A PRECONDITIONED INEXACT ACTIVE-SET METHOD FOR LARGE-SCALE NONLINEAR OPTIMAL CONTROL PROBLEMS

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Abstract. We provide a global convergence proof of the recently proposed sequential homotopy method with an inexact Krylov–semismooth-Newton method employed as a local solver. The resulting method constitutes an active-set method in function space. After discretization, it allows for efficient application of Krylov-subspace methods. For a certain class of optimal control problems with PDE constraints, in which the control enters the Lagrangian only linearly, we propose and analyze an efficient, parallelizable, symmetric positive definite preconditioner based on a double Schur complement approach. We conclude with numerical results for a badly conditioned and highly nonlinear benchmark optimization problem with elliptic partial differential equations and control bounds. The resulting method is faster than using direct linear algebra for the 2D benchmark and allows for the parallel solution of large 3D problems.

Key words. PDE-constrained optimization; Active-set method; Homotopy method; Preconditioned iterative method

AMS subject classifications. 49M37, 65F08, 65F10, 65K05, 90C30, 93C20

1. Introduction. We are interested in approximately solving optimization problems of the form
\[
\min \phi(x) \text{ over } x \in C \text{ subject to } c(x) = 0,
\]
where the objective functional \( \phi : X \to \mathbb{R} \) and the equality constraint \( c : X \to Y \) are twice continuously Fréchet-differentiable with real Hilbert spaces \( X, Y \). We model inequality constraints by the nonempty closed convex set \( C \subseteq X \).

A sequential homotopy method has recently been proposed \cite{48} for the approximate solution of (1.1), where the resulting linear saddle-point systems were numerically solved by direct methods based on sparse matrix decompositions. The aim of this article is to address the challenges that arise when the linear systems are solved only approximately by Krylov-subspace methods and to analyze and leverage novel preconditioners that exploit a multiple saddle-point structure, in particular double saddle-point form, which often arises in optimal control problems with partial differential equation (PDE) constraints \cite{37, 55, 41}.

The convergence analysis in this paper hinges (instead of using descent arguments for some merit function) on staying in a neighborhood of a suitably defined flow, which can be interpreted as the result of an idealized method with infinitesimal stepsizes. Flows of this kind were first used by Davidenko \cite{10} and later extended by various researchers as the basis for a plethora of globalization methods \cite{2, 11, 12, 32, 14, 7, 13, 46, 47, 6, 48}, often with a focus on affine invariance principles and partly to infinite dimensional problems. However, special care needs to be taken for most of these approaches when solving nonconvex optimization problems, as the Newton flow is attracted to saddle-points and maxima. Here we extend the sequential homotopy method of \cite{48}, which solves a sequence of projected backward Euler steps on a projected gradient/antigradient flow in Hilbert space, to allow for inexact...
linear system solutions and hence the use of Krylov-subspace methods. Salient properties of the sequential homotopy method are that the difficulties of nonconvexity and constraint degeneracy are handled on the nonlinear level by an implicit regularization similar to regularized/stabilized Sequential Quadratic Programming (see, e.g., [59, 20, 23, 21, 22] for the finite dimensional case). If semismooth Newton methods (see, e.g., [38, 49, 33, 56, 30, 31, 34, 29, 28]) are applied, the resulting methods can handle the inequality constraints in an active-set fashion. Active-set methods are of high interest, especially when a sequence of related problems needs to be solved, because warm-starts that reuse the solution from a previously solved problem can be easily accomplished. For approaches based on interior-point methods (see, e.g., [58, 52] for such methods in function space), efficient warm-starting is still an unsolved issue.

In addition to the presentation of this new inexact active-set approach and its convergence analysis, we propose and analyze new preconditioners for the resulting linear system at each iteration. Preconditioning PDE-constrained optimization problems has been a subject of considerable interest of late (see, e.g., [53, 50, 60, 44, 42, 43, 45, 40]), however relatively few such methods have made use of the double saddle-point structure. We refer the reader to recent, related work [37, 55, 41, 8]. We provide theoretical results on preconditioners for double saddle-point systems and, having arranged the linear systems obtained from the active-set approach to this form, we present efficient and flexible approximations to be applied within a Krylov-subspace solver.

This paper is structured as follows. Sections 2 and 3 state the sequential homotopy method and its Krylov-subspace active-set interpretation. Section 4 provides a convergence analysis for a homotopy method with inexact semismooth Newton corrector, and discusses the resulting active sets and linear systems which we need to solve. Section 5 gives results on preconditioners for double saddle-point matrices, the form of these systems, and Section 6 contains details of our implementation and approximations in our preconditioners. Section 7 presents a range of numerical results.

Notation. With \( B_X \) we denote the open unit ball in \( X \). As in [48], we denote with \( T(C, x) \) the tangent cone to a nonempty, closed, convex set \( C \) at \( x \in C \). We denote with \( K^- \) the polar cone of a nonempty, closed, convex cone \( K \subseteq X \). We generally use bold notation (such as \( x \)) for vectors; regular typeface (such as \( x \)) is used for continuous variables. When a matrix is written in calligraphic form (such as \( A \)), as opposed to \( A \)), the calligraphic form denotes a block matrix.

2. Sequential Homotopy Method. We briefly recapitulate the sequential homotopy method proposed in [48]. Let

\[
L^\rho(x, y) := \phi(x) + \frac{\rho}{2} \|c(x)\|_Y^2 + (y, c(x))_Y
\]

denote the augmented Lagrangian with some sufficiently large \( \rho \geq 0 \). The sequential homotopy method solves a sequence of subproblems that differ in \( (\hat{x}, \hat{y}) \in C \times Y \)

\[
F(x, y; \hat{x}, \hat{y}, \Delta t) := \begin{pmatrix}
x - PC(\hat{x} - \Delta t \nabla_x L^\rho(x, y)) \\
y - \hat{y} - \Delta tc(x)
\end{pmatrix} = 0
\]  

(2.1)

for the unknowns \((x, y) \in X \times Y\) by a homotopy in the parameter \( \Delta t \geq 0 \), where \( PC \) is the (in general nonsmooth) projection onto \( C \). By [48, Thm. 4], we know that for sufficiently small \( \Delta t \geq 0 \), equation (2.1) admits a unique solution provided that a Lipschitz condition on \( \nabla L^\rho \) holds. For \( \Delta t = 0 \), the solution to (2.1) is \((x, y) = (\hat{x}, \hat{y})\). If a continuation of solutions \((x(\Delta t), y(\Delta t))\) to (2.1) exists for \( \Delta t \to \infty \), then \( x(\Delta t), y(\Delta t) \) tends to a primal–dual solution to the original problem (1.1). If the solution \((x(\Delta t), y(\Delta t))\)
cannot be continued (or if we decide not to continue it) further than some finite \( \Delta t^* > 0 \), we can update the reference point \((\hat{x}, \hat{y}) = (x(\Delta t^*), y(\Delta t^*))\) and recommence the next homotopy leg (hence the name sequential homotopy method).

### 3. Krylov-Subspace Active-Set Interpretation of the Sequential Homotopy Method

There are two interesting interpretations of equation (2.1): First, it constitutes the projected backward Euler equations for the projected gradient/anti-gradient flow equations [48]:

\[
\frac{dx}{dt}(t) = P_{T(C, x(t))}(-\nabla_x L^\rho(x(t), y(t))), \quad \frac{dy}{dt}(t) = \nabla_y L^\rho(x(t), y(t)) = c(x(t)),
\]

whose equilibrium points are the critical points of (1.1). Moreover, under certain conditions, critical points that admit feasible descent curves are not asymptotically stable (see [48, Thm. 3]), so that convergence to maxima and saddle points of problem (1.1) is avoided. Second, equation (2.1) is a necessary optimality condition of a primal–dual proximally regularized and augmented version of (1.1), which reads with \( \lambda = 1/\Delta t \) as

\[
\min_{w \in Y, x \in C} \phi(x) + \frac{\rho}{2} ||c(x)||_Y^2 + \frac{\lambda}{2} \left[ ||x - \hat{x}||_X^2 + ||w - \hat{y}||_Y^2 \right] \text{ s.t. } c(x) + \lambda w = 0. \quad (3.1)
\]

Semismooth Newton methods (see, e.g., [56]) are an ideal candidate to solve (2.1) (see [48]). This approach can be interpreted as a Sequential Quadratic Programming (SQP) method for (3.1) that requires for each Quadratic Programming (QP) subproblem only one linear system solve while still facilitating aggressive active-set changes (determined by the semismooth Newton method). The application of conventional active-set QP solvers (e.g., [19]) would not be competitive here because their computational complexity is dependent on the number of active set changes between two consecutive QP subproblems, which for instance jeopardizes mesh-independence for discretizations of PDE-constrained optimization problems.

