(\cdot,\cdot)$). Nevertheless we insert some admissible control and its corresponding adjoint state into the reduced cost functional

$$j(u) = \int_0^T \frac{1}{2}\|Su - y_d\|^2_{L^2(\Omega)} + \frac{\nu}{2}\|u\|^2_{L^2(\Omega)} \,\mathrm{d}\,t$$

with the (linear) solution operator S of the initial boundary value problem (2)–(5).

The first derivative of this functional is

$$j'(u)(\varphi) = \int_0^T \nu(u,\varphi) + (S^\star(Su - y_d), \varphi) \,\mathrm{d}\,t$$

and can be written with the adjoint state as the optimality condition

$$j'(u(\cdot,t))(\varphi) = \int_0^T (\nu u(\cdot,t) - p(\cdot,t;u), \varphi) \,\mathrm{d}\,t.$$

Note that our adjoint state differs from the adjoint state of [19] or [21] in the sign while we follow the notation of [6]. The second derivative of the cost functional is

$$j''(u)(\varphi,\varphi) = \int_0^T \nu(\varphi,\varphi) + (S\varphi, S\varphi) \,\mathrm{d}\,t \geq \int_0^T \nu\|\varphi\|^2_{L^2(\Omega)} \,\mathrm{d}\,t$$

and therefore independent of u. For the discrete reduced cost functional

$$j_{h\tau}(J_\tau I_h u_{h,k-\frac{1}{2}}) = \frac{\tau}{2}\sum_{k=0}^{N-1} \|I_h S_h u_h - y_d\|^2_{L^2(\Omega)} + \frac{\nu\tau}{2}\sum_{k=0}^{N-1} \|I_h u_{h,k-\frac{1}{2}}\|^2_{L^2(\Omega)}$$

with the solution operator S_h of the discretized initial boundary value problem we have

$$\begin{aligned}
j'_{h\tau}(u(\cdot,\cdot))(\varphi) &= \sum_{k=0}^{N-1} \tau(\nu u(\cdot, t_{k+\frac{1}{2}}) - I_h p_{h,k+\frac{1}{2}}(\cdot; u), \varphi) \\
&= \int_0^T (\nu J_\tau u(\cdot,\cdot) - J_\tau I_h p_{h,\tau}(\cdot,\cdot; u), \varphi)\,\mathrm{d}\,t \\
j'_{h\tau}(J_\tau I_h u_{h,k-\frac{1}{2}})(\varphi) &= \sum_{k=0}^{N-1} \tau(\nu I_h u_{h,k+\frac{1}{2}}(\cdot) - I_h p_{h,k+\frac{1}{2}}(\cdot; J_\tau I_h u_{h,k+\frac{1}{2}}), \varphi) \\
&= \int_0^T (\nu J_\tau I_h u_{h,\tau}(\cdot,\cdot) - J_\tau I_h p_{h,\tau}(\cdot,\cdot; J_\tau I_h u_{h,k-\frac{1}{2}}), \varphi)\,\mathrm{d}\,t \\
\nu\|\varphi(\cdot,\cdot)\|^2_{L^2(Q)} &\le \int_0^T j''_{h\tau}(J_\tau I_h u(\cdot,\cdot))(\varphi,\varphi)\,\mathrm{d}\,t. \qquad (19)
\end{aligned}$$

The difference between the continuous and the discretized functional for a given control can be estimated by

$$\begin{aligned}
&|j'(u(\cdot,\cdot))(\varphi) - j'_{h\tau}(u(\cdot,\cdot))(\varphi)| = \\
&= \left| \int_0^T (\nu u(\cdot,\cdot) - p(\cdot,\cdot,u) - \nu J_\tau u(\cdot,\cdot) + J_\tau I_h p_{h,\tau}(\cdot,\cdot;u), \varphi)\,\mathrm{d}\,t \right| \le \\
&\le \|J_\tau I_h p_{h,\tau}(\cdot,\cdot;u) - p(\cdot,\cdot;u)\|_{L^2(Q)} \cdot \|\varphi\|_{L^2(Q)} + \nu\|J_\tau u(\cdot,\cdot) - u(\cdot,\cdot)\|_{L^2(Q)} \cdot \|\varphi\|_{L^2(Q)}. \qquad (20)
\end{aligned}$$

As $j'_{h\tau}$ is linear and bounded we obtain for any $u, q \in H^3((0,T), L^2(\Omega)) \cap H^3((0,T), H^2(\Omega))$

$$\left| j'_{h\tau}(u)(\varphi) - j'_{h\tau}(q)(\varphi) \right| \le C\|u - q\|_{L^2(Q)}\|\varphi\|_{L^2(Q)}. \qquad (21)$$

