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A fast solver for an H_1 regularized PDE-constrained optimization problem

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Abstract In this paper we consider a PDE-constrained optimization problem where an H_1 regularization control term is introduced. We address both time-independent and time-dependent versions. We introduce bound constraints on the state, and show how these can be handled by a Moreau-Yosida penalty function. We propose Krylov solvers and preconditioners for the different problems and illustrate their performance with numerical examples.

Keywords PDE-constrained optimization · Saddle point system · H_1 regularization · Preconditioning

1 Introduction

In recent years the development of numerical methods for optimal control problems with constraints given by partial differential equations (PDEs) has seen many contributions: see [40,23,21] and the references mentioned therein. At the heart of many techniques for solving the optimization problem, whether it is a linear problem or the linearization of some non-linear problem, lies the solution of a linear system. These systems are very often so-called saddle point matrices [2,11], i.e., they have the form

$$\mathcal{A} = \begin{bmatrix} A & B^T \\ B & 0 \end{bmatrix}. \tag{1}$$

The systems we consider in this paper have A which is symmetric positive semi-definite. Such matrices are invertible if $ker(A) \cap ker(B) = \{\mathbf{0}\}$: we will

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assume this condition holds for the remainder of this paper. We are then left with the challenge of efficiently solving systems of the form (1) in adequate time.

Direct solvers based on factorizations [10] can be effective in some cases, but for many large and, in particular, three-dimensional problems these are no longer sufficient. In such cases we turn to iterative solvers, namely Krylov subspace methods, which can deal with these large and sparse systems in an efficient manner. In order to achieve rapid convergence it is imperative to derive preconditioners that enhance the convergence behaviour, ideally independent of problem-dependent parameters, such as the mesh-size or the regularization parameter. For a general overview of preconditioners we refer to [35,13], and in the particular case of saddle point problems see [2,11,43].

A number of preconditioners which are robust with respect to regularization parameters and mesh-parameters have recently been developed [36,29, 28,39,25,9], although these methods are only applicable with an L_2 Tikhonov regularization term in the cost functional. A current challenge is to incorporate variations of the regularization term in these solution paradigms [16]. We address this issue here by adding an H_1 term for the control to the objective function and we present preconditioners that are robust with respect to the regularization parameter for this, more difficult, problem.

The paper is structured as follows. We start by stating the optimal control problem for both the time-independent case with distributed and boundary control as well as the time-dependent case with distributed control. We illustrate how the discretized first order conditions can be obtained from a so-called discretize-then-optimize approach. In Section 3 we show how the state constraints can be handled using a Moreau-Yosida penalty approach and show how handling the state constraints in this way can be incorporated into possible preconditioning strategies. In Section 4 we discuss the choice of possible Krylov solvers and introduce preconditioning strategies for both the time-dependent and time-independent control problem. Our numerical results shown in Section 5 illustrate the efficiency of our approach.

2 Problem setup and discretization

2.1 Time-independent control

First we consider the time-independent optimal control problem, where the following objective function should be minimized:

$$\begin{aligned}\mathcal{J}_1(y,u) &= \frac{1}{2}\left\|y-\bar{y}\right\|_{L^2(\Omega_1)} + \frac{\beta}{2}\left\|u\right\|_{H_1} &(2)\\ &= \frac{1}{2}\left\|y-\bar{y}\right\|_{L^2(\Omega_1)} + \frac{\beta}{2}\left\|u\right\|_{L^2(\Omega_2)} + \frac{\beta}{2}\left\|\nabla u\right\|_{L^2(\Omega_2)}, &(3)\end{aligned}$$

where both Ω_1 and Ω_2 are subdomains of $\Omega \in \mathbb{R}^d$ with $d = 2, 3$. The constraint is given by the following elliptic PDE

$$-\triangle y = u \tag{4}$$

together with Dirichlet boundary conditions, i.e. $y = g$ on $\partial\Omega$. We refer to y as the state and u as the corresponding control, which is used to drive the state variable as close as possible to the desired state (or observations) $\bar{y}$. The above problem is the so-called distributed control problem, as u defines the forcing of the PDE over the whole domain Ω. Another important case is given by the boundary control problem, where $\Omega_2 = \partial\Omega$ together with the PDE constraint

$$-\triangle y = f \tag{5}$$

$$\frac{\partial y}{\partial n} = u \text{ on } \partial\Omega \tag{6}$$

where f represents a fixed forcing term.

Problems of this type frequently appear in practical situations [21,31,8,32]. Additionally, many practical applications require the introduction of so-called box constraints on the control and/or the state, as it might be too expensive (time-wise, energy-wise, etc.) to allow for unconstrained minimization of the optimal control problem. The typical bounds for state and control would look like the following

$$u_a \leq u \leq u_b$$

for the control and

$$y_a \leq y \leq y_b$$

for the state. The numerical treatment of these constraints is by now well established [18,4] but nevertheless represents a challenge, in particular for the state constraints [7].

There are two approaches that can be taken to solve such PDE-constrained optimization problems numerically: discretize-then-optimize, where the infinite-dimensional problem is discretized and then optimized; and optimize-then-discretize, where we optimize first, and then discretize the first order optimality conditions accordingly (see [21]). Current research suggests we should use discretization schemes for which both approaches coincide [20].

At this stage we will follow the discretize-then-optimize approach and discretize the PDE and the objective function using finite elements [11,38]. We will discretize using $Q1$ finite elements, which are motivated by our choice of employing the deal.II [1] finite element package for our numerical experiments.

We start by discretizing the objective function $\mathcal{J}_1(y, u)$ to give

$$J_1(\mathbf{y}, \mathbf{u}) = \frac{1}{2}\left(\mathbf{y} - \bar{\mathbf{y}}\right)^T M_y \left(\mathbf{y} - \bar{\mathbf{y}}\right) + \frac{\beta}{2}\mathbf{u}^T M_u \mathbf{u} + \frac{\beta}{2}\mathbf{u}^T K_u \mathbf{u} \tag{7}$$

with M_y the mass matrix over Ω_1, M_u the mass matrix over Ω_2, and K_u a Neumann Laplacian over Ω_2, i.e.,

$$(K_u)_{ij} = \int_{\Omega_{2,h}} (\nabla u)^2 = \int_{\Omega_{2,h}} (\sum_j u_j \nabla\phi_j) \cdot (\sum_i u_i \nabla\phi_i) = \sum_j \sum_i u_j u_i \int_{\Omega_h} \nabla\phi_j \cdot \nabla\phi_j$$

We then discretize the associated PDE to get

$$K\mathbf{y} = M\mathbf{u} + \mathbf{d} \tag{8}$$

for the distributed control problem with $\mathbf{d}$ a vector representing the boundary contributions. For the boundary control problem we get

$$J_1(\mathbf{y},\mathbf{u}) = \frac{1}{2}\left(\mathbf{y}-\bar{\mathbf{y}}\right)^T M_y \left(\mathbf{y}-\bar{\mathbf{y}}\right) + \frac{\beta}{2}\mathbf{u}^T M_{u,b}\mathbf{u} + \frac{\beta}{2}\mathbf{u}^T K_{u,b}\mathbf{u} \tag{9}$$

together with

$$K\mathbf{y} = N\mathbf{u} + \mathbf{f}. \tag{10}$$

Here, $M_{u,b}$ and $K_{u,b}$ are the boundary mass matrix and Laplacian, respectively. The vector $\mathbf{f}$ represents the discretized forcing term, which for simplicity we take to be zero for the remainder of the paper. Note that K is the stiffness matrix over the domain Ω, M the mass matrix for that domain, and the matrix N consists of evaluations of inner products from the term $\int_{\partial\Omega} w\,\mathrm{tr}(v)$ with w a function on the boundary $\partial\Omega$, v a test function for the domain Ω and tr the trace operator.