From this vantage point, our investigation of inexact semismooth Newton methods for (2.1) provides a class of active-set SQP methods that are based on Krylov-subspace methods, which work particularly well in combination with suitable preconditioners such as those provided in Sec. 5.

### 4. Homotopy Method with Inexact Semismooth Newton Corrector

To avoid notational clutter, we use the abbreviations \( Z := X \times Y, z := (x, y), \) and \( \hat{z} := (\hat{x}, \hat{y}) \) in the following with the obvious meaning of

\[
F(z; \hat{z}, \Delta t) := F(x, y; \hat{x}, \hat{y}, \Delta t) = z - P_{C \times Y}(\hat{z} - \Delta t J \nabla L^\rho(z)),
\]

where \( J \) is the isomorphism \((x, y) \mapsto (x, -y)\) flipping the sign of the second component.

Considering that the solution algorithm provided in [48] employs only one semismooth Newton step plus one simplified (i.e., without updating the system matrices) semismooth Newton step, and then simultaneously updates the reference point \( \hat{z} \) and the steps size \( \Delta t \), we propose to analyze the sequential homotopy approach with inexact semismooth Newton methods as one monolithic (opposed to sequential) homotopy approach in the combined homotopy variables \((\hat{z}, \Delta t)\) (and not just \( \Delta t \) alone).

We first restrict the analysis to the case when only a single semismooth Newton step, without successive improvement by a simplified semismooth Newton step, is used. We shall later discuss the extension to additional simplified semismooth Newton steps for practical implementations.
4.1. Inexact semismooth Newton corrector steps. Let us recall some fundamental definitions for semismooth Newton methods (following the setting in [56]). For a function \( f : Z \to Z \) and a set-valued mapping \( \partial^* f : Z \rightrightarrows L(Z) \), we call \( f \) semismooth (or, more precisely, weakly \( \partial^* f \)-semismooth) at \( z \in Z \) if \( f \) is continuous in a neighborhood of \( z \) and

\[
\sup_{A \in \partial^* f(z+s)} \| f(z+s) - f(z) - As \|_Z = o(\| s \|_Z) \quad \text{as} \quad \| s \|_Z \to 0.
\]

We generate a sequence \((z_k)_{k \in \mathbb{N}}\) by iterating the following steps for \( k = 0, 1, \ldots \):

1. Choose \( \Delta t_k > 0 \)
2. Compute \( F_k = F(z_k; z_k, \Delta t_k) \)
3. Compute \( A_k \in \partial^* F(z_k; z_k, \Delta t_k) \)
4. Compute \( \Delta z_k \in Z_0 \) satisfying \( \| A_k \Delta z_k + F_k \|_Z \leq \kappa_k \| F_k \|_Z \) for some tolerance \( \kappa_k \in [0, \bar{\kappa}] \) with given \( \bar{\kappa} < 1 \)
5. Set \( z_{k+1} = z_k + \Delta z_k \)
6. Project \( z_{k+1} = P_{C \times Y}(z_{k+1}^0) \)

For simplicity, we skip the use of an additional smoothing step before the projection (cf. [48]). It is not needed in the example considered in Sec. 7.

The following result shows that if the sequence \((z_k)\) becomes stationary then we have obtained a critical point of (1.1).

**Lemma 4.1.** Let the range of \( c'(x) \) be closed in \( Y \) and let the Guignard Constraint Qualification (GCQ) hold for all feasible \( x \in C \) (cf. [48] Ass. 1 and Def. 4)). If \( \Delta t_k > 0 \) and \( z_{k+1} = z_k \), then \( z_k = (x_k, y_k) \) is a critical point of (1.1).

**Proof.** If \( z_{k+1} = z_k \Rightarrow \bar{z} \), then \( \Delta z_k = 0 \) and \( F_k = F(\bar{z}; \bar{z}, \Delta t_k) = 0 \), which implies by (2.1) and \( \Delta t_k > 0 \) that \( c(\bar{x}) = 0 \) and \( \bar{x} = P_C(\bar{x} - \Delta t L^\rho(\bar{z})) \). Hence, \( \bar{x} = P_{T(C;\bar{x})}(\bar{x} - \Delta t L^\rho(\bar{z})) \) and by [5] Prop. 6.28 we have that \( -\nabla c(x) - \nabla c(x)\bar{y} = -\nabla L^\rho(\bar{z}) \in T^- (C, \bar{x}) \). By [48] Def. 5, \( \bar{z} = z_k \) is a critical point. \( \square \)

In the remainder of this section we state reasonable assumptions that imply convergence of \((z_k)\) to a critical point of (1.1). Instead of stating the assumptions upfront, we shall develop and state them as they are required in the steps of the proof. The overarching strategy of the convergence proof consists in the following steps. First, the gradient/antigradient flow [48] reaches into the region of local convergence in finite time. Second, for small enough \( \Delta t_k \), solutions to the projected backward Euler equations (2.1) exist uniquely in a neighborhood of the flow. Third, the deviation of the projected backward Euler solution from projected gradient/antigradient flows can be bounded. Fourth, we derive a bound for the distance of one inexact semismooth Newton step to the solution of the projected backward Euler iterate. Fifth, a finite number of projected backward Euler steps suffice to stay close to the flow until it reaches the region of local convergence, and the linear system termination tolerance \( \bar{\kappa} \in (0, 1) \) can be chosen such that also the inexact iterates \((z_k)\) reach the region of local convergence, too.

**Step 1.** We assume that given \( z_0 \in C \times Y \), there exists a gradient/antigradient flow emanating from \( z_0 \):

**Assumption 1.** There exists an absolutely continuous curve \( z^0 : [0, \infty) \to C \times Y \) that is the unique solution of the initial value problem

\[
\frac{dz^0}{dt}(t) = P_{T(C \times Y; z^0(t))}(-J \nabla L^\rho(z^0(t))), \quad z^0(0) = z_0,
\]

and converges to \( z^* := \lim_{t \to \infty} z^0(t) \).
A sufficient condition for the existence of $z^0$ (but without its convergence) is given in [43, Thm. 2].

Next, we postulate that there is a region of local convergence around $z^*$:

**Assumption 2.** There exist constants $\Delta t_{max}^loc > \Delta t_{min} > 0$, $\bar{\kappa} \in (0, 1)$, and $\varepsilon > 0$ such that if for some $N \in \mathbb{N}$ it holds that $z_N \in z^* + \varepsilon B_Z$ and $\Delta t_k \in [\Delta t_{min}, \Delta t_{max}^loc]$ for all $k \geq N$, then $z_k \to z^*$ for $k \to \infty$.

To understand that Ass. 2 is reasonable, let us consider for $\Delta t \geq 0$ and bounded with constant $\bar{\kappa}$.

**Lemma 4.2.** Let Ass. 1 and 2 hold. Then, there exists $\Delta t_{max}^N > 0$ such that there exists a unique solution $z^+(\tilde{z}, \Delta t) \in \mathcal{N}_2$, i.e., $F(z^+(\tilde{z}, \Delta t); \tilde{z}, \Delta t) = 0$, for all $\tilde{z} \in \mathcal{N}_1$ and $\Delta t \leq \Delta t_{max}^N$. Moreover, it holds that

$$
\|z^+(\tilde{z}, \Delta t) - z^+\|_Z \leq 2\tilde{M} \Delta t \leq \varepsilon.
$$

**Proof.** The technique is a refinement of an argument in the proof of [43, Thm. 4]. Let $0 < \Delta t_{max}^N \leq \min \{ \frac{1}{\bar{\kappa} \Delta t_{min}}, \frac{1}{2\tilde{M}} \}$ and define

$$
\Phi(z) := P_{C \times Y}(\tilde{z} - \Delta t J \nabla L^\rho(z)).
$$

For $\Delta t \leq \Delta t_{max}^N$, $\Phi$ is a contraction on $\mathcal{N}_2$ because

$$
\|\Phi(z) - \Phi(\tilde{z})\|_Z \leq \Delta t \omega \|z - \tilde{z}\|_Z \leq \Delta t_{max}^N \omega \|z - \tilde{z}\|_Z \leq \frac{1}{2} \|z - \tilde{z}\|_Z.
$$

To show that the fixed point iteration with $\Phi$ stays in $\mathcal{N}_2$, we can estimate the initial increment as

$$
\|\Phi(\tilde{z}) - \tilde{z}\|_Z = \|P_{C \times Y}(\tilde{z} - \Delta t J \nabla L^\rho(\tilde{z})) - P_{C \times Y}(\tilde{z})\|_Z \leq \Delta t \|\nabla \rho(\tilde{z})\| \leq \Delta t \tilde{M},
$$
which implies by induction over \( k \in \mathbb{N} \) that
\[
\|\Phi^k(\hat{z}) - \hat{z}\|_2 \leq \sum_{i=0}^{k-2} 2^{-i} \|\Phi(\hat{z}) - \hat{z}\|_2 \leq 2 \Delta t \overline{M} \leq \varepsilon.
\]

Because \( \hat{z} \in \mathcal{N}_1 \), there exists \( t \geq 0 \) such that \( \|\hat{z} - z^0(t)\|_2 \leq \varepsilon \). Hence, \( \|\Phi^k(\hat{z}) - z^0(t)\|_2 \leq \|\Phi(\hat{z}) - \hat{z}\|_2 \leq 2\varepsilon \), implying \( \Phi^k(\hat{z}) \in \mathcal{N}_2 \) for all \( k \in \mathbb{N} \). Using Banach’s fixed point theorem, we finally obtain the unique existence of \( z^+(\hat{z}, \Delta t) \in \mathcal{N}_2 \).