For the error between the projection of the exact solution and the numerical approximation we have with any $\varphi \in H^3((0,T), L^2(\Omega)) \cap H^3((0,T), H^2(\Omega))$

$$\begin{aligned}
&\nu\|R_h\bar{u}(\cdot,\cdot) - J_\tau I_h \bar{u}_{h,\tau}(\cdot,\cdot)\|^2_{L^2(Q)} \le \\
&\overset{(19)}{\le} j''_{h\tau}(\varphi)(R_h\bar{u}(\cdot,\cdot) - J_\tau I_h \bar{u}_{h,\tau}(\cdot,\cdot), R_h\bar{u}(\cdot,\cdot) - J_\tau I_h \bar{u}_{h,\tau}(\cdot,\cdot)) \\
&= j'_{h\tau}\left(R_h\bar{u}(\cdot,\cdot)\right)\left(R_h\bar{u}(\cdot,\cdot) - J_\tau I_h \bar{u}_{h,\tau}(\cdot,\cdot)\right) - j'_{h\tau}\left(J_\tau I_h \bar{u}_{h,\tau}(\cdot,\cdot)\right)\left(R_h\bar{u}(\cdot,\cdot) - J_\tau I_h \bar{u}_{h,\tau}(\cdot,\cdot)\right).
\end{aligned}$$

Due to the optimality conditions

$$\begin{aligned}
j'_{h\tau}(J_\tau I_h \bar{u}_{h,\tau})(\varphi(\cdot)) &= 0 & \forall \varphi \in V_h(\Omega), \\
j'(\bar{u}(\cdot,\cdot))(\varphi(\cdot)) &= 0 & \forall \varphi \in L^2(\Omega) \supset V_h(\Omega),
\end{aligned}$$

this is equal to

$$\begin{aligned}
&\nu\|R_h\bar{u}(\cdot,\cdot) - J_\tau I_h \bar{u}_{h,\tau}(\cdot,\cdot)\|^2_{L^2(Q)} \le \\
&\le j'_{h\tau}(R_h\bar{u}(\cdot,\cdot))\left(R_h\bar{u}(\cdot,\cdot) - J_\tau I_h \bar{u}_{h,\tau}(\cdot)\right) - j'_{h\tau}(\bar{u}(\cdot,\cdot))\left(R_h\bar{u}(\cdot,\cdot) - J_\tau I_h \bar{u}_{h,\tau}(\cdot)\right) + \\
&+ j'_{h\tau}(\bar{u}(\cdot,\cdot))\left(R_h\bar{u}(\cdot,\cdot) - J_\tau I_h \bar{u}_{h,\tau}(\cdot)\right) - j'(\bar{u}(\cdot,\cdot))\left(R_h\bar{u}(\cdot,\cdot) - J_\tau I_h \bar{u}_{h,\tau}(\cdot,\cdot)\right).
\end{aligned}$$

The last two terms can be estimated with the estimate (20). As the functional $j'_{h\tau}$ is linear and bounded (see (21)) we obtain

$$
\begin{aligned}
&\nu\|R_h\bar{u}(\cdot,\cdot) - J_\tau I_h\bar{u}_{h,\tau}(\cdot,\cdot)\|^2_{L^2(Q)} \leq \\
&\overset{(20),(21)}{\leq} C\|R_h\bar{u}(\cdot,\cdot) - \bar{u}(\cdot,\cdot)\|_{L^2(Q)}\|R_h\bar{u}(\cdot,\cdot) - J_\tau I_h\bar{u}_{h,\tau}(\cdot,\cdot)\|_{L^2(Q)} \\
&+ \|J_\tau I_h p_{h,\tau}(\cdot,\cdot;\bar{u}) - \bar{p}(\cdot,\cdot;\bar{u})\|_Q\|R_h\bar{u}(\cdot,\cdot) - J_\tau I_h\bar{u}_{h,\tau}(\cdot,\cdot)\|_{L^2(Q)} \\
&+ \nu\|J_\tau\bar{u}(\cdot,\cdot) - \bar{u}(\cdot,\cdot)\|_{L^2(Q)}\|R_h\bar{u}(\cdot,\cdot) - J_\tau I_h\bar{u}_{h,\tau}(\cdot,\cdot)\|_{L^2(Q)}.
\end{aligned}
$$

Thus we proved for the error between the projection of the optimal control and its numerical approximation the estimate

$$
\begin{aligned}
&\nu\|R_h\bar{u}(\cdot,\cdot) - J_\tau I_h\bar{u}_{h,\tau}(\cdot,\cdot)\|_{L^2(Q)} \leq \\
&\quad\leq C\|R_h\bar{u}(\cdot,\cdot) - \bar{u}(\cdot,\cdot)\|_{L^2(Q)} + \|J_\tau I_h p_{h,\tau}(\cdot,\cdot;\bar{u}) - \bar{p}(\cdot,\cdot;\bar{u})\|_{L^2(Q)} + \nu\|J_\tau\bar{u}(\cdot,\cdot) - \bar{u}(\cdot,\cdot)\|_{L^2(Q)}.
\end{aligned}
$$

The error between the optimal control and its numerical approximation can be estimated with the the triangle inequality. This yields

$$
\begin{aligned}
&\|\bar{u}(\cdot,\cdot) - J_\tau I_h\bar{u}_{h,\tau}(\cdot,\cdot)\|_{L^2(Q)} \leq \\
&\leq \|\bar{u}(\cdot,\cdot) - R_h\bar{u}(\cdot,\cdot)\|_{L^2(Q)} + \|R_h\bar{u}(\cdot,\cdot) - J_\tau I_h\bar{u}_{h,\tau}(\cdot,\cdot)\|_{L^2(Q)} \\
&\lesssim \|R_h\bar{u}(\cdot,\cdot) - \bar{u}(\cdot,\cdot)\|_{L^2(Q)} + \|J_\tau I_h p_{h,\tau}(\cdot;\bar{u}) - \bar{p}(\cdot,\cdot;u)\|_{L^2(Q)} + \nu\|J_\tau\bar{u}(\cdot,\cdot) - \bar{u}(\cdot,\cdot)\|_{L^2(Q)}.
\end{aligned}
$$

The error between the optimal control and its projection can be bounded as in Lemma 3.6, the second term is bounded by the convergence result of the adjoint state with a given state, given by Lemma 3.5 and 3.6 and the last term is bounded by the interpolation result (18). □

All together we have proven Theorem 3.2.