We now want to clarify the matrix structure of the problem by considering the continuous problem with homogeneous Dirichlet boundary conditions. We consider objective function (2) subject to (4). We now formally consider the Lagrangian

$$\mathcal{L} = \mathcal{J}_1(y,u) - \int_\Omega (-\triangle y - u)p_1\,dx - \int_{\partial\Omega} yp_2\,ds \tag{11}$$

and the Fréchet derivative with respect to y in the direction h:

$$\begin{aligned} D_y\mathcal{L}(y,u,p_1,p_2)h &= \int_\Omega (y-\bar{y})h\,dx - \int_\Omega -\triangle h\,p_1\,dx - \int_{\partial\Omega} p_2 h\,ds \\ &= \int_\Omega (y-\bar{y})h\,dx + \int_\Omega h\,\triangle p_1\,dx - \int_{\partial\Omega}\frac{\partial h}{\partial n}p_1\,ds \\ &\quad + \int_{\partial\Omega} h\frac{\partial p_1}{\partial n}\,ds - \int_{\partial\Omega} p_2 h\,ds. \end{aligned}$$

For a minimum we must have that the optimal control and state, denoted by u^* and y^* respectively, must satisfy

$$D_y\mathcal{L}(y^*,u^*,p_1,p_2)h = 0 \quad \forall h \in H^1(\Omega). \tag{12}$$

In particular, we must have $D_y\mathcal{L}(y^*,u^*,p_1,p_2)h = 0$ for all $h \in C_0^\infty(\Omega)$. In this case $h|_{\partial\Omega} = 0 = \frac{\partial h}{\partial n}|_{\partial\Omega}$, and so the expression above reduces to

$$\int_\Omega (y^* - \bar{y} + \triangle p_1)h\,dx \quad \forall\ h \in C_0^\infty(\Omega),$$

and so, applying the fundamental lemma of the Calculus of Variations, we get that

$$-\triangle p_1 = y - \hat{y} \quad \text{in } \Omega.$$

Now consider $h \in H_0^1(\Omega)$, so that $h|_{\partial\Omega} = 0$. Then we get

$$\int_{\partial\Omega} \frac{\partial h}{\partial n} p_1 \, ds = 0 \quad \forall h \in H_0^1(\Omega)$$

so we have

$$p_1 = 0 \quad \text{on } \partial\Omega.$$

The remaining equations give us the link between p_1 and p_2, namely

$$p_2 = \frac{\partial p_1}{\partial n} \quad \text{on } \partial\Omega.$$

If we label $p_1 = p$, then we can write the adjoint equation as

$$-\triangle p = y - \hat{y} \quad \text{in } \Omega \tag{13}$$

$$p = 0 \qquad \text{on } \partial\Omega, \tag{14}$$

which is the continuous adjoint equation. Now consider optimality with respect to the control, u. The optimal control and state satisfy

$$D_u \mathcal{L}(y^*, u^*, p_1, p_2)h = 0 \quad \forall h \in H^1(\Omega).$$

This gives us that

$$\int_\Omega \beta \left(u^* h + \frac{\partial u^*}{\partial x}\frac{\partial h}{\partial x} + \frac{\partial u^*}{\partial y}\frac{\partial h}{\partial y} + \frac{\partial u^*}{\partial z}\frac{\partial h}{\partial z} \right) + ph \, dx = 0 \quad \forall h \in H^1(\Omega),$$

$$\int_\Omega \beta u^* h dx - \int_\Omega \beta \triangle u h + \int_{\partial\Omega} \left(\frac{\partial u}{\partial x} + \frac{\partial u}{\partial y} + \frac{\partial u}{\partial z} \right) h dz + \int_\Omega ph dx = 0 \quad \forall h \in H^1(\Omega).$$

In particular, this holds for $h \in C_0^\infty(\Omega)$, so as above we must have almost everywhere

$$\beta(u^* - \triangle u^*) + p = 0. \tag{15}$$

Note that this is different to the case when the control appears in the objective function in the $\mathcal{L}_2$ norm. In particular, if $p = 0$ on the boundary, we do not necessarily have that $u^* = 0$ on the boundary, which was shown to be the case for the $\mathcal{L}_2$ case (see [40,34]).

We consider the discretize-then-optimize approach: suppose we want to find $y_h \in Y_0^h \subset H_0^1(\Omega)$ and $u_h \in U^h \subset H^1(\Omega)$ which satisfy

$$\min_{y_h, u_h} \frac{1}{2}||y_h - I_h \bar{y}||^2_{L^2(\Omega)} + \frac{\beta}{2}||u_h||^2_{H^1(\Omega)},$$

$$\text{s.t.} \qquad \int_\Omega \nabla y_h \cdot \nabla v_h + u_h = \int_\Omega v_h, \ \forall v_h \in Y_0^h.$$

Then if $Y_0^h = \langle \phi_1 \ldots \phi_n \rangle$, and we use the same basis for $U^h = \langle \phi_1 \ldots \phi_n, \phi_{n+1}, \phi_{n+\partial n} \rangle$, which is extended as we don't know $\mathbf{u} = \mathbf{0}$ on the boundary, then we can write the optimization problem in terms of matrices as

$$\min_{\mathbf{y},\mathbf{u}} \frac{1}{2}\mathbf{y}^T M_y \mathbf{y} - \mathbf{y}^T \mathbf{b} + \frac{\beta}{2}\mathbf{u}^T M_u \mathbf{u} + \frac{\beta}{2}\mathbf{u}^T K_u \mathbf{u} \tag{16}$$

$$\text{s.t. } K\mathbf{y} = M\mathbf{u}, \tag{17}$$

where

$$M_y = \begin{bmatrix} M_I & 0 \\ 0 & 0 \end{bmatrix}, \; M_u = \begin{bmatrix} M_I & X^T \\ X & M_B \end{bmatrix}, \; K_u = \begin{bmatrix} K_I & Y^T \\ Y & K_B \end{bmatrix}$$
$$M = \begin{bmatrix} M_I & 0 \\ 0 & 0 \end{bmatrix}, \text{ and } K = \begin{bmatrix} K_I & 0 \\ 0 & I \end{bmatrix}.$$

Note that here the subscript I indicates interior nodes and the subscript B the boundary contributions; X and Y represent the contributions from both interior and boundary nodes. The first order conditions lead to the following saddle point system

$$\begin{bmatrix} M_y & 0 & -K \\ 0 & \beta M_u + \beta K_u & M \\ -K & M & 0 \end{bmatrix}.$$

If we have non-homogeneous boundary conditions, then all that changes is that the Discretized PDE becomes

$$K\mathbf{u} = M\mathbf{y} + \mathbf{d}.$$

We argued in [34] that it is not convenient to work with matrices on the interior as most finite element packages will assemble the matrices on the whole of the domain and then apply Dirichlet boundary conditions by making the matrix diagonal on the part corresponding to the boundary degrees of freedom. It can also be seen – assuming all matrices are in this form – that, if the variables $\mathbf{y}$, $\mathbf{u}$, and $\boldsymbol{p}$ contain zeros in the boundary parts, these zeros are maintained throughout any Krylov solver. This means that M_y, M_u, and M could simply be the mass matrices assembled on the boundary and interior of the domain with diagonal components corresponding to Dirichlet nodes. In our case, the matrix $\beta M_u + \beta K_u$ is not diagonal, which would not guarantee that the zero Dirichlet conditions for the state and adjoint state are maintained. This leads us to the following matrix structure

$$\begin{bmatrix} M_y & 0 & -K^T \\ 0 & \beta M_u + \beta K_u & M \\ -K & M & 0 \end{bmatrix} \begin{bmatrix} \mathbf{y} \\ \mathbf{u} \\ \boldsymbol{p} \end{bmatrix} = \begin{bmatrix} M_y \bar{\mathbf{y}} \\ 0 \\ \mathbf{d} \end{bmatrix} \tag{18}$$

with

$$M_y = \begin{bmatrix} M_I & 0 \\ 0 & M_B \end{bmatrix}, \; M_u = \begin{bmatrix} M_I & X^T \\ X & M_B \end{bmatrix}, \; K_u = \begin{bmatrix} K_I & Y^T \\ Y & K_B \end{bmatrix}$$
$$M = \begin{bmatrix} M_I & 0 \\ 0 & 0 \end{bmatrix}, \text{ and } K = \begin{bmatrix} K_I & 0 \\ 0 & I \end{bmatrix},$$

with all mass matrices being lumped. Note that all these matrices are readily available from common finite element packages and the zero block in M can implicitly be created as part of the matrix vector multiplication involving M.