The a-priori estimate of Banach’s fixed point theorem yields with (4.2) that
\[
\|\hat{z} - z^+(\hat{z}, \Delta t)\|_2 \leq \frac{1}{1 - T} \|\Phi(\hat{z}) - \hat{z}\|_2 \leq 2 \overline{M} \Delta t \leq \varepsilon. \quad \Box
\]

**Step 3.** We derive a bound for the deviation of the projected backward Euler step from neighboring projected gradient/antigradient flows, whose existence we postulate in the following assumption.

**Assumption 4.** There exists a function \( \bar{z} : \mathcal{N}_1 \times [0, \infty) \to C \times Y \) that is absolutely continuous in its second argument and the unique solution of the initial value problems
\[
\frac{\partial \bar{z}}{\partial t}(z, t) = P_{T(C \times Y, \bar{z}(z, t))}(-J \nabla L^\rho(\bar{z}(z, t))), \quad \bar{z}(z, 0) = z
\]
for all \( z \in \mathcal{N}_1, t \geq 0 \).

We can now derive the following estimate:

**Lemma 4.3.** Let Ass. 1–4 hold. Then, there exists a function \( \varphi : \mathcal{N}_1 \times (0, \Delta t_{\text{max}}^N] \to \mathbb{R}_{\geq 0} \) satisfying \( \lim_{t \to 0^+} \varphi(z, t) = 0 \) for all \( z \in \mathcal{N}_1 \) such that
\[
\|z^+(z, t) - \bar{z}(z, t)\|_2 \leq t \varphi(z, t) e^{\omega t}.
\]

**Proof.** We use the abbreviations \( f(z) := -J \nabla L^\rho(z), \Pi(z) := P_{T(C \times Y, z)}(\cdot), \) and \( \Pi_-(\cdot) = P_{T-(C \times Y, z)}(\cdot) \) for convenience. The proof is based on an estimate for a projected forward Euler step and then estimating the distance between the projected backward and forward Euler steps. With
\[
z^f(z, t) := z + \int_0^t \Pi_{C \times Y(z + tf(z))}(f(z)),
\]
we then obtain for almost all \( t \in [0, \Delta t_{\text{max}}^N] \) that
\[
\frac{d}{dt} \left( \frac{1}{2} \left\|z^f(z, t) - P_{C \times Y}(z + tf(z)) \right\|_2^2 \right) = (z^f(z, t) - P_{C \times Y}(z + tf(z)), \Pi_{C \times Y(z + tf(z))}(f(z)) - \Pi_{P_{C \times Y}(z + tf(z))}(f(z)))_Z = 0.
\]

Using the differential form of Gronwall’s inequality together with \( z^f(z, 0) = z = P_{C \times Y}(z) \), we obtain that \( z^f(z, t) = P_{C \times Y}(z + tf(z)) \) is a projected forward Euler step and that it is a solution (uniqueness is guaranteed by [9 Thm. 3.1]) of the initial value problem with constant \( f(z) \) on the right-hand side
\[
\frac{\partial}{\partial t} \zeta(z, t) = \Pi_{\zeta(z, t)}(f(z)), \quad \zeta(z, 0) = z.
\]

Dropping the arguments \( z, t \) of \( \bar{z} \) and \( z^f \) (and further below in the proof also \( z^+ \)) for notational convenience, we can use Moreau’s decomposition, monotonicity of the
set-valued map \( z \mapsto T^-(C \times Z, z) \) (see [[1] Lem. 2.1]), the Cauchy–Schwarz inequality, and Lipschitz-continuity of \( f \) to derive

\[
\frac{d}{dt} \| \bar{z} - z^f \|^2_Z = 2 \left( \bar{z} - z^f, \frac{\partial \bar{z}}{\partial t} - \frac{\partial z^f}{\partial t} \right)_Z = 2 \left( \bar{z} - z^f, \Pi_z(f(z)) - \Pi_z(f(z)) \right)_Z \\
= 2 \left( \bar{z} - z^f, f(\bar{z}) - f(z) \right)_Z - 2 \left( \bar{z} - z^f, \Pi_z^*(f(z)) - \Pi_z^*(f(z)) \right)_Z \geq 0 \text{ by monotonicity}
\]

(4.3)

\[
\leq 2 \left( \bar{z} - z^f, f(\bar{z}) - f(z) \right)_Z + 2 \left( \bar{z} - z^f, f(z^f) - f(z) \right)_Z \\
\leq 2\omega \| \bar{z} - z^f \|^2_Z + 2\omega \| \bar{z} - z^f \|_Z \| z^f - z \|_Z 
\]

For the penultimate term in (4.3), we have the estimate

\[
\| \bar{z} - z^f \|_Z = \left\| \int_0^t \Pi_z(z, \tau)(f(z(\bar{z}, \tau))) - \Pi_z(z, \tau)(f(z)) \, d\tau \right\|_Z \leq 2Mt \tag{4.4}
\]

by virtue of Ass. 3. For the last term in the same equation, we recall that

\[
\lim_{t \to 0^+} \frac{z^f(t, z) - z}{t} = \lim_{t \to 0^+} \frac{P_{C \times Y}(z + tf(z)) - z}{t} = \Pi_z(f(z)),
\]

from which we can deduce the existence of a function \( \tilde{\varphi}(z, t) \) that is monotonic in \( t \) and satisfies \( \lim_{t \to 0^+} \tilde{\varphi}(z, t) = 0 \) such that

\[
\| z^f - z \|_Z = t \left\| \frac{z^f - z}{t} \right\|_Z \leq tM \tilde{\varphi}(z, t). \tag{4.5}
\]

Combining equations (4.3), (4.4), and (4.5), we obtain

\[
\frac{d}{dt} \| \bar{z} - z^f \|^2_Z \leq 2\omega \| \bar{z} - z^f \|^2_Z + 4\omega M^2 t^2 \tilde{\varphi}(z, t).
\]

Applying Gronwall’s inequality in differential form, and taking the square root, yields

\[
\| \bar{z} - z^f \|_Z \leq 2Mt \sqrt{\omega \tilde{\varphi}(z, t)} e^{\omega t}.
\]

We finally bound the local truncation error of the projected backward Euler step by

\[
\| z^+ - \bar{z} \|_Z \leq \| z^+ - z^f \|_Z + \| z^f - \bar{z} \|_Z \\
\leq \| P_{C \times Y}(z + tf(z^+)) - P_{C \times Y}(z + tf(z)) \|_Z + \| z^f - \bar{z} \|_Z \\
\leq t\omega \| z^+ - z \|_Z + \| z^f - \bar{z} \|_Z \\
\leq t^2\omega \left\| \frac{P_{C \times Y}(z + tf(z^+)) - z}{t} \right\|_Z + 2Mt \sqrt{\omega \tilde{\varphi}(z, t)} e^{\omega t} =: t\varphi(z, t) e^{\omega t}.
\]

This finishes the proof. \( \square \)

Moreover, Gronwall’s inequality can be used to show the following result about neighboring flows:

**Lemma 4.4.** Let Ass. 3, 4 hold and let \( z, \tilde{z} \in \mathcal{N}_1 \). If \( \bar{z}(z, \tau), \tilde{z}(\tilde{z}, \tau) \in \mathcal{N}_2 \) for all \( \tau \in [0, t] \), then

\[
\| \bar{z}(z, t) - \tilde{z}(\tilde{z}, t) \|_Z \leq e^{\omega t} \| z - \tilde{z} \|_Z.
\]
Proof. We reuse the abbreviations introduced in the proof of the previous lemma. Using Moreau’s decomposition \( f(\cdot) = \Pi_z(f(\cdot)) + \Pi_\Delta(f(\cdot)) \), we obtain
\[
\frac{d^2}{dt^2} \| z(t) - \tilde{z}(t) \|^2_Z = 2 \left( \tilde{z}(t), t \right) \Pi_{z(t)}(f(\tilde{z}(t))) - \Pi_{\tilde{z}(t)}(f(\tilde{z}(t))) \bigg) Z \\
= 2 \left( \tilde{z}(t), t \right) \Pi_{\tilde{z}(t)}(f(\tilde{z}(t))) - f(\tilde{z}(t)) \bigg) Z \\
- 2 \left( \tilde{z}(t), t \right) \Pi_{\tilde{z}(t)}(f(\tilde{z}(t))) - f(\tilde{z}(t)) \bigg) Z \\
\leq 2 \omega \| z(t) - \tilde{z}(t) \|^2_Z,
\]
because the inner product involving the \( \Pi_\Delta \) terms is non-negative by monotonicity \[9\] Lem. 2.1. Application of Gronwall’s inequality in differential form and taking the square root complete the proof. \( \square \)

Step 4. To bound the distance between the solution \( z^+(z_k, \Delta t_k) \) to (2.1) and one single inexact semismooth Newton iteration \( z_{k+1} \), we adapt the results from \[56\] to our setting. We thus require the following assumption:

**Assumption 5.** The function \( z \mapsto F(z; \tilde{z}, \Delta t) \) is semismooth for all \( z, \tilde{z} \in \mathcal{N}_2 \) and \( \Delta t \in [0, \Delta t^N_{\max}] \).