Proof of Theorem 3.2. The convergence of the control follows with Lemma 3.7. The convergence of the control implies the convergence of the state (Lemma 3.5), which implies the convergence of the adjoint state (3.6). □

Finally we transfer the result to the other schemes.

Remark 3.8. We have not shown that the schemes (OC G2) and (OC CN2) are second order schemes. The schemes only differ from (OC CN1) in the right hand side of the adjoint state and for the nonfinal time steps we have (by Taylor expansion)

$$
\begin{aligned}
\frac{\frac{y_{i-1}+y_i}{2} - \frac{y_{d,i-1}+y_{d,i}}{2}}{2} + \frac{\frac{y_i+y_{i+1}}{2} - \frac{y_{d,i}+y_{d,i+1}}{2}}{2} &= y_i - y_{d,i} + \mathcal{O}(\tau^2), \\
\frac{y_{i-1} - y_{d,i-1}}{6} + \frac{4}{6}(y_i - y_{d,i}) + \frac{y_{i+1} - y_{d,i+1}}{6} &= y_i - y_{d,i} + \mathcal{O}(\tau^2).
\end{aligned}
$$

Therefore the assumptions of Lemma 3.6 hold for these time steps. But for the final step we can only show

$$
\begin{aligned}
\frac{\frac{y_{N-1}+y_N}{2} - \frac{y_{d,N}+y_{d,N-1}}{2}}{2} &= \frac{y_N - y_{d,N}}{2} + \mathcal{O}(\tau), \\
\frac{1}{6}(y_{N-1} - y_{d,N-1}) + \frac{2}{6}(y_N - y_{d,N}) &= \frac{y_N - y_{d,N}}{2} + \mathcal{O}(\tau).
\end{aligned}
$$

by Taylor expansions. Nevertheless we see in the numerical example in Section 5.2 that all the schemes seem to be of second order.

For Crank-Nicolson discretizations of parabolic partial differential equation with irregular initial data it is known that even two first order implicit Euler starting steps do not destroy the convergence [27, Theorem 2]. We hope that we can transfer similar results to the schemes (OC G2) and (CN2). This is work of further research.

4 Variable time step size

As mentioned before, it is well known that for higher regularity of the solution of parabolic partial differential equations additional compatibility conditions for the initial and boundary data are needed, see e. g. [12, Theorem 7.1.5, 7.1.6 and 7.1.7] or [32, Theorem 27.2 and 27.3]. If the compatibility conditions are not fulfilled or the initial data are non-smooth, graded time step sizes are in use, see e. g. [30, Section 5.2] for the h-version (or better τ-version in this context) of a discontinuous Galerkin scheme in time or [26] for different approaches for the Crank-Nicolson scheme and non-smooth initial data.

These incompatibilities can appear in the state for $t = 0$ and in the adjoint state for $t = T$. Therefore the error analysis for appropriate time step generating function is done in Section 4.2.

4.1 Generalization to variable time step sizes

With the interpretation as continuous Galerkin method we are able to generalize the method to variable time step sizes.

Therefore let $\tau_i = t_i - t_{i-1}$ for $i = 1, \cdots, N$. The discretization of the forward equation of (9) leads to the Crank-Nicolson scheme with τ_i instead of τ, see the previous section. For the backward equation of (9) we compute the integrals with the midpoint rule and get

$$\begin{aligned} -\bar{p}_{i-\frac{1}{2}} + \bar{p}_{i+\frac{1}{2}} + A\frac{\tau_i \bar{p}_{i-\frac{1}{2}} + \tau_{i+1}\bar{p}_{i+\frac{1}{2}}}{2} &= \\ &= \frac{\left(\bar{y}_i - y_{d,i} + \bar{y}_{i-1} - y_{d,i-1}\right)\tau_i}{4} + \frac{\left(\bar{y}_i - y_{d,i} + \bar{y}_{i+1} - y_{d,i+1}\right)\tau_{i+1}}{4}. \end{aligned}$$

For the last equation we discuss the backward equation on the interval $[t_{N-1/2}, T + \frac{\tau_N}{2}]$ to get

$$-\bar{p}_{N-\frac{1}{2}} - A\frac{\bar{p}_{N-\frac{1}{2}}}{2}\tau_N = \frac{\frac{\bar{y}_N - y_{d,N}}{2} + \frac{\bar{y}_{N-1} - y_{d,N-1}}{2}}{2}\tau_N$$

4.2 Convergence analysis

In this section we show that second order convergence is also possible in the case of variable time step sizes. The Lemmas 3.6 and 3.5 of the previous section, which also discuss perturbed approximations, are the key to our analysis.