In case of the boundary control problem we obtain the following first order system

$$\begin{bmatrix} M_y & 0 & -K^T \\ 0 & \beta M_{u,b} + \beta K_{u,b} & N^T \\ -K & N & 0 \end{bmatrix} \begin{bmatrix} \mathbf{y} \\ \mathbf{u} \\ \boldsymbol{p} \end{bmatrix} = \begin{bmatrix} M_y \bar{\mathbf{y}} \\ 0 \\ 0 \end{bmatrix}. \tag{19}$$

2.2 Time-dependent problem

We now present a time-dependent version, which is of wide practical interest. The objective function is now given by

$$\mathcal{J}_2(y,u) = \frac{1}{2}\int_0^T \int_{\Omega_1} (y-\bar{y})^2 dxdt + \frac{\beta}{2}\int_0^T \int_{\Omega_2} u^2 dxdt + \frac{\beta}{2}\int_0^T \int_{\Omega_2} (\nabla u)^2 dxdt, \tag{20}$$

where all functions are simply time-dependent versions of their steady counterparts presented above. The constraint is given by the following time-dependent parabolic PDE

$$y_t - \triangle y = u$$

for the distributed control problem with Dirichlet boundary conditions, i.e. $y(\mathbf{x},t) = g(\mathbf{x},\mathbf{t})$ on $\partial\Omega$ for some prescribed function g. In case of a boundary control problem, we consider the following PDE constraint

$$y_t - \triangle y = f \tag{21}$$

$$\frac{\partial y}{\partial n} = u \text{ on } \partial\Omega. \tag{22}$$

For the discretization of the time-dependent objective function we use the trapezoidal rule for the time integral and finite elements in space to give

$$J_2(\mathbf{y},\mathbf{u}) = \frac{1}{2}(\mathbf{y}-\bar{\mathbf{y}})^T \mathcal{M}_y (\mathbf{y}-\bar{\mathbf{y}}) + \frac{\beta}{2}\mathbf{u}^T \mathcal{M}_u \mathbf{u} + \frac{\beta}{2}\mathbf{u}^T \mathcal{K}_u \mathbf{u} \tag{23}$$

where

$$\mathcal{M}_y = \text{blkdiag}(1/2M_y, M_y, \dots, M_y, 1/2M_y),$$
$$\mathcal{M}_u = \text{blkdiag}(1/2M_u, M_u, \dots, M_u, 1/2M_u)$$

and

$$\mathcal{K}_u = \text{blkdiag}(1/2K_u, K_u, \dots, K_u, 1/2K_u),$$

which are simply block-variants of the previously defined matrices over the domains Ω_1 and Ω_2. Note that in the time-dependent case we abuse the notation $\mathbf{y}$ previously used, i.e., $\mathbf{y} = \left[\mathbf{y}_1^T, \mathbf{y}_2^T, \dots, \mathbf{y}_{N_T}^T\right]^T$. Using this notation and a backward Euler scheme, we can write down a one-shot discretization of the time-dependent PDE as follows

$$\begin{bmatrix} L & & & \\ -M & L & & \\ & \ddots & \ddots & \\ & & -M & L \end{bmatrix} \mathbf{y} - \tau \mathcal{M}\mathbf{u} = \mathbf{c} \tag{24}$$

with $L = M + \tau K$ and $\mathbf{c}$ representing the boundary conditions for the heat equation.

Again, we form the Lagrangian and write down the first order conditions in a linear system,

$$\begin{bmatrix} \tau\mathcal{M}_y & 0 & -\mathcal{K}^T \\ 0 & \tau\beta(\mathcal{M}_u + \mathcal{K}_u) & \tau\mathcal{M} \\ -\mathcal{K} & \tau\mathcal{M} & 0 \end{bmatrix} \begin{bmatrix} \mathbf{y} \\ \mathbf{u} \\ \boldsymbol{p} \end{bmatrix} = \begin{bmatrix} \tau\mathcal{M}_y\bar{\mathbf{y}} \\ 0 \\ \mathbf{c} \end{bmatrix}, \tag{25}$$

in the case of the distributed control problem, and

$$\begin{bmatrix} \tau\mathcal{M}_y & 0 & -\mathcal{K}^T \\ 0 & \tau\beta(\mathcal{M}_{u,b} + \mathcal{K}_{u,b}) & \tau\mathcal{N}^T \\ -\mathcal{K} & \tau\mathcal{N} & 0 \end{bmatrix} \begin{bmatrix} \mathbf{y} \\ \mathbf{u} \\ \boldsymbol{p} \end{bmatrix} = \begin{bmatrix} M_y\bar{\mathbf{y}} \\ 0 \\ 0 \end{bmatrix} \tag{26}$$

for boundary control. Note that we have a slight abuse of notation here as we use $\mathbf{y}$ and also $\mathbf{u}$ and $\boldsymbol{p}$ for both the time-independent problem as well as the time-dependent problem, but we believe that it will be clear from the context which of the two we are currently considering.

3 Handling the state constraints

Box constraints both for the control $\mathbf{u}$ and the state $\mathbf{y}$ can be dealt with efficiently using a penalty term. For the case of constraints on both the control and the state of an optimal control problem the Moreau-Yosida penalty function has proven to be a viable tool: see [22, 16, 28] and the references mentioned therein. The modified objective function becomes

$$\mathcal{J}_{MY}(y,u) = \mathcal{J}(y,u) + \frac{1}{2\varepsilon}\left\|\max\{0, y - y_b\}\right\|^2 + \frac{1}{2\varepsilon}\left\|\min\{0, y - y_a\}\right\|^2 \tag{27}$$

for the state constrained case and similarly for control constraints. In accordance with [16] this approach we can employ a semi-smooth Newton scheme that leads to the following linear system

$$\begin{bmatrix} M_y + \varepsilon^{-1}G_{\mathcal{A}}M_yG_{\mathcal{A}} & 0 & -K^T \\ 0 & \beta M_u + \beta K_u & M \\ -K & M & 0 \end{bmatrix} \begin{bmatrix} \mathbf{y} \\ \mathbf{u} \\ \boldsymbol{p} \end{bmatrix} = \begin{bmatrix} M_y\bar{\mathbf{y}} + \varepsilon^{-1}\left(G_{\mathcal{A}_+}M_yG_{\mathcal{A}_+}y_b + G_{\mathcal{A}_-}M_yG_{\mathcal{A}_-}y_a\right) \\ 0 \\ c \end{bmatrix} \tag{28}$$

where we define the active sets as $\mathcal{A}_+ = \{i : \mathbf{y}_i > (y_b)_i\}$, and $\mathcal{A}_-\ \{i : \mathbf{y}_i < (y_a)_i\}$, and $\mathcal{A} = \mathcal{A}_+ \cup \mathcal{A}_-$; the matrices G are diagonal matrix variants of the characteristic function for the corresponding sets, i.e.,

$$(G_{\mathcal{A}})_{ii} = \begin{cases} 1 & \text{for } i \in \mathcal{A} \\ 0 & \text{otherwise.} \end{cases}$$

Our focus is on the efficient solution of the linear systems (28), which are of saddle point type. Note that the active sets defined above within an iterative process such as the semi-smooth Newton scheme are computed based on the state computed at the previous time-step, but for simplicity we neglect any indices. For more details of semi-smooth Newton methods we refer to [23,41, 21]; there is also recent theory introducing path following approaches for the penalty parameter ε [19].

4 Preconditioning

4.1 Choice of Krylov solver and handling the (1, 1)-block

As mentioned in the introduction, the use of iterative schemes is imperative for the solution of the linear systems arising from PDE-constrained optimization. The combination of a state-of-the-art solver with an efficient preconditioning technique is crucial. In this section we derive preconditioners for each of the problems presented earlier, but first focus on the introduction of the iterative scheme. Krylov solvers are for most applications the method of choice, as they are cheap to apply — at each step they only require a matrix vector product, the evaluation of the preconditioners, and the evaluation of inner products. These methods build up a low-dimensional subspace that can be used to approximate the solution to the linear system.