We can now show invertibility of the linearizations \( A_k \) for \( k \in \mathbb{N} \):

**Lemma 4.5.** Let Ass. 1–5 hold. Then, all \( A \in \partial^* F(z; \tilde{z}, \Delta t) \) are invertible with \( \| A^{-1} \|_{\mathcal{L}(Z)} \leq 2 \) for all \( z, \tilde{z} \in \mathcal{N}_2 \) and \( \Delta t \in [0, \Delta t^N_{\max}] \).

**Proof.** By construction of \( F \), we have that \( A = I_Z - \mathcal{M} \) with
\[
\mathcal{M} = \partial^* [PC_{\times Y}(\tilde{z} - \Delta tJ\nabla L^\rho(z))].
\]
The chain rule for semismooth functions \[56\] Prop. 3.7] yields \( \mathcal{M} = \mathcal{M}_2 \mathcal{M}_1 \) with \( \mathcal{M}_1 = -\Delta tJ\nabla^2 L^\rho(z) \) and \( \mathcal{M}_2 \in \partial^* PC_{\times Y}((\tilde{z} - \Delta tJ\nabla L^\rho(z)) \). With the corresponding Lipschitz constants (i.e., 1 for the projector \( PC_{\times Y} \) and \( \omega \) for \( J\nabla L^\rho \)) and the choice of \( \Delta t^N_{\max} \) from the proof of Lem. 4.2 we obtain
\[
\| \mathcal{M} \|_{\mathcal{L}(Z)} \leq \| \mathcal{M}_2 \|_{\mathcal{L}(Z)} \cdot \| \mathcal{M}_1 \|_{\mathcal{L}(Z)} \leq 1 \cdot \Delta t\omega \leq \Delta t^N_{\max} \omega \leq \frac{1}{2}.
\]
The Neumann series \( A^{-1} = \sum_{k=0}^{\infty} \mathcal{M}^k \) yields the desired result. \( \square \)

In addition to \( F_k, A_k, \Delta z_k, z_k^0 \), and \( z_k \) introduced at the beginning of Sec. 4.1 we use for \( k \in \mathbb{N} \) the additional notation
\[
v_k^0 = z_{k+1}^0 - z^+(z_k, \Delta t_k), \quad v_k^+ = z_k - z^+(z_k, \Delta t_k), \quad v_{k+1} = z_{k+1} - z^+(z_k, \Delta t_k).
\]

We are now prepared to prove the following result:

**Lemma 4.6.** Let Ass. 1–5 hold. Then, there exists a function \( \psi : \mathbb{R}_{\geq 0} \times \mathcal{N} \times [0, \Delta t^N_{\max}] \to \mathbb{R}_{\geq 0} \) with \( \lim_{h \to 0^+} \psi(h; z, \Delta t) = 0 \) such that
\[
\| v_{k+1} \|_Z \leq 2 \left( \gamma_A k \omega + \psi(\| v_k^+ \|_Z; z_k, \Delta t_k) \right) \| v_k^+ \|_Z
\]
for all \( z \in \mathcal{N}_2, \Delta t \in [0, \Delta t^N_{\max}] \).

**Proof.** We start by observing that the Lipschitz constant of \( F(\cdot; z_k, \Delta t_k) \) on \( \mathcal{N}_2 \) is \( 1 + \Delta t\omega \), which can be used together with \( F(z^+(z_k, \Delta t_k); z_k, \Delta t_k) = 0 \) to bound
\[
\| F_k \|_Z = \| F(z_k; z_k, \Delta t_k) - F(z^+(z_k, \Delta t_k); z_k, \Delta t_k) \|_Z \leq (1 + \Delta t\omega) \| v_k^+ \|_Z.
\]
By simple rearrangements, we obtain
\[ A_k v_k^0 = A_k (\Delta z_k + z_k - z^+(z_k, \Delta t_k)) \]
\[ = (A_k \Delta z_k + F_k) - [F(z_k; z_k, \Delta t_k) - F(z^+(z_k, \Delta t_k); z_k, \Delta t_k) - A_k v_k^+] . \]

Because \( F(\cdot; z_k, \Delta t_k) \) is semismooth, the term in brackets is \( o(\|v_k^+\|) \) and we can suitably define \( \psi \) to obtain
\[ \|A_k v_{k+1}^0\|_Z \leq \kappa_k \|F_k\|_Z + \psi(\|v_k^+\|_Z ; z_k, \Delta t_k) \|v_k^+\|_Z. \] (4.7)

Combining Lem. 4.5 with equations (4.7) and (4.6) yields
\[ \|v_{k+1}\|_Z = \|z_{k+1} - z^+(z_k, \Delta t_k)\|_Z = \|P_{C \times Y}(z_{k+1}^0) - P_{C \times Y}(z^+(z_k, \Delta t_k))\|_Z \]
\[ \leq \|z_{k+1}^0 - z^+(z_k, \Delta t_k)\|_Z = \|A_k^{-1}A_k v_{k+1}^0\|_Z \leq 2 \|A_k v_{k+1}^0\|_Z \]
\[ \leq 2 \left[ (1 + \Delta t_k \omega) + \psi(\|v_k^+\|_Z ; z_k, \Delta t_k) \right] \|v_k^+\|_Z . \]

This ends the proof. \( \square \)

**Step 5.** Our aim in this final step is to combine the results of the previous steps to establish that \((z_k)\) eventually reaches the region of local convergence \(z^* + \varepsilon B z\). We restrict our analysis to the case that the bounds of Lem. 4.3 and 4.6 are uniform:

**Assumption 6.** There exist non-decreasing functions \( \varphi, \psi : \mathbb{R} \to \mathbb{R} \) with \( \lim_{t \to 0^+} \varphi(t) = \lim_{h \to 0^+} \psi(h) = 0 \) such that \( \varphi(z, t) \leq \varphi(t) \) and \( \psi(h; z, t) \leq \psi(h) \) for all \( z \in \mathcal{N}_1 \), \( t \in (0, \Delta t_{\text{max}}) \), and \( h \in \mathbb{R}_{>0} \).

We can finally prove the global convergence theorem.

**Theorem 4.7** (Global convergence). Let Ass. 4.7 hold. Then, there exist constants \( \Delta t_{\text{max}} > 0 \) and \( \bar{\kappa} \in (0, 1) \) such that for any stepsize sequence \((\Delta t_k)\) satisfying \( \sum_{k=0}^{\infty} \Delta t_k = \infty \) and
\[ \Delta t_k \leq \Delta t_{\text{max}} \quad \text{for all } k \text{ such that } \sum_{i=0}^{k} \Delta t_i \leq \bar{\kappa}, \]
the smallest integer \( N \) with \( \sum_{i=0}^{N} \Delta t_i > \bar{\kappa} \) satisfies \( \|z_N - z^*\|_Z \leq \varepsilon. \) Furthermore, if \( \Delta t_k \in [\Delta t_{\text{min}}, \Delta t_{\text{max}}^{\text{lo}}] \) for all \( k \geq N \), then \((z_k)\) converges to \( z^* \).