The forward equation is the same as in the case of constant time step sizes. Therefore we achieve second order convergence if $\bar{p}_{i+\frac{1}{2}}$ is a second order approximation.

So we only need to discuss the approximation of the backward equation. If we show second order convergence for $\bar{p}_{i+\frac{1}{2}}$ we are done. We only have problems if the time-step sizes change. In these cases the midpoint of the interval $[t_{i-\frac{1}{2}}, t_{i+\frac{1}{2}}]$ and t_i do not coincide anymore (see Figure

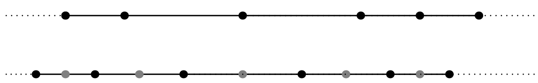


Figure 3: Comparison of the discretization time nodes of y and p. Midpoints of the intervals $[p_{i-\frac{1}{2}}, p_{i+\frac{1}{2}}]$ are additionally inserted in grey. First line y, second line p

3). The time step size between $\bar{p}_{i-\frac{1}{2}}$ and $\bar{p}_{i+\frac{1}{2}}$ is equal to $\frac{\tau_{i+1}+\tau_i}{2} = \frac{t_{i+1}-t_{i-1}}{2}$. We introduce the notation $\underline{\tau} = \min_i \left\{\tau_i,\ \frac{\tau_{i+1}+\tau_i}{2}\right\}$ and $\overline{\tau} = \max_i \left\{\tau_i,\ \frac{\tau_{i+1}+\tau_i}{2}\right\}$ for the minimal and the maximal time step size in the discretization.

For simplicity and shortness we assume again $y_{d,i} = 0$. All the arguments for y_i carry over to $y_{d,i}$ if y_d is smooth enough. So we discuss the scheme

$$-\bar{p}_{i-\frac{1}{2}} + p_{i+\frac{1}{2}} + A\frac{\tau_i \bar{p}_{i-\frac{1}{2}} + \tau_{i+1}\bar{p}_{i+\frac{1}{2}}}{2} = \\ = \frac{(\bar{y}_i + \bar{y}_{i-1})\,\tau_i}{4} + \frac{(\bar{y}_i + \bar{y}_{i+1})\,\tau_{i+1}}{4}$$

for $\bar{p}_{i-\frac{1}{2}}$ and show that this scheme is a $\mathcal{O}\left(\overline{\tau}_i^2\right)$ perturbation of the midpoint-rule

$$\frac{-\bar{p}_{i-\frac{1}{2}} + \bar{p}_{i+\frac{1}{2}}}{\frac{t_{i+1}-t_{i-1}}{2}} + A\bar{p}\left(\frac{t_{i-\frac{1}{2}} + t_{i+\frac{1}{2}}}{2}\right) = \bar{y}\left(\frac{\frac{t_{i-1}+t_i}{2} + \frac{t_i+t_{i+1}}{2}}{2}\right).$$

If we have proven this we can use Theorem 3.6 and are done. Therefore we divide our scheme by the time step size $\frac{t_{i+1}-t_{i-1}}{2}$

$$\frac{-\bar{p}_{i-\frac{1}{2}} + \bar{p}_{i+\frac{1}{2}}}{\frac{t_{i+1}-t_{i-1}}{2}} + \frac{1}{\frac{t_{i+1}-t_{i-1}}{2}} A\frac{\tau_i \bar{p}_{i-\frac{1}{2}} + \tau_{i+1}\bar{p}_{i+\frac{1}{2}}}{2} = \\ = \frac{\bar{y}_i\,(t_{i+1} - t_{i-1}) + \bar{y}_{i-1}\,(t_i - t_{i-1}) + \bar{y}_{i+1}\,(t_{i+1} - t_i)}{2\,(t_{i+1} - t_{i-1})}.$$

Lemma 4.1. *If the changes of time step size are of order $\tau_i - \tau_{i+1} = \mathcal{O}\left(\overline{\tau}^2\right)$, then*

$$y\left(\frac{\frac{t_{i-1}+t_i}{2} + \frac{t_i+t_{i+1}}{2}}{2}\right) - \frac{y_i\,(t_{i+1} - t_{i-1}) + y_{i-1}\,(t_i - t_{i-1}) + y_{i+1}\,(t_{i+1} - t_i)}{2\,(t_{i+1} - t_{i-1})} = \mathcal{O}\left(\overline{\tau}^2\right),$$

$$Ap\left(\frac{t_{i-\frac{1}{2}} + t_{i+\frac{1}{2}}}{2}\right) - \frac{1}{\frac{t_{i+1}-t_{i-1}}{2}} A\frac{\tau_i p_{i-\frac{1}{2}} + \tau_{i+1} p_{i+\frac{1}{2}}}{2} = \mathcal{O}\left(\overline{\tau}^2\right).$$

Proof. For the proof we compare the Taylor expansions.

$$\frac{y_i\,(t_{i+1} - t_{i-1}) + y_{i-1}\,(t_i - t_{i-1}) + y_{i+1}\,(t_{i+1} - t_i)}{2\,(t_{i+1} - t_{i-1})} = \\ = \frac{1}{2}y_i + \frac{1}{2}y_i\frac{t_i - t_{i-1}}{t_{i+1} - t_{i-1}} - \frac{1}{2}\dot{y}_i\frac{(t_i - t_{i-1})^2}{t_{i+1} - t_{i-1}} + h.o.t. \\ + \frac{1}{2}y_i\frac{t_{i+1} - t_i}{t_{i+1} - t_{i-1}} + \frac{1}{2}\dot{y}_i\frac{(t_i - t_{i+1})^2}{t_{i+1} - t_{i-1}} + h.o.t. \\ = y_i + \dot{y}_i\frac{t_{i+1} - 2t_i + t_{i-1}}{2} + h.o.t..$$