There are a variety of Krylov subspace methods, and the most effective to use depends on the properties of the linear system. For symmetric and positive definite matrices the conjugate gradient (CG) method of Hestenes and Stiefel [17] – in combination with a symmetric and positive definite preconditioner – is typically the method of choice. For symmetric and indefinite problems, such as the ones we are dealing with here, the minimal residual method (MINRES) introduced by Paige and Saunders [27], as well as modified variations of the CG method [6], lend themselves to the task of approximating the solution to the linear system effectively. We will apply MINRES for the remainder of this paper, as its only requirements are that $\mathcal{A}$ is symmetric and the preconditioner is positive definite.

We now want to describe preconditioners which have proven to be efficient for solving systems of the form (1) in combination with MINRES. As the system matrix is indefinite it is not immediately obvious that a good preconditioner can be found that is symmetric and positive definite. Murphy *et al.* [26] show that the preconditioned matrix $\mathcal{P}^{-1}\mathcal{A}$ with $\mathcal{P} = \text{blkdiag}(A, S)$, where $S := BA^{-1}B^T$ is the Schur-complement of $\mathcal{A}$, has three eigenvalues. This results in the termination of MINRES after at most three steps. Note that, for the types of problems we consider here, the $(1, 1)$-block is a block-diagonal matrix, e.g. for the time-dependent case given by $A = \text{blkdiag}(\tau\mathcal{M}, \tau\beta(\mathcal{M}_u + \mathcal{K}_u))$. The constraint B is, for the time-dependent case, given by $B = [-\mathcal{K}, \tau\mathcal{N}]$. Naturally, this $\mathcal{P}$ is too expensive for any realistic problem but it illustrates that if we can find good approximations to both the $(1,1)$-block and the Schur-complement of $\mathcal{A}$, then the method will converge in a small number of steps.

We have now reduced the issue of approximating the solution of the linear system to finding good approximations to the $(1,1)$-block and the Schur-complement of $\mathcal{A}$. The $(1,1)$-block in most of the cases presented here consists of lumped mass matrices and can simply be inverted. If the mass matrices are consistent we can use the Chebyshev semi-iteration [42] and if the $(1,1)$-block is only semi-definite we can add a small perturbation to make it positive definite so the above applies, i.e., we replace the zero blocks in A by blocks of the form ηI with η a small parameter greater than zero. Note that this technique can also be used for an approximation of the Schur-complement in case the $(1,1)$-block is semi-definite [3,37]. For the rest of the paper we assume that our preconditioner is given by $\mathcal{P} = \text{blkdiag}(\hat{A}, \hat{S})$ where $\hat{A}$ approximates the $(1,1)$-block and $\hat{S}$ the Schur-complement. We discuss appropriate approaches for the approximation of the Schur-complement next.

4.2 Time-independent problem

No state constraints

We are interested in finding a good preconditioner for the matrix

$$\begin{bmatrix} M_y & 0 & -K^T \\ 0 & \beta M_u + \beta K_u & M \\ -K & M & 0 \end{bmatrix}.$$

We assume that we can deal with the blocks M_y and $\beta M_u + \beta K_u$ efficiently. In more detail, the mass matrix M_y can be approximated by the Chebyshev semi-iteration in the consistent case and simply inverted whenever it is lumped. The inverse of $\beta M_u + \beta K_u$ can efficiently be approximated using (algebraic) multigrid.

The performance of our preconditioner therefore depends on having a good approximation of the Schur-complement

$$S = K M_y^{-1} K^T + M(\beta M_u + \beta K_u)^{-1} M.$$

One possible approximation would be

$$\hat{S}_1 = K M_y^{-1} K^T$$

(see [33]), which neglects the second term in the Schur-complement. This typically results in good convergence properties for relatively large β, but performance deteriorates as β approaches zero. Another approach [30], that for certain setups can overcome or weaken this dependence on the regularization parameter, is given by

$$\hat{S}_2 = (K + \hat{M}) M_y^{-1} (K^T + \hat{M}^T),$$

where the matrix $\hat{M}$ is chosen to approximate the second term in the Schur-complement well. In more detail, we construct $\hat{M}$ such that

$$\hat{M}M_y^{-1}\hat{M}^T = M(\beta M_u + \beta K_u)^{-1}M,$$

which is the case for $\hat{M} = M(\beta M_u + \beta K_u)^{-1/2}M_y^{1/2}$. Note that with this choice we cannot easily form and invert $(K + \hat{M})$. We instead choose the diagonal $\operatorname{diag}(K_u)$ as an approximation for K_u. Note that the approximation of K_u by its diagonal is, in the case of a forward Poisson problem, not ideal as no mesh-independence can be expected. Nevertheless, the inverse of $(K + \hat{M})$ needs to be approximated cheaply and, as we are using lumped mass matrices, we now get

$$\hat{M} = M(\beta M_u + \beta D_K)^{-1/2}M_y^{1/2},$$

where $D_K = \operatorname{diag}(K_u)$. This allows us to form $K + \hat{M}$, whose inverse in turn can be approximated using an algebraic or geometric multigrid preconditioner.

State constraints

We are now interested in finding a good preconditioner for the matrix coming from the state constrained problem treated with a Moreau-Yosida penalty term,

$$\begin{bmatrix} L & 0 & -K^T \\ 0 & \beta M_u + \beta K_u & M \\ -K & M & 0 \end{bmatrix},$$

where $L = M_y + \varepsilon^{-1}G_{\mathcal{A}}M_yG_{\mathcal{A}}$. Due to the diagonal nature of the mass matrices the matrix L is simply a diagonal matrix and can be treated trivially in the preconditioner. For the block $\beta M_u + \beta K_u$ we can again use a multigrid process to approximate the inverse within the preconditioner. This leaves us again with finding an efficient way to approximate the Schur-complement

$$S = KL^{-1}K + M(\beta M_u + \beta K_u)^{-1}M. \tag{29}$$

We want to employ the technique used for the case without state constraints. We start by looking for an approximation of the form

$$\hat{S} = (K + \hat{M})L^{-1}(K + \hat{M})^T, \tag{30}$$

where we have to determine the matrix $\hat{M}$ in such a way that the second term in S is accounted for. For this we want

$$\hat{M}L^{-1}\hat{M}^T \approx M(\beta M_u + \beta K_u)^{-1}M.$$

In order to simplify this process we make the following approximation

$$\beta M_u + \beta K_u \approx \beta M_u + \beta D_K := D_u,$$

where $D_K = \operatorname{diag}(K_u)$ and hence D_u is a diagonal matrix. We now proceed to

$$\hat{M}L^{-1}\hat{M}^T = MD_u^{-1}M \Rightarrow \hat{M} = MD_u^{-1/2}L^{1/2}$$

as all matrices involved are diagonal matrices and hence commute, i.e., $\hat{M} = MD_u^{-1/2}L^{1/2} = L^{1/2}D_u^{-1/2}M$.