**Proof.** We start with choosing \( \beta > 0 \) such that
\[ \bar{\kappa} e\bar{\omega} \beta \leq \frac{\varepsilon}{3}. \] (4.8)

Next, we choose \( \Delta t_{\text{max}} \in (0, \Delta t_{\text{max}}^{\text{lo}}] \) satisfying
\[ \bar{\kappa} e\bar{\omega} \bar{\varphi}(\Delta t_{\text{max}}) \leq \frac{\varepsilon}{3} \quad \text{and} \quad 4 \bar{M} \bar{y}(2M \Delta t_{\text{max}}) \leq \frac{\beta}{2}. \] (4.9)

Finally, we choose \( \bar{\kappa} \in (0, 1) \) such that
\[ 4 \bar{M} (1 + \Delta t_{\text{max}} \omega) \bar{\kappa} \leq \frac{\beta}{2}. \] (4.10)

Lem. 4.2 delivers \( \|v_k^+\|_Z \leq 2 \bar{M} \Delta t_k \) and by Lem. 4.6 together with (4.9) and (4.10) we then get
\[ \|z_{k+1} - z^+(z_k, \Delta t_k)\|_Z = \|v_{k+1}\|_Z \leq 2 \left[ (1 + \Delta t_{\text{max}} \omega) \bar{\kappa} + \tilde{\psi}(\|v_k^+\|_Z) \right] \|v_k^+\|_Z \leq \beta \Delta t_k . \] (4.11)

We now prove by induction that for \( k \leq N \) it holds that
\[ \|z_k - \bar{z} \left( \bar{\omega}, \sum_{i=0}^{k-1} \Delta t_i \right)\|_Z \leq [\beta + \bar{\varphi}(\Delta t_{\text{max}})] e\omega \sum_{i=0}^{k-1} \Delta t_i \sum_{i=0}^{k-1} \Delta t_i . \] (4.12)
For $k = 0$, both sides of (4.12) are equal to zero. For the induction step, we obtain by the triangle inequality, (4.11), Lem. 4.3 and 4.4 and the induction hypothesis (4.12):

\[
\begin{align*}
\|z_{k+1} - \tilde{z}(z_0, \sum_{i=0}^{k} \Delta t_i)\|_Z \\
\leq \|z_{k+1} - z^+\Delta z_k, \Delta t_k\|_Z + \|z^+\Delta z_k - \tilde{z}(z_0, \sum_{i=0}^{k} \Delta t_i)\|_Z \\
+ \|\tilde{z}(z_k, \Delta t_k) - \tilde{z}(z_0, \sum_{i=0}^{k-1} \Delta t_i)\|_Z \\
\leq \beta \Delta t_k + \Delta t_k \bar{\varphi}(\Delta t_{\max}) \epsilon^{\omega \Delta t_k} + \epsilon^{\omega \Delta t_k} \|z_k - \tilde{z}(z_0, \sum_{i=0}^{k-1} \Delta t_i)\|_Z \\
\leq \beta \Delta t_k \epsilon^{\omega \Delta t_k} + \Delta t_k \bar{\varphi}(\Delta t_{\max}) \epsilon^{\omega \Delta t_k} + \epsilon^{\omega \Delta t_k} [\beta + \bar{\varphi}(\Delta t_{\max})] \epsilon^{\omega \sum_{i=0}^{k-1} \Delta t_i} \sum_{i=0}^{k-1} \Delta t_i \\
\leq [\beta + \bar{\varphi}(\Delta t_{\max})] \epsilon^{\omega \sum_{i=0}^{k-1} \Delta t_i} \sum_{i=0}^{k-1} \Delta t_i.
\end{align*}
\]

Abbreviating $t^* = \sum_{i=0}^{N-1} \Delta t_i \leq \bar{t}$ and $t = \sum_{i=0}^{N} \Delta t_i \geq \bar{t}$, we can then use (4.12), (4.1), (4.8), and (4.9) to deduce that for $k = N$ it holds that

\[
\begin{align*}
\|z_N - z^*\|_Z \\
\leq \|z_N - \tilde{z}(z_0, \Delta t_k)\|_Z + \|\tilde{z}(z_0, \Delta t_k) - z^*\|_Z \\
\leq \beta + \bar{\varphi}(\Delta t_{\max}) t^* e^{\omega t^*} + \|\tilde{z}(z_0, \Delta t_k) - z^*\|_Z \leq \frac{\varepsilon}{3} + \frac{\varepsilon}{3} + \frac{\varepsilon}{3} \leq \varepsilon.
\end{align*}
\]

The final assertion follows from Ass. 2.

**4.2. Implications for practical implementations.** The nature of the proof of global convergence (Thm. 4.7) is more that of a theoretical guarantee and we do not advise to use the estimates for the choice of parameters in a practical implementation of the algorithm. This would anyway be impossible, because central constants such as the Lipschitz constant $\omega$ or the time $t$ are unavailable. Some qualitative properties are, however, useful in practice:

1. We can control the condition number $\|A_k^{-1}\|_{L(Z)} \|A_k\|_{L(Z)}$ of the linear systems by reducing $\Delta t_k$ (see Lem. 4.5). For practical implementations, however, we advise to use larger $\Delta t_k$ (violating $\Delta t_k \omega \leq \frac{1}{2}$), so that usually $\|A_k^{-1}\|_{L(Z)} > 2$ holds.

2. The choice of the linear system termination tolerance $\kappa_k \leq \bar{\kappa}$ must be balanced with $\Delta t_k$. A smaller $\kappa_k$ means more work on the linear algebra level but allows more progress (i.e., larger $\Delta t_k$) on the nonlinear level. In our experience, it is advantageous to use a larger $\kappa_k$ when $\Delta t_k$ is small.

3. One main ingredient of the convergence proof is Lem. 4.6, which we can interpret as choosing $\Delta t_k$ small enough so that $z_k$ stays in the region of local convergence for the inexact semismooth Newton method on $F(z; z_k, \Delta t_k)$.

**4.3. Inexact simplified semismooth Newton corrector steps.** As a practical implementation, we use Alg. 1, with the only modification that the linear systems are solved approximately. We remark that the stepsize control is performed on $\lambda_k = 1/\Delta t_k$ instead of $\Delta t_k$. The relative termination tolerance is chosen as

$$
\kappa_k = \max \left( \kappa_{\min}, \min \left( \kappa_{\max} + (\kappa_{\min} - \kappa_{\max}) \frac{\lambda_k - \lambda_0}{\lambda_0/\lambda^*}, \kappa_{\max} \right) \right).
$$

The values for the numerical experiments were set to $\kappa_{\min} = 10^{-7}$, $\kappa_{\max} = 10^{-3}$, $\lambda_0^* = 1$, $\lambda^* = 10^{-7}$. We further enforce $\lambda_k \geq \lambda_{\min} = 10^{-7}$ in the adaptive stepsize control.
The numerical criterion for evaluating whether we keep inside the region of local convergence is the same increment monotonicity test as described in [38, Alg. 1], which also serves as the basis for the adaptive stepsize control. The stepsize proportional-integral (PI) controller constants are the same as in [38, Alg. 1].

4.4. Discretized linear systems and active sets. We now address how the discretized linear systems required for the computation of the inexact semismooth Newton increments can be set up and solved. We denote by $M^h_X \in \mathbb{R}^{n \times n}$ and $M^h_Y \in \mathbb{R}^{m \times m}$ the symmetric positive definite matrices that are the discretizations of the inner products on $X$ and $Y$. With the discretized objective $\phi_h : \mathbb{R}^n \to \mathbb{R}$ and constraint function $c_h : \mathbb{R}^n \to \mathbb{R}^m$, the discretized augmented Lagrangian reads as

$$L^\rho_h(x, y) = \phi_h(x) + \frac{\rho}{2} c_h(x)^T M^h_Y c_h(x) + y^T M^h_Y c_h(x).$$

Because the gradient is the Riesz representation of the derivative (cf. the discussion in [25]), we also need to scale the discrete derivative to obtain the gradients

$$\nabla_x L^\rho_h(x, y) = (M^h_X)^{-1} \frac{\partial L^\rho_h(x, y)}{\partial x}^T, \quad \nabla_y L^\rho_h(x, y) = (M^h_Y)^{-1} \frac{\partial L^\rho_h(x, y)}{\partial y}^T.$$

We restrict the presentation to the important special case in which the discretization of $C$ has the form

$$C^h = \{ x \in \mathbb{R}^n \mid x^l_i \leq x_i \leq x^u_i \text{ for } i = 1, \ldots, n \}$$

with lower and upper variable bounds $x^l, x^u \in \mathbb{R}^n$, whose entries may take on values of $\pm \infty$. Because the projection operator must respect the scalar product of $X$, it becomes

$$P_{C^h}(v) = \arg \min_{w \in C^h} \frac{1}{2} (w - v)^T M^h_X (w - v).$$

The optimization problem (4.14) can be solved efficiently using a few steps of the primal–dual active set strategy [30] or of a sequential homotopy method with a Euclidean projector and constant step size, which greatly simplifies because there are no equality constraints, just variable bounds. Both approaches yield the active set $V(v) := \{ i \in \mathbb{N} \mid P_{C^h}(v)_i \in \{ x^l_i, x^u_i \} \}$ of the projection (4.14), which we use for the discretized linearization of $F$ around $(x, y)$. Locally, i.e., for constant $V(v)$, the solution $w = P_{C^h}(v)$, the solution $w = P_{C^h}(v)$ solves the optimality conditions

$$\begin{pmatrix} M^h_X & I_{V(v)} \\ I_{V(v)}^T & 0 \end{pmatrix} \begin{pmatrix} w \\ \nu_{V(v)} \end{pmatrix} = \begin{pmatrix} M^h_X v_{V(v)} \\ x^l_{V(v)} \end{pmatrix},$$

where $I_{V(v)}$ are the columns of the $n$-by-$n$ identity matrix corresponding to the active indices in $V(v)$ and $\nu_{V(v)}$ is an appropriately dimensioned Lagrange multiplier.