On the other hand

$$y\left(\frac{\frac{t_{i-1}+t_i}{2}+\frac{t_i+t_{i+1}}{2}}{2}\right)=y_i+\dot{y}_i\frac{t_{i-1}-2t_i+t_{i+1}}{4}+h.o.t.$$

If we subtract both extensions, the terms of zeroth order in front of y_i vanish and the terms in front of $\dot{y}_i$ are of order $\mathcal{O}\left(\overline{\tau}_i^2\right)$

For the other term we compare again Taylor expansions

$$\begin{aligned}\frac{1}{\frac{t_{i+1}-t_{i-1}}{2}}A\frac{\tau_i p_{i-\frac{1}{2}}+\tau_{i+1}p_{i+\frac{1}{2}}}{2}&=\frac{1}{\tau_i+\tau_{i+1}}A\left(\tau_i\left(p_i-\frac{\tau_i}{2}\dot{p}_i+h.o.t.\right)+\tau_{i+1}\left(p_i+\frac{\tau_i}{2}\dot{p}_i+h.o.t.\right)\right)\\&=Ap_i+\frac{\tau_{i+1}^2-\tau_i^2}{\tau_i+\tau_{i+1}}\frac{1}{2}A\dot{p}_i+h.o.t.=Ap_i+\frac{\tau_{i+1}-\tau_i}{2}A\dot{p}_i+h.o.t.\end{aligned}$$

and

$$\begin{aligned}Ap\left(\frac{t_{i-\frac{1}{2}}+t_{i+\frac{1}{2}}}{2}\right)&=Ap_i+A\dot{p}_i\left(\frac{t_i+t_{i-1}+t_i+t_{i+1}}{4}-t_i\right)+h.o.t.\\&=Ap_i+A\dot{p}_i\left(\frac{\tau_{i+1}-\tau_i}{4}\right)+h.o.t.\end{aligned}$$

As above the difference of the two is of order $\mathcal{O}\left(\overline{\tau}_i^2\right)$. □

Altogether we have proven

Theorem 4.2. *The scheme with variable time step sizes is a second order scheme if*

$$\tau_{i+1}-\tau_i=\mathcal{O}\left(\overline{\tau}^2\right). \tag{22}$$

Corollary 4.3. Last we mention a method to provide a variable time step distribution which fulfills equation (22). Therefore we choose a monotone mesh generating function k which fulfills

$$k\in\mathcal{C}^2\left([0,1],[0,T]\right)\qquad k(0)=0\qquad k(1)=T\qquad t_i=k\left(\frac{i}{N}\right).$$

The resulting time step sizes τ_i fulfill the condition (22) of theorem 4.2.

Proof. We use Taylor expansions of both sides of (22). For the left hand side we have

$$\begin{aligned}\tau_{i+1}-\tau_i=t_{i+1}-2t_i+t_{i-1}&=k\left(\frac{i+1}{N}\right)-2k\left(\frac{i}{N}\right)+k\left(\frac{i-1}{N}\right)\\&=k\left(\frac{i}{N}\right)+k'\left(\frac{i}{N}\right)\frac{1}{N}+\frac{1}{2}k''\left(\xi_1\right)\frac{1}{N^2}-2k\left(\frac{i}{N}\right)\\&\quad+k\left(\frac{i}{N}\right)-k'\left(\frac{i}{N}\right)\frac{1}{N}+\frac{1}{2}k''\left(\xi_2\right)\frac{1}{N^2}\\&=\frac{1}{2}\left(k''\left(\xi_1\right)+k''\left(\xi_2\right)\right)\frac{1}{N^2}=\mathcal{O}\left(\frac{1}{N^2}\right).\end{aligned}$$

And for the right hand side we compute

$$\begin{aligned}\tau_i = t_i - t_{i-1} &= k\left(\frac{i}{N}\right) - \left(k\left(\frac{i}{N}\right) - k'\left(\frac{i}{N}\right)\frac{1}{N} + \frac{1}{2}k''(\xi_3)\frac{1}{N^2}\right)\\ &= k'\left(\frac{i}{N}\right)\frac{1}{N} - \frac{1}{2}k''(\xi_3)\frac{1}{N^2} = \mathcal{O}\left(\frac{1}{N}\right).\end{aligned}$$

This finishes this proof as $\tau_{i+1} - \tau_i$ is of higher order then needed for (22). □

Remark 4.4. Rösch discusses in [28] a parabolic optimal control problem with a terminal objective functional and control constraints. He uses

$$k(t) = T - T(1-t)^4$$

as grading function. He shows that with this grading towards $t = T$ the convergence of the control is of order $\frac{3}{2}$.