Boundary control

In the boundary control problem the saddle point matrix is given by

$$\begin{bmatrix} M_y & 0 & -K^T \\ 0 & \beta M_{u,b} + \beta K_{u,b} & N^T \\ -K & N & 0 \end{bmatrix} \tag{31}$$

with a $(1,1)$-block that can be handled by the previous techniques. The Schur-complement here is

$$S = KM_y^{-1}K^T + N(\beta M_{u,b} + \beta K_{u,b})^{-1}N^T.$$

We again approximate the Laplacian by its diagonal to get

$$S \approx KM_y^{-1}K^T + N(\beta M_{u,b} + \beta D_{K,b})^{-1}N^T = KM_y^{-1}K^T + ND_u^{-1}N^T.$$

Once again we proceed by assuming that an approximation of the form

$$\hat{S} = (K + \hat{M})M_y^{-1}(K + \hat{M})^T$$

will give a good approximation to the Schur-complement, with

$$\hat{M}M_y^{-1}\hat{M}^T = ND_u^{-1}N^T. \tag{32}$$

Since the mass matrices are lumped, we can assume that all the matrices are diagonal, and we get an expression for the diagonal elements of (32) corresponding to boundary degrees of freedom. Note that $ND_u^{-1}N^T$ is a diagonal matrix with non-zero entries only for boundary nodes. We also do not account for the difference in scalings with respect to the mesh parameter h between a boundary mass matrix and a mass matrix on the whole domain. The diagonal elements of $\hat{M}$ can be obtained from

$$m_{ii}\hat{m}_{ii}^2 = \frac{m_{ii}^2}{d_{u,ii}}$$

or equivalently

$$\hat{m}_{ii}^2 = \frac{m_{ii}^3}{d_{u,ii}} \Rightarrow \hat{m}_{ii} = \frac{m_{ii}^{3/2}}{\sqrt{d_{u,ii}}}. \tag{33}$$

We already mentioned that the boundary mass matrix scales differently compared to the mass matrix on the whole domain by on order of h. We first consider the case when we only have an L^2-term for the control, i.e. $K_u = 0$, and want to compute $\hat{M}$ such that

$$\hat{M}M_y^{-1}\hat{M} = \beta^{-1}NM_u^{-1}N^T$$

and using the approximations $M_y \approx h^2 I$ and $M_u \approx hI$ we get

$$h^{-2}\hat{M}^2 \approx \hat{M}M_y^{-1}\hat{M} = \beta^{-1}NM_u^{-1}N^T \approx \beta^{-1}h^{-1}NN^T.$$

Since all matrices in the last expression are diagonal (remember N is a rectangular matrix with entries only when boundary degree of freedom is paired with boundary degree of freedom) we get

$$\hat{m}_{ii}^2 = h\beta^{-1} m_{ii}^2 \Rightarrow \hat{m}_{ii} = \sqrt{h\beta^{-1}} m_{ii}.$$

Based on this analysis we proceed by multiplying $\hat{m}_{ii}$ in (33) with $\sqrt{h}$ to account for the different orders of the boundary matrices and the matrices over the whole domain to finally get

$$\hat{m}_{ii} = \frac{\sqrt{h} m_{ii}^{3/2}}{\sqrt{d_{u,ii}}}.$$

4.3 Time-dependent problem

We now extend the previous techniques to the time-dependent case.

No state constraints

Recall that the first order conditions of the time-dependent problem are represented by the following saddle point system

$$\begin{bmatrix} \tau\mathcal{M}_y & 0 & -\mathcal{K}^T \\ 0 & \tau\beta(\mathcal{M}_u + \mathcal{K}_u) & \tau\mathcal{M} \\ -\mathcal{K} & \tau\mathcal{M} & 0 \end{bmatrix} \begin{bmatrix} \mathbf{y} \\ \mathbf{u} \\ \boldsymbol{p} \end{bmatrix} = \begin{bmatrix} \tau\mathcal{M}_y\bar{\mathbf{y}} \\ 0 \\ d \end{bmatrix} \tag{34}$$

and assume that $\mathcal{M}_y$ and $\tau\beta(\mathcal{M}_u + \mathcal{K}_u)$ are invertible so we can form the Schur-complement

$$S = \tau^{-1}\mathcal{K}\mathcal{M}_y^{-1}\mathcal{K}^T + \tau\mathcal{M}(\beta\mathcal{M}_u + \beta\mathcal{K}_u)^{-1}\mathcal{M}.$$

For strategies to handle a semi-definite $\mathcal{M}_y$ we refer to [37]. Again we approximate S via

$$\hat{S} = \tau^{-1}(\mathcal{K} + \hat{\mathcal{M}})\mathcal{M}_y^{-1}(\mathcal{K} + \hat{\mathcal{M}})^T,$$

with a not yet specified but symmetric matrix $\hat{\mathcal{M}}$. As we want $\hat{\mathcal{M}}\mathcal{M}_y^{-1}\hat{\mathcal{M}}$ to resemble the second block in the Schur-complement S we obtain

$$\hat{\mathcal{M}}\mathcal{M}_y^{-1}\hat{\mathcal{M}}^T \approx \mathcal{M}(\beta\mathcal{M}_u + \beta\mathcal{K}_u)^{-1}\mathcal{M}.$$

As all matrices are block-diagonal, we want that

$$\tau^{-1}\hat{M}M_y^{-1}\hat{M}^T \approx \tau M(\beta M_u + \beta K_u)^{-1}M.$$

Using again the approximation

$$\beta M + \beta K_u \approx \beta M + \beta D_K := D_u,$$

we get

$$\tau^{-1}\hat{M}M^{-1}\hat{M}^T = \tau M D_u^{-1} M \Rightarrow \hat{M} = \tau M D_u^{-1/2} M_y^{1/2}.$$

State constraints

The system obtained from the state constrained case has a change in the $(1,1)$-block, i.e.,

$$\begin{bmatrix} \tau\mathcal{L} & 0 & -\mathcal{K}^T \\ 0 & \tau\beta(\mathcal{M}_u + \mathcal{K}_u) & \tau\mathcal{M} \\ -\mathcal{K} & \tau\mathcal{M} & 0 \end{bmatrix} \begin{bmatrix} \mathbf{y} \\ \mathbf{u} \\ \boldsymbol{p} \end{bmatrix} = \begin{bmatrix} \tau\mathcal{M}_y\bar{\mathbf{y}} \\ 0 \\ d \end{bmatrix} \tag{35}$$

where $\mathcal{L} = \text{blkdiag}(L_i)$ with the $L_i = M_y + \varepsilon^{-1}G_{\mathcal{A}^{(i)}}M_yG_{\mathcal{A}^{(i)}}$ and $\mathcal{A}^{(i)}$ the active sets for a grid point in time. Assuming invertibility of $\mathcal{L}$, the Schur-complement now becomes

$$S = \tau^{-1}\mathcal{K}\mathcal{L}^{-1}\mathcal{K}^T + \tau\mathcal{M}(\beta\mathcal{M}_u + \beta\mathcal{K}_u)^{-1}\mathcal{M}.$$

We again want to derive an approximation of the form

$$\hat{S} = \tau^{-1}(\mathcal{K} + \hat{\mathcal{M}})\mathcal{L}^{-1}(\mathcal{K}^T + \hat{\mathcal{M}}^T)$$

that resembles the Schur-complement as closely as possible. As we again want $\tau^{-1}\hat{\mathcal{M}}\mathcal{L}^{-1}\hat{\mathcal{M}}$ to resemble the second block in the Schur-complement S we obtain

$$\tau^{-1}\hat{\mathcal{M}}\mathcal{L}^{-1}\hat{\mathcal{M}}^T \approx \tau\mathcal{M}(\beta\mathcal{M}_u + \beta\mathcal{K}_u)^{-1}\mathcal{M}.$$

As all matrices are block-diagonal we want that for all blocks ($i = 1, \dots, n$)

$$\tau^{-1}\hat{M}L_i^{-1}\hat{M}^T \approx \tau M(\beta M_u + \beta K_u)^{-1}M.$$

and with the approximation

$$\beta M + \beta K_u \approx \beta M + \beta D_K := D_u,$$

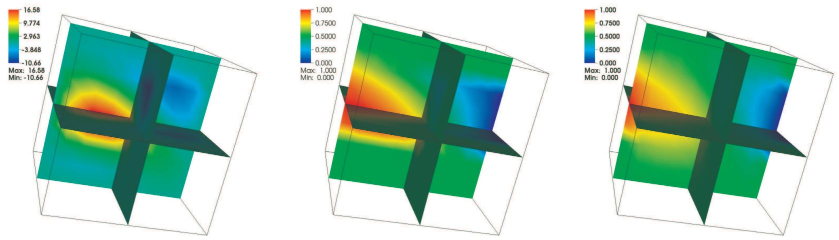
we get

$$\tau^{-1}\hat{M}L_i^{-1}\hat{M}^T = \tau M D_u^{-1}M \Rightarrow \hat{M} = \tau M D_u^{-1/2}L_i^{1/2}.$$

Note that now the blocks of $\mathcal{L}$ are different for each grid point in time as the active sets will be different for each i. In an efficient implementation this issue has to be addressed as recomputing the preconditioner with each application is not feasible. We have not done this for the results presented in Section 5.