It is now convenient to augment the discretization of $F$ (see equation (2.1)) by the projection conditions (4.15) for $v = \hat{x} - \Delta t \nabla_x L^\rho_h(x, y)$, which yields

$$M^h_X w + I_{V(v)} \nu_{V(v)} - M^h_X (\hat{x} - \Delta t \nabla_x L^\rho_h(x, y)) = 0, \quad (4.16a)$$

$$I_{V(v)}^T w - x^l_{V(v)} = 0, \quad (4.16b)$$

$$x - w = 0, \quad (4.16c)$$

$$y - \hat{y} - \Delta t \nabla_y L^\rho_h(x, y) = 0. \quad (4.16d)$$

PRECONDITIONED INEXACT ACTIVE-SET METHOD

11
Equation \([4.16c]\), which derives from the first component of \(F\) in \([2.4]\) with \(w = \text{R}_c h(v)\), can be directly eliminated. There are three disadvantages to equation \([4.16]\): First, equation \([4.16]\) is very badly scaled for large values of \(\Delta t\). Second, its Jacobian matrix is not symmetric. Third, in PDE-constrained optimization, the matrices \(M_X^h\) and \(M_Y^h\) are usually large and sparse, while their inverses (required for the gradients of \(L_h^\rho\)) are not sparse. All three can be remedied by appropriately premultiplying the rows of \([4.16]\) by \(\lambda\) and \(-\lambda M_Y^h\) and scaling of the projection Lagrange multiplier \(\hat{\nu}_{W(v)} := \lambda \nu_{W(v)}\) to obtain

\[
\begin{align*}
\lambda M_X^h (\mathbf{x} - \hat{\mathbf{x}}) + \frac{\partial L^\rho_c}{\partial x} (\mathbf{x}, \mathbf{y})^T + I_{W(v)} \hat{\nu}_{W(v)} &= 0, \\
-\lambda M_Y^h (\mathbf{y} - \hat{\mathbf{y}}) + \frac{\partial L^\rho_c}{\partial y} (\mathbf{x}, \mathbf{y})^T &= 0, \\
I_{W(v)}^T \mathbf{x} - \mathbf{x}_{1/n} &= 0.
\end{align*}
\]

Because we are not interested in the value of \(\hat{\nu}_{W(v)}\), it is actually more convenient to first setup the problem disregarding the variable bounds as

\[
\lambda M^h (\mathbf{z} - \hat{\mathbf{z}}) + \frac{\partial L^\rho_c}{\partial z} (\mathbf{z})^T = 0
\]

with the short notation \(\mathbf{z} = (\mathbf{x}, \mathbf{y})\) and \(M^h = \text{diag}(M_X^h, -M_Y^h)\) and then use \([4.17c]\) to eliminate the active variables. Equation \([4.18]\) has a symmetric Jacobian because it is the derivative of the proximal, augmented Lagrangian

\[
L_h^\rho(\mathbf{x}, \mathbf{y}; \hat{\mathbf{x}}, \hat{\mathbf{y}}) := \frac{1}{2} (\mathbf{x} - \hat{\mathbf{x}})^T M_X^h (\mathbf{x} - \hat{\mathbf{x}}) - \frac{1}{2} (\mathbf{y} - \hat{\mathbf{y}})^T M_Y^h (\mathbf{y} - \hat{\mathbf{y}}) + L_h^\rho (\mathbf{x}, \mathbf{y}).
\]

For the linearization around \((\mathbf{x}, \mathbf{y})\), we remark that with \(G := \frac{\partial L^\rho_c}{\partial z}(\mathbf{x})\) and \(H := \frac{\partial^2 L^\rho_c}{\partial z^2}(\mathbf{x}, \mathbf{rho}(\mathbf{x}) + \mathbf{y})\) the derivatives of the augmented Lagrangian \(L_h^\rho\) can be expressed in the respective derivatives of the unaugmented Lagrangian \(L_h^\rho\) according to

\[
\frac{\partial L^\rho_c}{\partial x}(\mathbf{x}, \mathbf{y}) = \frac{\partial L^\rho_c}{\partial x}(\mathbf{x}, \rho c_h(\mathbf{x}) + \mathbf{y}), \quad \frac{\partial^2 L^\rho_c}{\partial x^2}(\mathbf{x}, \mathbf{y}) = \rho c_h(\mathbf{y}) + H + \rho G^T M_Y^h G, \quad \frac{\partial^2 L^\rho_c}{\partial x \partial y}(\mathbf{x}, \mathbf{y}) = M_Y^h G, \quad \frac{\partial^2 L^\rho_c}{\partial y \partial x}(\mathbf{x}, \mathbf{y}) = 0.
\]

This leads to the linearized system

\[
\begin{pmatrix}
\lambda M_X^h + H + \rho G^T M_Y^h G & G^T M_Y^h \\
M_Y^h & -\lambda M_Y^h
\end{pmatrix}
\begin{pmatrix}
\Delta \mathbf{x} \\
\Delta \mathbf{y}
\end{pmatrix}
= -\begin{pmatrix}
b_1 \\
b_2
\end{pmatrix},
\]

where \(b_1 := \lambda M_X^h (\mathbf{x} - \hat{\mathbf{x}}) + \frac{\partial L^\rho_c}{\partial x}(\mathbf{x}, \rho c_h(\mathbf{x}) + \mathbf{y})\) and \(b_2 := -\lambda M_Y^h (\mathbf{y} - \hat{\mathbf{y}}) + M_Y^h c_h(\mathbf{x})\). To further reduce issues of fill-in and bad scaling, we can use a nonlinear transformation \([45]\) Sec. 5.1] and solve instead the linear system

\[
\begin{pmatrix}
\lambda M_X^h + H & G^T M_Y^h \\
M_Y^h & -\frac{\lambda}{1 + \rho \lambda} M_Y^h
\end{pmatrix}
\begin{pmatrix}
\Delta \mathbf{x} \\
\Delta \mathbf{y}
\end{pmatrix}
= -\begin{pmatrix}
b_1 \\
b_2
\end{pmatrix},
\]

together with the nonlinear backtransformation

\[
\Delta \mathbf{y} = \frac{1}{1 + \rho \lambda} (\Delta \hat{\mathbf{y}} + \rho (M_Y^h)^{-1} b_2) = \frac{1}{1 + \rho \lambda} (\Delta \hat{\mathbf{y}} - \rho \lambda (\mathbf{y} - \hat{\mathbf{y}}) + \rho c_h(\mathbf{x})).
\]

We remark that this reformulation might require an additional computation of a Riesz representation of \(b_2\) via solving an additional linear system with \(M_Y^h\) if the
computational evaluation of the constraint function is only available with implicit premultiplication with \( M_H^b \) as \( M_H^{bc_b}(x) \).

Before solving (4.19), we need to modify it to accommodate for the current active set \( \mathcal{W}(v) \) by replacing the \( i \)-th row of the system matrix with an entry of one on the diagonal and zeros on all off-diagonal entries and replacing the \( i \)-th component of \( b_i \) by \( x_i - x_i^v \). Obviously, this masking of rows destroys the symmetry of the system matrix, but can be remedied: after splitting into \( n_a \) active and \( n_i \) inactive variables and applying a suitable symmetric permutation, the system has the form

\[
\begin{pmatrix}
I_{n_a} & 0 & \lambda \tilde{M}_X^b + \tilde{H} & 0 \\
* & \tilde{M}_Y^b \tilde{G} & -\tilde{G}^T M_V^b & \Delta x^a \\
* & \tilde{M}_Y^b \tilde{G} & -\tilde{G}^T M_V^b & \Delta x^i \\
* & 0 & \tilde{M}_Y^b \tilde{G} & -\tilde{G}^T M_V^b \\
\end{pmatrix}
\begin{pmatrix}
\Delta x^a \\
\Delta x^i \\
\Delta \tilde{y} \\
\end{pmatrix} =
\begin{pmatrix}
b_i^a \\
b_i^i \\
\frac{1}{1 + \rho} b_2 \\
\end{pmatrix},
\]

where \( \tilde{G} \) comprises only the columns of \( G \) that belong to inactive variables, and \( \tilde{M}_X^b \) and \( \tilde{H} \) comprise only the rows and columns that belong to inactive variables. When a symmetric Krylov-subspace method is started with an initial guess that solves the first block row exactly, then the generated Krylov subspace will only depend on the symmetric 2-by-2 block in the lower right and symmetric Krylov-subspace methods can safely be used.