Remark 4.5. For the simulation of parabolic partial differential equations with discontinuous Galerkin schemes as time discretization, Schötzau and Schwab introduce

$$k(t) = T \cdot t^{(2r+3)/\theta}$$

as mesh generating function in [30, Section 5.2]. The constant r is the polynomial degree of the discontinuous Galerkin scheme in time and the constant $\theta \in (0, 1]$ corresponds to the smoothness of the initial data, so that $y_0 \in H^\theta(\Omega)$. Clearly this function fulfills also our conditions.

5 Numerical examples

5.1 Solution algorithm

As we discuss a problem without control or state constraints it is possible to eliminate the optimality condition in the discrete system. Altogether for (OC CN1) we have to solve the linear system

$$\left(\begin{array}{cccc|cccc} K & & & & -\frac{M}{\nu} & & & \\ L & K & & & & \ddots & & \\ & \ddots & \ddots & & & & \ddots & \\ & & L & K & & & & -\frac{M}{\nu} \\ \hline -M & & & & -K & -L & & \\ & \ddots & & & & \ddots & \ddots & \\ & & -M & & & & -K & -L \\ & & & -\frac{M}{2} & & & & -K \end{array}\right) \left(\begin{array}{c} \bar{y}_1 \\ \vdots \\ \vdots \\ \bar{y}_N \\ \hline \bar{p}_{i+\frac{1}{2}} \\ \vdots \\ \vdots \\ \bar{p}_{N-\frac{1}{2}} \end{array}\right) = \left(\begin{array}{c} -Ly_0 \\ 0 \\ \vdots \\ 0 \\ \hline -My_{d,1} \\ \vdots \\ -My_{d,N-1} \\ -M\frac{y_{d,N}}{2} \end{array}\right). \tag{23}$$

with $K = \frac{M}{\tau} + \frac{A}{2} \in \mathbb{R}^{n\times n}$ and $L = -\frac{M}{\tau} + \frac{A}{2} \in \mathbb{R}^{n\times n}$, where M is the mass matrix and A the stiffness matrix.

The system-matrix is a $2 \cdot N \cdot n \times 2 \cdot N \cdot n$ matrix where N is the number of time-steps and n is the dimension of y and p. Each of the 4 big sub-matrices has the dimension $N \cdot n \times N \cdot n$.

If we choose (OC CN2) the lower left sub-matrix and the lower part of the right hand side have to be replaced by

$$\begin{pmatrix} -\frac{M}{2} & -\frac{M}{4} & & & \\ -\frac{M}{4} & -\frac{M}{2} & -\frac{M}{4} & & \\ & \ddots & \ddots & \ddots & \\ & & -\frac{M}{4} & -\frac{M}{2} & -\frac{M}{4} \\ & & & -\frac{M}{4} & -\frac{M}{4} \end{pmatrix} \text{ and } \begin{pmatrix} -M\frac{y_{d,0}+2y_{d,1}+y_{d,2}}{4} \\ \vdots \\ -M\frac{y_{d,N-2}+2y_{d,N-1}+y_{d,N}}{4} \\ -M\frac{y_{d,N-1}+y_{d,N}}{4} \end{pmatrix}.$$

And if we choose (OC G1) the lower matrices are replaced by

$$\begin{pmatrix} -\frac{4}{6}M & -\frac{M}{6} & & & \\ -\frac{M}{6} & -\frac{4}{6}M & -\frac{M}{6} & & \\ & \ddots & \ddots & \ddots & \\ & & -\frac{M}{6} & -\frac{4}{6}M & -\frac{M}{6} \\ & & & -\frac{M}{6} & -\frac{2}{6}M \end{pmatrix} \text{ and } \begin{pmatrix} -M\frac{y_{d,0}+4y_{d,1}+y_{d,2}}{6} \\ \vdots \\ -M\frac{y_{d,N-2}+4y_{d,N-1}+y_{d,N}}{6} \\ -M\frac{y_{d,N-1}+2y_{d,N}}{6} \end{pmatrix}.$$

5.2 Example

We choose a test problem with parabolic partial differential equations with homogeneous Neumann boundary conditions

$$\left.\begin{aligned} \min \frac{1}{2}\int_0^1 \|y-y_d\|^2_{L^2(\Omega)} + \frac{\nu}{2}\|u\|^2_{L^2(\Omega)}\ \mathrm{d}\,t \\ y_{,t} - \Delta y = u \qquad & \text{in } \Omega\times(0,T], \\ \frac{\partial}{\partial n} y = 0 \qquad & \text{on } \partial\Omega\times(0,T], \\ y = 0 \qquad & \text{in } \Omega\times\{0\}. \end{aligned}\right\} \tag{24}$$

For our numerical example we study $\Omega\times(0,T] = (0,1)^2\times(0,1]$.

We measure the error by

$$\max_{t_i\in[0:\tau:1]} \left((\bar{y}_{hi} - \bar{y}(t_i,x))^T M (\bar{y}_{hi} - \bar{y}(t_i,x)) \right)^{1/2},$$

$$\text{and} \max_{t_{i+\frac{1}{2}}\in\left[\frac{\tau}{2}:\tau:1-\frac{\tau}{2}\right]} \left(\left(\bar{p}_{hi+\frac{1}{2}} - \bar{p}(t_{i+\frac{1}{2}},x)\right)^T M \left(\bar{p}_{hi+\frac{1}{2}} - \bar{p}(t_{i+\frac{1}{2}},x)\right) \right)^{1/2}.$$

For these expressions we have proven error bounds of order τ^2 in Section 3. It can be interpreted as a discretization of the $L^\infty\left([0,T], L^2(\Omega)\right)$-error between the numerical approximation and the interpolant of the exact solution.