5 Numerical Results

We now want to illustrate how the preconditioners presented above perform when applied to a variety of problem setups. As mentioned earlier we employ a finite element discretization, here done with the finite element package deal.II [1]. We discretize the state, control and adjoint state variables using **Q1** elements. We stop all computations when the pseudo-residual minimized in MINRES falls below a certain tolerance, typically 10^{-4} or 10^{-6}. For the algebraic multigrid preconditioner we use the Trilinos ML package [12] that



(a) Control (b) Desired state (c) Computed state

Fig. 1: Control, desired state, and state for time-independent distributed control with $\beta = 10^{-6}$.

implements a smoothed aggregation AMG. Within the algebraic multigrid we typically used 10 steps of a Chebyshev smoother in combination with the application of two V-cycles. Note that, especially in the time-dependent case with state constraints, our implementation at this point is only a proof-of-concept as we are simply recomputing the preconditioner for every active set. Future research should address the issue of efficiently updating the AMG preconditioner or employing a geometric multigrid method that takes the changes of the active set into account.

For time-dependent problems we show the degrees of freedom only for one grid point in time (i.e. for a single time-step) and we are implicitly solving a linear system of dimension 3 times the number of time-steps (N_t) times the degrees of freedom of the spatial discretization (n). For example, a spatial discretization with 274625 unknowns and 20 time-steps corresponds to an overall linear system of dimension 16 477 500. All results are performed on a Centos Linux machine with Intel(R) Xeon(R) CPU X5650 @ 2.67GHz CPUs and 48GB of RAM.

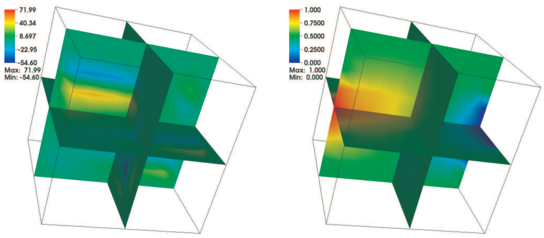
5.1 The time-independent case

No state constraints

In this section we show numerical results for the time-independent control problem. The desired state is given by

$$\bar{\mathbf{y}} = \begin{cases} \sin(2\pi x_0 x_1 x_2) & \text{if } x_0, x_1 \in [0.2, 0.7] \\ 0.5 & \text{otherwise.} \end{cases}$$

with the Dirichlet condition that $y = 0$ on $\partial\Omega$. The desired state, computed control and computed state for $\beta = 10^{-6}$ are shown in Figure 1. We show the results for a variety of β parameters in Table 1 and the tolerance 10^{-4} for the pseudo-residual.



(a) Control (b) Computed state

Fig. 2: Control and computed state for time-independent distributed control with $\beta = 10^{-6}$ and no H_1-term.

DoF	MINRES(T)	MINRES(T)	MINRES(T)
	$\beta = 10^{-2}$	$\beta = 10^{-4}$	$\beta = 10^{-6}$
729	5(0.23)	10(0.99)	17(0.82)
4913	6(2.07)	10(2.51)	22(5.37)
35937	8(9.16)	10(7.76)	24(18.14)
274625	8(60.89)	10(74.38)	24(161.36)
2146689	8(547.15)	10(660.26)	26(1853.41)

Table 1: Results obtained with Schur complement approximation $\hat{S}$ and β.

We see from the results in Table 1 that there is some benign growth in the iteration numbers with respect to the regularization parameter and no dependence with respect to the mesh-parameter h.

State constraints

In the next example we consider the introduction of state constraints for the time-independent control problem. As was shown in [24] the quality of the preconditioner can have a significant influence on the convergence of the Newton scheme. In our experience for smaller values of β and ε the tolerance of 10^{-4} was not always sufficient for the Newton method to reach convergence and the results shown in Table 2 are computed for the tolerance 10^{-6}. We also employed a nested-iteration technique [16], which starts by solving the optimal control problem on a coarse mesh and then transferring the solution to the next finer mesh as an initial guess for the Newton method. As can be seen from Table 2 this leads to a small number of Newton steps on the fine meshes. We here consider

$$\bar{\mathbf{y}} = -\sin(2\pi x_0 x_1 x_2)\exp\left(-\left((x_0-0.5)^2+(x_1-0.5)^2+(x_2-0.5)^2\right)\right)$$

and the Dirichlet condition is defined as $y = P_{[y_a,y_b]}(\bar{\mathbf{y}})$ on $\partial\Omega$ as the projection of the desired state onto the feasible region. Here we only consider the lower bound given by $y_a = -0.7$. We show the results for two different values of ε using $\beta = 10^{-6}$ in Table 2 and it can be seen that the number of Newton iterations is very similar and the MINRES iterations grow slightly with the reduction of ε.

DoF	AS	MINRES (tl/av)	T	AS	MINRES (tl/av)	T
	$\varepsilon = 10^{-2}$			$\varepsilon = 10^{-4}$		
729	5	145/29	11.38	5	156/31	12.23
4913	4	137/34	78.21	5	280/56	158.79
35937	4	154/39	285.59	5	351/70	689.61
274625	4	164/41	3589.12	6	448/74	10795.51

Table 2: Results obtained for state-constrained problem for different values of the penalty parameter. Total and average number of MINRES iterations for all Newton steps are shown as well as the timings for $\beta = 10^{-6}$.

Boundary control

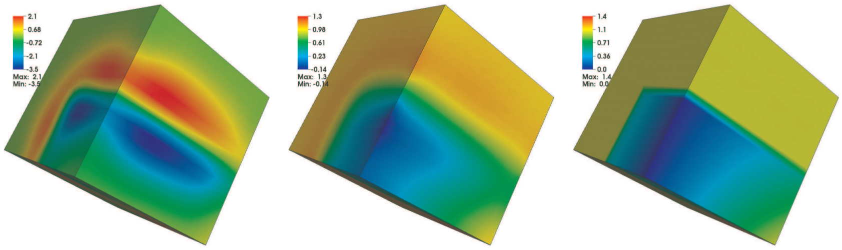
The control of the PDE via the boundary of the domain represents a relevant and interesting scenario. We will now illustrate how our preconditioner performs for this case. The desired state is given by

$$\bar{\mathbf{y}} = \begin{cases} \sin(x_1) + x_2 x_0 & \text{if } x_0 > 0.5 \text{ and } x_1 < 0.5 \\ \quad 1 & \text{otherwise.} \end{cases}$$

Table 3 shows the MINRES iteration numbers and timings for different meshes and values of β. It can be seen that there is a slight mesh-dependence and also a slight dependence on β. As the PDE-constraint involves a Neumann Laplacian for which already the forward problems is expected to show mesh-dependence [5] it is not surprising this continues into the inverse problem. We have so far not considered state-constraints using this boundary control approach but we believe that the techniques presented here carry over to this case as well.

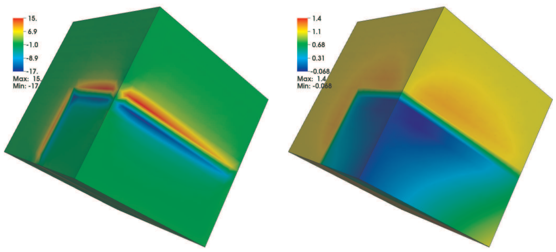
DoF	MINRES(T)	MINRES(T)	MINRES(T)
	$\beta = 10^{-2}$	$\beta = 10^{-4}$	$\beta = 10^{-6}$
729	22(0.1)	20(0.1)	16(0.2)
4913	26(1)	28(1)	22(1)
35937	30(7)	38(9)	30(6)
274625	34(99)	48(176)	48(133)
2146689	38(1212)	60(1789)	64(1863)

Table 3: MINRES timings and iteration numbers for the boundary control case and varying mesh sizes as well as different values of the regularization parameter β.



(a) Control (b) Computed state (c) Desired state

Fig. 3: Desired state, computed state and control for a boundary control problem with $\beta = 10^{-6}$.