Hence, preconditioners are only required for the symmetric part of (4.20).

5. Preconditioned Iterative Methods for Double Saddle-Point Systems.

To derive efficient preconditioners, it is important to exploit additional problem structure. We take interest here in a special property of a large class of PDE-constrained optimal control problems:

\[
\begin{align*}
\min & \quad \frac{1}{2} \| u - u_d \|_V^2 + \frac{\gamma}{2} \| q - q_d \|_U^2 \\
\text{over} & \quad (q, u) \in C_Q \times U, \\
\text{s.t.} & \quad c((u, q)) = c((u, 0)) + c_q((0, 0))q = 0,
\end{align*}
\]

in which the matrix \( H \) is of block diagonal form, because the control and state variables are separated in the objective function and the control enters the (possibly nonlinear) state equation only affine linearly. We assume that \( X = Q \times U \) comprises controls \( q \in C_Q \subset Q \) and states \( u \in C_U = U \) with a tracking term in a space \( V \) with \( U \hookrightarrow V \hookrightarrow U^* \), while \( y \in Y \) are the adjoint variables. We can model control bounds in \( C_Q \), whose discretization \( C_Q^b \) is of the form (4.13).

Following the obvious extension of variable naming above, a symmetric permutation of (4.20) leads to

\[
\begin{pmatrix}
I_{n_a} & 0 & \lambda \tilde{M}_X^b + \tilde{H}_Q & 0 \\
* & \tilde{M}_Y^b \tilde{G}_Q & \tilde{G}^T M_Y^b & \tilde{G}^T M_V^b \\
* & \tilde{M}_Y^b \tilde{G}_Q & -\tilde{G}^T M_Y^b & \tilde{M}_Y^b G_U \\
* & 0 & \tilde{M}_Y^b \tilde{G}_Q & \tilde{M}_Y^b \tilde{G}_Q \\
\end{pmatrix}
\begin{pmatrix}
\Delta q^a \\
\Delta q^i \\
\Delta \tilde{y} \\
\Delta u \\
\end{pmatrix} =
\begin{pmatrix}
b_i^a \\
b_i^i \\
\frac{1}{1 + \rho} b_2 \\
\end{pmatrix}.
\]

In this section we provide some theory of preconditioning matrices of the form

\[
A = \begin{pmatrix}
A_1 & B_1^T & 0 \\
B_1 & -A_2 & B_2^T \\
0 & B_2 & A_3
\end{pmatrix},
\]

which are frequently referred to as double saddle-point systems. This is important, as the systems we are required to solve in this paper are of the form (5.3). Specifically,
after (trivially) eliminating the first block-row in \((5.2)\), we obtain a system of the form \((5.3)\) from the lower right 3-by-3 blocks of \((5.2)\). It is important that the proposed preconditioners are robust with respect to the augmented Lagrangian coefficient \(\rho > 0\) and the proximity parameter \(\lambda\), which may typically vary between \(10^{-12}\) and \(10^{1}\).

We highlight that there has been much previous work on preconditioners for double saddle-point systems, see for example \([20, 37, 1, 55]\). In particular \([55]\) provides a comprehensive description of eigenvalues of preconditioned double saddle-point systems on the continuous level (i.e., by the operators involved). What follows in this section is an analysis for discretized double saddle-point systems, inspired by the logic of the proof given in \([37, \text{Thm. 4}]\).

For our forthcoming analysis we will make use of the following result, which concerns eigenvalues for generalized saddle-point systems preconditioned by a block-diagonal matrix. The bounds described in the following theorem can be found elsewhere in the literature: for instance, the lower bounds on the negative and positive eigenvalues were found in \([3, \text{Cor. 1}]\), and the upper bounds on the negative and positive eigenvalues are a consequence of \([54, \text{Lem. 2.2}]\); see also \([39, \text{Thm. 4}]\).

**Theorem 5.1.** Let

\[
\mathcal{A}_2 = \begin{pmatrix} A_1 & B^T \\ B & -A_2 \end{pmatrix}, \quad \mathcal{P}_2 = \begin{pmatrix} A_1 & 0 \\ 0 & S_1 \end{pmatrix},
\]

where \(A_1, S_1 = A_2 + BA_1^{-1}B^T\) are assumed to be symmetric positive definite, and \(A_2\) is assumed to be symmetric positive semi-definite. Then all eigenvalues of \(\mathcal{P}_2^{-1}\mathcal{A}_2\) satisfy

\[
\mu(\mathcal{P}_2^{-1}\mathcal{A}_2) \in \left[-1, \frac{3}{2}(1 - \sqrt{5})\right] \cup \left[1, \frac{3}{2}(1 + \sqrt{5})\right].
\]

We now analyze a block-diagonal preconditioner for matrix systems of the form \((5.3)\), in the simplified setting that \(A_3 = 0\), using the logic of \([37, \text{Thm. 4}]\).

**Theorem 5.2.** Let

\[
\mathcal{A}_0 = \begin{pmatrix} A_1 & B_1^T & 0 \\ B_1 & -A_2 & B_2^T \\ 0 & B_2 & 0 \end{pmatrix}, \quad \mathcal{P}_D = \begin{pmatrix} A_1 & 0 & 0 \\ 0 & S_1 & 0 \\ 0 & 0 & S_2 \end{pmatrix},
\]

where \(A_1, S_1 = A_2 + B_1A_1^{-1}B_1^T, S_2 = B_2S_1^{-1}B_2^T\) are assumed to be symmetric positive definite, and \(A_2\) is assumed to be symmetric positive semi-definite. The matrix \(B_2\) must therefore have at least as many columns as rows, and have full row rank. Then all eigenvalues of \(\mathcal{P}_D^{-1}\mathcal{A}_0\) satisfy:

\[
\mu(\mathcal{P}_D^{-1}\mathcal{A}_0) \in \left[-\frac{1}{2}(1 + \sqrt{5}), 2\cos\left(\frac{5\pi}{4}\right)\right] \cup \left[-1, \frac{1}{2}(1 - \sqrt{5})\right] \cup \left[2\cos\left(\frac{5\pi}{4}\right), \frac{1}{2}(\sqrt{5} - 1)\right] \cup \left[1, 2\cos\left(\frac{5\pi}{4}\right)\right],
\]

which to 3 decimal places are \([-1.618, -1.247] \cup [-1, -0.618] \cup [0.445, 0.618] \cup [1, 1.802]\).

**Proof.** Examining the associated eigenproblem

\[
\begin{pmatrix} A_1 & B_1^T & 0 \\ B_1 & -A_2 & B_2^T \\ 0 & B_2 & 0 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \mu \begin{pmatrix} A_1 & 0 & 0 \\ 0 & S_1 & 0 \\ 0 & 0 & S_2 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix},
\]

we obtain that

\[
A_1x_1 + B_1^Tx_2 = \mu A_1x_1, \quad B_1x_1 - A_2x_2 + B_2^Tx_3 = \mu S_1x_2, \quad B_2x_2 = \mu S_2x_3.
\]
We now prove the result by contradiction, that is we assume there exists an eigenvalue outside the stated intervals. From (5.4a), we see that

\[ pA_1x_1 + B_1^Tx_2 = 0 \quad \Rightarrow \quad px_1 = -A_1^{-1}B_1^Tx_2, \quad (5.5) \]

where \( p = 1 - \mu \neq 0 \) by assumption. Substituting (5.5) into (5.4b) tells us that

\[
0 = p \left[ B_1x_1 - (1 + \mu)A_2x_2 + B_2^Tx_3 - \mu B_1A_1^{-1}B_1^Tx_2 \right]
= -B_1A_1^{-1}B_1^Tx_2 - p(1 + \mu)A_2x_2 + pB_2^Tx_3 - \mu pB_1A_1^{-1}B_1^Tx_2
= -[qB_1A_1^{-1}B_1^T + rA_2]x_2 + pB_2^Tx_3, \quad (5.6)
\]

where \( q = 1 + \mu p = 1 + \mu - \mu^2 \neq 0, r = p(1 + \mu) = 1 - \mu^2 \neq 0 \) by assumption. Now, for the cases \( \mu \in (-\infty, -1), \mu \in (\frac{1}{2}(1 - \sqrt{5}), 1), \) and \( \mu \in (\frac{1}{2}(1 + \sqrt{5}), +\infty), \) \( q \) and \( r \) have the same signs (negative, positive, and negative, respectively), so \( qB_1A_1^{-1}B_1^T + rA_2 \) is a definite (and hence invertible) matrix. Thus, in these cases, (5.6) tells us that

\[ x_2 = p[qB_1A_1^{-1}B_1^T + rA_2]^{-1}B_2^Tx_3, \]

which we may then substitute into (5.4c) to yield that

\[ 0 = pB_2[qB_1A_1^{-1}B_1^T + rA_2]^{-1}B_2^Tx_3 - \mu B_2[1 + A_1^{-1}B_1^T + A_2]^{-1}B_2^Tx_3. \quad (5.7) \]