Inspired by [21], where a Dirichlet problem is given as numerical example, we choose for our

(a) Coefficients for y

c_1	c_2	c_3	$c_4 = c_5 = c_6$
$\frac{-5\left(5\,\mathrm{e}^{-\frac{1}{3}\pi^2}-6\right)}{-6+7\,\mathrm{e}^{\frac{1}{3}\pi^2}}$	5	$-\frac{1}{4}\frac{7+141\,\mathrm{e}^{\frac{1}{3}\pi^2}+7\left(\mathrm{e}^{\frac{1}{3}\pi^2}\right)^2-6-106\,\mathrm{e}^{-\frac{1}{3}\pi^2}}{-6+7\,\mathrm{e}^{\frac{1}{3}\pi^2}}$	$\frac{1}{4}$

(b) Coefficients $c_7,\ c_8, c_9,\ \ c_{10},\ c_{11},\ c_{12}$ for y_d

c_7	c_8	c_9	$c_{10} = c_{11} = c_{12}$
$-\frac{5}{9}\frac{\left(9+35\nu\pi^4\right)\left(5\,\mathrm{e}^{-\frac{1}{3}\pi^2}-6\right)}{-6+7\,\mathrm{e}^{\frac{1}{3}\pi^2}}$	$5+\frac{175}{9}\nu\pi^4$	$4\cdot c_3\cdot c_{10}$	$\frac{1}{4}+\nu\pi^4$

Table 1: Coefficients for the numerical example (25), (26).

Scheme	Color	Mark
(OC CN1) $\equiv$ (OC G2)	blue	square
(OC CN2)	red	diamond
(OC G1)	magenta	triangle

Table 2: Colors and marks in the convergence plots .

Neumann problem

$$\begin{aligned} y_d(t,x_1,x_2) &= c_7 w_a(t,x_1,x_2) + c_8 w_b(t,x_1,x_2) + \\ &+ c_9 w_a(0,x_1,x_2) + c_{10} w_b(0,x_1,x_2) + \\ &+ c_{11} w_a(1,x_1,x_2) + c_{12} w_b(1,x_1,x_2) \qquad (25) \\ \text{with } w_a(t,x_1,x_2) &= \mathrm{e}^{\frac{1}{3}\pi^2 t}\cos(\pi x_1)\cos(\pi x_2) \\ \text{and } w_b(t,x_1,x_2) &= \mathrm{e}^{-\frac{1}{3}\pi^2 t}\cos(\pi x_1)\cos(\pi x_2). \end{aligned}$$

The exact solution (y,p) of this optimal control problem can be represented by a linear combination of $w_a(t,x_1,x_2)$, $w_b(t,x_1,x_2)$, $w_a(0,x_1,x_2)$, $w_b(0,x_1,x_2)$, $w_a(1,x_1,x_2)$ and $w_b(1,x_1,x_2)$,

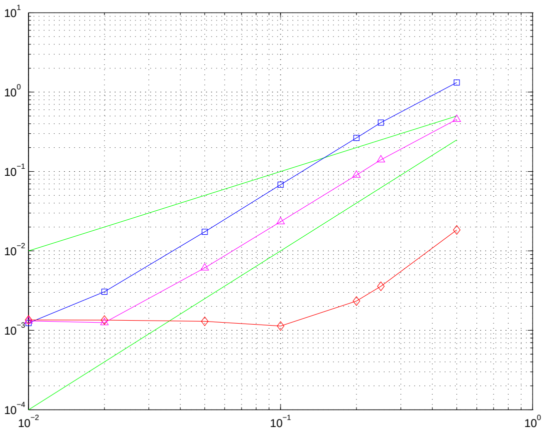
$$\begin{aligned} \bar{y}(t,x_1,x_2) &= c_1 w_a(t,x_1,x_2) + c_2 w_b(t,x_1,x_2) + \\ &+ c_3 w_a(0,x_1,x_2) + c_4 w_b(0,x_1,x_2) + c_5 w_a(1,x_1,x_2) + c_6 w_b(1,x_1,x_2). \qquad (26) \end{aligned}$$

The coefficients must be chosen such that the optimality system is satisfied. The choice of the coefficients is not unique, using Maple we computed the solution displayed in Table 1.

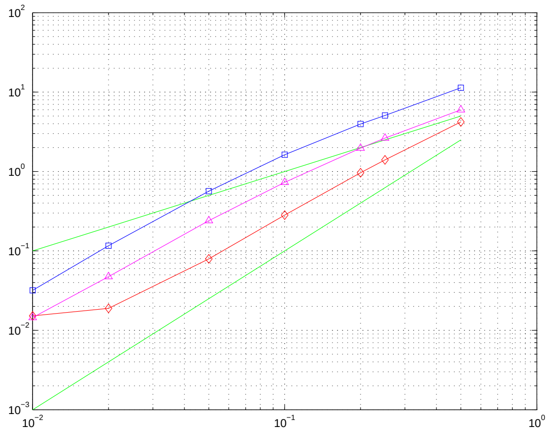
5.3 Numerical results

For clarity of presentation of the numerical results we have split the convergence plots into two parts. On the left hand side we always plot the error in the state $\bar{y}$, on right hand side the error of the adjoint state $\bar{p}$.