(a) Control (b) Computed state

Fig. 4: Same setup as in Figure 3 only with L_2 instead of H_1 term.

5.2 The time-dependent case

No state constraints

In this Section we show results for the time-dependent case. First, we consider the case when no state constraints are present. Here, we work with a fixed time-step $\tau = 0.05$, which results in 20 time-steps. In all tables we only show the degrees of freedom associated with the discretization of the spatial domain. The overall system that we are implicitly solving is then of dimension $N_t * n * 3$, e.g. $20 * 274625 * 3 = 16477500$ degrees of freedom. The desired state is now given by

$$\bar{\mathbf{y}} = -\exp(t)\sin(2\pi x_0 x_1 x_2)\exp\left(-\left((x_0-0.5)^2+(x_1-0.5)^2+(x_2-0.5)^2\right)\right)$$

and $\mathbf{y} = \bar{\mathbf{y}}$ on $\partial\Omega$. The results for this setup are shown in Table 4 for various mesh-parameters and values of the regularization parameter β. We can see that the results now depend on the regularization parameter but that the growth seen is rather benign as we are able to solve for relatively small values of β and a large number of unknowns in a reasonable number of iterations.

DoF	MINRES(T)	MINRES(T)	MINRES(T)
	$\beta = 10^{-2}$	$\beta = 10^{-4}$	$\beta = 10^{-6}$
729	4(2)	19(8)	55(21)
4913	5(15)	19(46)	70(158)
35937	7(146)	20(359)	79(1324)
274625	7(1167)	21(3007)	85(11326)

Table 4: MINRES iteration numbers and timings for various meshes and varying regularization parameter β.

State constraints

We now present results for the time-dependent case in the presence of state-constraints. We again consider the unit square with the desired state defined by

$$\bar{\mathbf{y}} = -\exp(t)\sin(2.0\pi x_1 x_2 x_3)\exp\left(-\left((x_0-0.5)^2+(x_1-0.5)^2+(x_2-0.5)^2\right)\right).$$

The iteration numbers for the outer active set method and MINRES are shown in Table 5. We only show results for two small mesh-sizes as our implementation is currently only a proof-of-concept implementation that does not update the preconditioner for each active set but rather recompute it during each iteration, which in practice will be too expensive. As a comparison we show

DoF	AS	MINRES (tl/av)	AS	MINRES (tl/av)
	$\varepsilon = 10^{-2}$		$\varepsilon = 10^{-4}$	
729	7	500/71	10	2221/222
4913	5	395/79	6	1561/260

Table 5: Results obtained for state-constrained problem for different values of the penalty parameter. Total and average number of MINRES iterations for all Newton steps are shown as well as the timings for $\beta = 10^{-4}$.

the iteration numbers for the same problem with an L_2-term instead of the H_1-term for the control in Table 6. It can be seen that both problems need an increasing number of iterations to reach the desired tolerance for decreasing values of the penalty parameter. Nevertheless, the number of iterations for the case without H_1-term shows only moderate growth in the iteration numbers and the iteration numbers for the H_1 are still feasible, as the values for β and ε are both chosen rather small.

DoF	AS	MINRES (tl/av)	AS	MINRES (tl/av)
	$\varepsilon = 10^{-2}$		$\varepsilon = 10^{-4}$	
729	5	156/31	6	427/71
4913	4	137/36	5	558/112

Table 6: Results obtained for state-constrained L_2-problem for different values of the penalty parameter. Total and average number of MINRES iterations for all Newton steps are shown as well as the timings for $\beta = 10^{-4}$.

Boundary control

We now show results for the boundary control case when we are dealing with a time-dependent problem. The desired state is given by

$$\bar{\mathbf{y}} = -\exp(t)\sin(2\pi x_0 x_1 x_2)\exp\left(-\left((x_0-0.5)^2+(x_1-0.5)^2+(x_2-0.5)^2\right)\right).$$

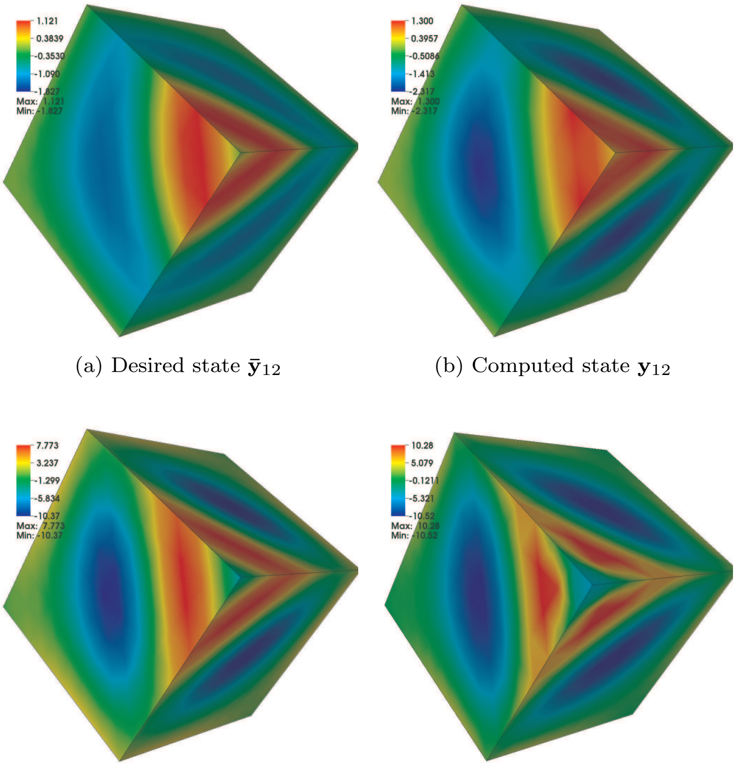
The results for this setup with varying mesh-size and regularization parameter β are shown in Table 7. These results show that there exists a β-dependence but also that for relatively small regularization parameters the iteration numbers are bounded and rather small. In addition, the iteration numbers do not increase with refining the mesh.

DoF	MINRES(T)	MINRES(T)	MINRES(T)	MINRES(T)
	$\beta = 10^{-2}$ $N_T = 20$	$\beta = 10^{-4}$ $N_T = 20$	$\beta = 10^{-6}$ $N_T = 20$	$\beta = 10^{-6}$ $N_T = 100$
729	16(5)	28(8)	50(11)	48(61)
4913	12(17)	24(32)	44(54)	44(230)
35937	10(70)	20(124)	46(310)	42(1270)

Table 7: MINRES iteration numbers and timings for various meshes and varying regularization parameter β.

6 Conclusions and Outlook

In this paper we presented optimal control problems subject to Poisson problem or the heat equation in a distributed or boundary control setup. The control was added to the objective function as a regularization term in the H_1 norm. We introduced the corresponding discrete optimality system and introduced preconditioners for both the steady as well as the transient problem. Due to the Laplacian term coming from the H_1 norm we were not able to introduce preconditioners that are fully independent of the regularization parameter but for the simple preconditioners we introduced the dependence on the regularization parameter seemed rather weak. We also showed that our approach works for state-constrained problems, which were treated using a



(a) Desired state $\bar{\mathbf{y}}_{12}$ (b) Computed state $\mathbf{y}_{12}$

(c) Control $\mathbf{y}_{12}$ with H_1-term. (d) Control $\mathbf{y}_{12}$ with L_2-term.

Fig. 5: Control with and without H_1 term as well as desired state and state for time-dependent boundary control with $\beta = 10^{-6}$.

Moreau-Yosida penalty approach. Numerical results showed that our preconditioners provided satisfactory results when applied to three-dimensional test problems.

The method presented here has not focused on the storage efficiency of our all-at-once approach. One might employ checkpointing [14] techniques when alternatingly solving forward and adjoint PDEs. Multiple shooting approaches are one way of splitting up the time-interval [15] and can lead to the same type of system. A possible way forward is to compute suboptimal solutions on a sequential splitting of the time-interval [15] or to use a parallel implementation of our approach. It is also possible to reduce the storage requirements by performing block-eliminations of some form, usually via a Schur-complement approach.

References

1. Bangerth, W., Hartmann, R., Kanschat, G.: deal.II—a general-purpose object-oriented finite element library. ACM Trans. Math. Software **33**(4), Art. 24, 27 (2007)
2. Benzi, M., Golub, G.H., Liesen, J.: Numerical solution of saddle point problems. Acta Numer **14**, 1–137 (2005)
3. Benzi, M., Haber, E., Taralli, L.: A preconditioning technique for a class of PDE-constrained optimization problems. Advances in Computational Mathematics **35**, 149–173 (2011)
4. Bergounioux, M., Ito, K., Kunisch, K.: Primal-dual strategy for constrained optimal control problems. SIAM J. Control Optim. **37**(4), 1176–1194 (1999)
5. Bochev, P., Lehoucq, R.: On the finite element solution of the pure neumann problem. SIAM review **47**(1), 50–66 (2005)
6. Bramble, J.H., Pasciak, J.E.: A preconditioning technique for indefinite systems resulting from mixed approximations of elliptic problems. Math. Comp **50**(181), 1–17 (1988)
7. Casas, E.: Control of an elliptic problem with pointwise state constraints. SIAM J. Control Optim. **24**(6), 1309–1318 (1986). DOI 10.1137/0324078. URL http://dx.doi.org/10.1137/0324078
8. Christofides, P.: Nonlinear and robust control of PDE systems: Methods and applications to transport-reaction processes. Birkhauser (2001)
9. Du, X., Sarkis, M., Schaerer, C.E., Szyld, D.B.: Inexact and truncated parareal-in-time krylov subspace methods for parabolic optimal control problems. Tech. Rep. 12-02-06, Department of Mathematics, Temple University (2012)
10. Duff, I.S., Erisman, A.M., Reid, J.K.: Direct methods for sparse matrices. Monographs on Numerical Analysis. The Clarendon Press Oxford University Press, New York (1989)
11. Elman, H.C., Silvester, D.J., Wathen, A.J.: Finite elements and fast iterative solvers: with applications in incompressible fluid dynamics. Numerical Mathematics and Scientific Computation. Oxford University Press, New York (2005)
12. Gee, M., Siefert, C., Hu, J., Tuminaro, R., Sala, M.: ML 5.0 smoothed aggregation user's guide. Tech. Rep. SAND2006-2649, Sandia National Laboratories (2006)
13. Greenbaum, A.: Iterative methods for solving linear systems, *Frontiers in Applied Mathematics*, vol. 17. Society for Industrial and Applied Mathematics (SIAM), Philadelphia, PA (1997)
14. Griewank, A., Walther, A.: Algorithm 799: revolve: an implementation of checkpointing for the reverse or adjoint mode of computational differentiation. ACM Transactions on Mathematical Software (TOMS) **26**(1), 19–45 (2000)
15. Heinkenschloss, M.: A time-domain decomposition iterative method for the solution of distributed linear quadratic optimal control problems. J. Comput. Appl. Math. **173**(1), 169–198 (2005). DOI 10.1016/j.cam.2004.03.005
16. Herzog, R., Sachs, E.W.: Preconditioned conjugate gradient method for optimal control problems with control and state constraints. SIAM J. Matrix Anal. Appl. **31**(5), 2291–2317 (2010)
17. Hestenes, M.R., Stiefel, E.: Methods of conjugate gradients for solving linear systems. J. Res. Nat. Bur. Stand **49**, 409–436 (1953) (1952)
18. Hintermüller, M., Ito, K., Kunisch, K.: The primal-dual active set strategy as a semismooth Newton method. SIAM J. Optim. **13**(3), 865–888 (2002)
19. Hintermüller, M., Kunisch, K.: Path-following methods for a class of constrained minimization problems in function space. SIAM J. Optim. **17**(1), 159–187 (2006)
20. Hinze, M., Köster, M., Turek, S.: A Hierarchical Space-Time Solver for Distributed Control of the Stokes Equation. Tech. rep., SPP1253-16-01 (2008)
21. Hinze, M., Pinnau, R., Ulbrich, M., Ulbrich, S.: Optimization with PDE Constraints. Mathematical Modelling: Theory and Applications. Springer-Verlag, New York (2009)
22. Ito, K., Kunisch, K.: Semi-smooth Newton methods for state-constrained optimal control problems. Systems Control Lett. **50**(3), 221–228 (2003). DOI 10.1016/S0167-6911(03)00156-7
23. Ito, K., Kunisch, K.: Lagrange multiplier approach to variational problems and applications, *Advances in Design and Control*, vol. 15. Society for Industrial and Applied Mathematics (SIAM), Philadelphia, PA (2008)

24. Kanzow, C.: Inexact semismooth Newton methods for large-scale complementarity problems. Optimization Methods and Software **19**(3-4), 309–325 (2004). DOI 10.1080/10556780310001636369. URL http://www.tandfonline.com/doi/abs/10.1080/10556780310001636369
25. Kollmann, M., Kolmbauer, M.: A Preconditioned MinRes Solver for Time-Periodic Parabolic Optimal Control Problems. Sumitted,Numa-Report 2011-06 (August 2011)
26. Murphy, M.F., Golub, G.H., Wathen, A.J.: A note on preconditioning for indefinite linear systems. SIAM J. Sci. Comput **21**(6), 1969–1972 (2000)
27. Paige, C.C., Saunders, M.A.: Solutions of sparse indefinite systems of linear equations. SIAM J. Numer. Anal **12**(4), 617–629 (1975)
28. Pearson, J.W., Stoll, M., Wathen, A.: Preconditioners for state constrained optimal control problems with Moreau-Yosida penalty function. Submitted (2011)
29. Pearson, J.W., Stoll, M., Wathen, A.J.: Regularization-robust preconditioners for time-dependent PDE-constrained optimization problems. To appear SIAM J. Matrix Anal.Appl (2012)
30. Pearson, J.W., Wathen, A.J.: A new approximation of the schur complement in preconditioners for pde-constrained optimization. Numerical Linear Algebra with Applications **19**, 816–829 (2012). DOI 10.1002/nla.814. URL http://dx.doi.org/10.1002/nla.814
31. Peirce, A., Dahleh, M., Rabitz, H.: Optimal control of quantum-mechanical systems: Existence, numerical approximation, and applications. Physical Review A **37**(12), 4950 (1988)
32. Pironneau, O.: Optimal shape design for elliptic systems. System Modeling and Optimization pp. 42–66 (1982)
33. Rees, T., Dollar, H.S., Wathen, A.J.: Optimal solvers for PDE-constrained optimization. SIAM Journal on Scientific Computing **32**(1), 271–298 (2010). DOI http://dx.doi.org/10.1137/080727154
34. Rees, T., Stoll, M., Wathen, A.: All-at-once preconditioners for PDE-constrained optimization. Kybernetika **46**, 341–360 (2010)
35. Saad, Y.: Iterative methods for sparse linear systems. Society for Industrial and Applied Mathematics, Philadelphia, PA (2003)
36. Stoll, M.: All-at-once solution of a time-dependent time-periodic PDE-constrained optimization problems. Submitted (July 2011)
37. Stoll, M., Wathen, A.: All-at-once solution of time-dependent PDE-constrained optimization problems. Submitted (2010)
38. Strang, G., Fix, G.: An Analysis of the Finite Element Method 2nd Edition, 2nd edn. Wellesley-Cambridge (2008)
39. Takacs, S., Zulehner, W.: Convergence analysis of multigrid methods with collective point smoothers for optimal control problems. Computing and Visualization in Science **14**, 131– 141 (2011)
40. Tröltzsch, F.: Optimal Control of Partial Differential Equations: Theory, Methods and Applications. Amer Mathematical Society (2010)
41. Ulbrich, M.: Semismooth Newton Methods for Variational Inequalities and Constrained Optimization Problems. SIAM Philadelphia (2011)
42. Wathen, A.J., Rees, T.: Chebyshev semi-iteration in preconditioning for problems including the mass matrix. Electronic Transactions in Numerical Analysis **34**, 125–135 (2008)
43. Zulehner, W.: Analysis of iterative methods for saddle point problems: a unified approach. Math. Comp **71**(238), 479–505 (2002)