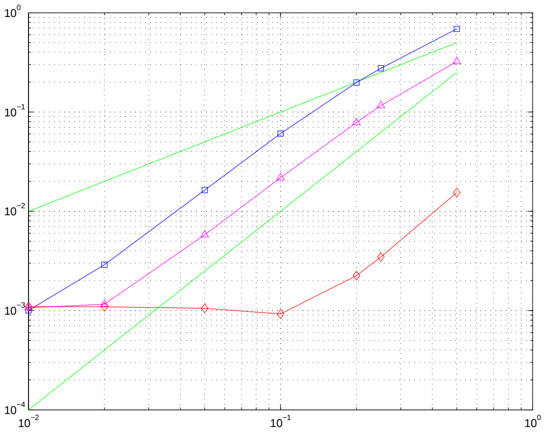
We nicely observe second order convergence for different ν in Figure 4 for the example (24), (25), (26). As the same spatial discretization is used for all examples the error is dominated by



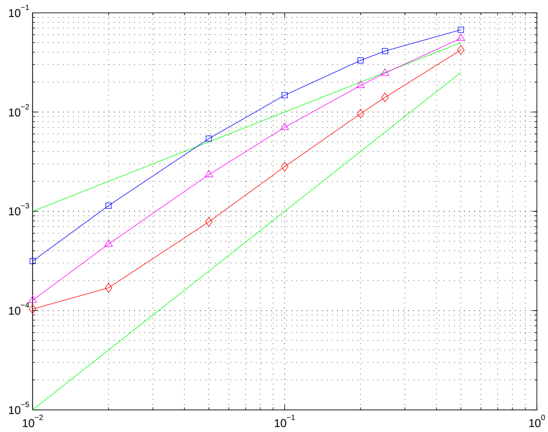
(a) Convergence of y for $\nu = 1$



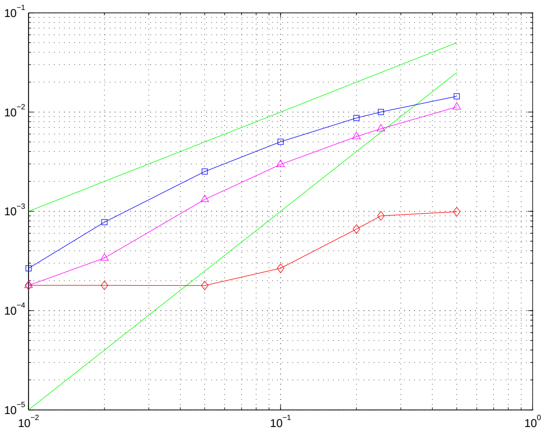
(b) Convergence of p for $\nu = 1$



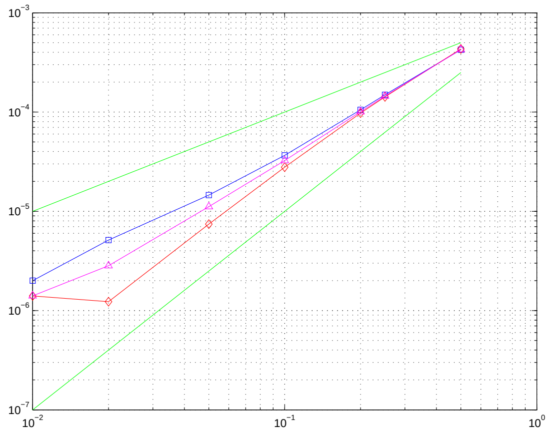
(c) Convergence of y for $\nu = 1 \cdot 10^{-2}$



(d) Convergence of p for $\nu = 1 \cdot 10^{-2}$



(e) Convergence of y for $\nu = 1 \cdot 10^{-4}$



(f) Convergence of p for $\nu = 1 \cdot 10^{-4}$

Figure 4: Plot of the error against the step size τ for different ν for the example with both errors. Spatial discretization is for all time step sizes the same. Left hand side y, right hand side p. Green τ, τ^2, other colors according to Table 2.

this for small time step sizes. We see also that different problems are solved for different ν.and that the error constants become larger for decreasing ν.

6 Conclusion

In this paper we have developed a family of three slightly different second order schemes for optimal control problems with evolution equations. The schemes are introduced as Crank-Nicolson discretizations. One of the schemes can also be interpreted as the Störmer-Verlet scheme. The main feature of the schemes is that discretization and optimization can be interchanged.

Firstly two schemes are based on a time stepping scheme, later on we show that two of the schemes are also Galerkin methods. We prove second order convergence for the optimal control problems in the time discretization points for constant step sizes and also graded time meshes. The expected and the numerical convergences rates coincide nicely for the constant time mesh step size. For a (re)construction of the control over the full time interval the Galerkin approach suggests the use of piecewise constant functions in time, but one would expect that piecewise continuous linear functions in time may yield better convergence properties. Meidner and Vexler discuss this for the case of finitely many time dependent controls in [23].

An advice which of the methods will perform better in general seems not to be possible. It depends on the problem and the time step size.

We did not discuss constraints. The interchangeability of discretization and optimization is not affected by control constraints but the convergence order should be discussed.

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