We now highlight that \( \mu \neq 0 \); otherwise (5.7) would read that

\[ 0 = B_2[1 + A_1^{-1}B_1^T + A_2]^{-1}B_2^Tx_3 = S_2x_3 \quad \Rightarrow \quad x_3 = 0, \]

which means that

\[
\begin{pmatrix}
A_1 & B_1^T \\
B_1 & -A_2
\end{pmatrix}
\begin{pmatrix}
x_1 \\
x_2
\end{pmatrix} = \mu
\begin{pmatrix}
A_1 & 0 \\
0 & S_1
\end{pmatrix}
\begin{pmatrix}
x_1 \\
x_2
\end{pmatrix},
\]

holds (along with \( B_2x_2 = 0 \)). Applying Thm. 5.1 then gives that \( \mu \in [-1, \frac{1}{2}(1 - \sqrt{5})] \cup [\frac{1}{2}(1 + \sqrt{5}), 1], \) yielding a contradiction. Using that \( \mu \neq 0, \) as well as that \( p \neq 1 \) by assumption, we may divide (5.7) by \( p \mu \) to obtain that

\[
0 = B_2[\mu qB_1A_1^{-1}B_1^T + \mu rA_2]^{-1}B_2^Tx_3 - B_2[pB_1A_1^{-1}B_1^T + pA_2]^{-1}B_2^Tx_3
= B_2[sB_1A_1^{-1}B_1^T + tA_2]^{-1}B_2^Tx_3 - B_2[pB_1A_1^{-1}B_1^T + pA_2]^{-1}B_2^Tx_3,
\]

where \( s = \mu q = \mu + \mu^2 - \mu^3 \) and \( t = \mu r = \mu - \mu^3. \) As the situation \( x_3 = 0 \) reduces the problem to that of Thm. 5.1 where \( \mu \) is contained within a subset of the intervals claimed here, we may reduce the analysis to the case \( x_3 \neq 0 \) and write

\[ 0 = x_3^TB_2[(sB_1A_1^{-1}B_1^T + tA_2]^{-1} - [pB_1A_1^{-1}B_1^T + pA_2]^{-1}) B_2^Tx_3 =: x_3^T\Psi x_3, \quad (5.8) \]

with both \( B_1A_1^{-1}B_1^T \) and \( A_2 \) symmetric positive semi-definite. We now consider different cases (we have already excluded the possibility that \( \mu = 0 \)):

- \( \mu \in (-\infty, -\frac{1}{2}(1 + \sqrt{5})) : \) Here \( p, s, t > 0, \) such that \( s > p, t > p. \) Hence \( sB_1A_1^{-1}B_1^T + tA_2 > pB_1A_1^{-1}B_1^T + pA_2 \) (meaning \( [sB_1A_1^{-1}B_1^T + tA_2] - [pB_1A_1^{-1}B_1^T + pA_2] \) is positive definite), and \( \Psi \) is negative definite. This yields a contradiction with (5.8), so there is no \( \mu \in (-\infty, -\frac{1}{2}(1 + \sqrt{5})). \)
\[ \mu \in (2 \cos(\frac{5\pi}{6}), -1) : \text{Here } p, s, t > 0, \text{ such that } s < p, t < p. \text{ Hence } sB_1A_1^{-1}B_1^T + tA_2 < pB_1A_1^{-1}B_1^T + pA_2 \text{ (meaning } [sB_1A_1^{-1}B_1^T + tA_2] - [pB_1A_1^{-1}B_1^T + pA_2] \text{ is negative definite), and } \Psi \text{ is positive definite. Similarly to above, this yields a contradiction.} \]

\[ \mu \in (\frac{1}{2}(1 - \sqrt{5}), 0) : \text{Here, } p, s, t > 0, \text{ such that } s < p, t < p. \text{ Hence } sB_1A_1^{-1}B_1^T + tA_2 < pB_1A_1^{-1}B_1^T + pA_2, \text{ and } \Psi \text{ is positive definite, yielding a contradiction.} \]

\[ \mu \in (0, 2 \cos(\frac{3\pi}{4})) : \text{Here } p, s, t > 0, \text{ such that } s < p, t < p. \text{ Hence } sB_1A_1^{-1}B_1^T + tA_2 > pB_1A_1^{-1}B_1^T + pA_2, \text{ and } \Psi \text{ is negative definite, yielding a contradiction.} \]

\[ \mu \in (2 \cos(\frac{\pi}{4}), +\infty) : \text{Here } p, s, t > 0, \text{ such that } s < p, t < p. \text{ Hence } sB_1A_1^{-1}B_1^T + tA_2 \text{ and } pB_1A_1^{-1}B_1^T + pA_2 \text{ are both negative definite, such that } sB_1A_1^{-1}B_1^T + tA_2 < pB_1A_1^{-1}B_1^T + pA_2. \text{ Therefore } [sB_1A_1^{-1}B_1^T + tA_2]^{-1} > [pB_1A_1^{-1}B_1^T + pA_2]^{-1}, \text{ and } \Psi \text{ is positive definite, yielding a contradiction.} \]

The result is thus proved by contradiction. \( \square \)

Making the proof of the proof of Thm. 5.2 we now briefly analyze the analogous block-diagonal preconditioner for (5.3), for the more general case that \( A_3 \) is symmetric positive semi-definite. This guarantees a fixed rate of convergence for preconditioned MINRES applied to systems of the form (5.3) with properties stated below.

**Theorem 5.3.** Let

\[ \mathcal{P}_D = \begin{pmatrix} A_1 & 0 & 0 \\ 0 & S_1 & 0 \\ 0 & 0 & S_2 \end{pmatrix}, \]

with \( A \) as defined in (5.3), where \( A_1, S_1 = A_2 + B_1A_1^{-1}B_1^T, S_2 = A_3 + B_2A_1^{-1}B_2^T \) are assumed to be symmetric positive definite, and \( A_2, A_3 \) are assumed to be symmetric positive semi-definite. Then all eigenvalues of \( \mathcal{P}_D^{-1}A \) satisfy:

\[ \mu (\mathcal{P}_D^{-1}A) \in \left[ -\frac{1}{2}(1 + \sqrt{5}), \frac{1}{2}(1 - \sqrt{5}) \right] \cup \left[ 2 \cos \left( \frac{5\pi}{6} \right), 2 \cos \left( \frac{\pi}{4} \right) \right], \]

which to 3 decimal places are \( [-1.618, -0.618] \cup [0.445, 1.802] \).

**Proof.** Simple algebra tells us that (5.4a), (5.4b) hold, along with

\[ B_2x_2 + A_3x_3 = \mu S_2x_3. \]

(5.9)

Applying the working of Thm. 5.2 tells us that \( x_2 = \rho [qB_1A_1^{-1}B_1^T + rA_2]^{-1}B_2^T x_3 \) whenever \( \mu \in (-\infty, -1) \cup \left( \frac{1}{2}(1 - \sqrt{5}), 1 \right) \cup \left( \frac{1}{2}(1 + \sqrt{5}), +\infty \right) \), so using (5.9):

\[ 0 = pB_2[qB_1A_1^{-1}B_1^T + rA_2]^{-1}B_2^T x_3 - \mu B_2[B_1A_1^{-1}B_1^T + A_2]^{-1}B_2^T x_3 + pA_3x_3. \]

(5.10)

We may again argue that \( \mu \neq 0; \) if it were then (5.10) would inform us that \( x_3 = 0 \), so the problem reduces to that of Thm. 5.1. As \( \mu \neq 0 \) and \( p \neq 1 \), we may divide (5.10) by \( \mu p \) and pre-multiply by \( x_3^T \) to obtain:

\[ 0 = x_3^T B_2 \left( [sB_1A_1^{-1}B_1^T + tA_2]^{-1} - [pB_1A_1^{-1}B_1^T + pA_2]^{-1} \right) B_2^T x_3 + \frac{1}{\mu} x_3^T A_3 x_3 \]

\[ =: x_3^T \left( \Psi + \frac{1}{\mu} A_3 \right) x_3. \]

(5.11)

Considering different cases once again (we have already excluded the possibility that \( \mu = 0 \)), we may demonstrate contradictions with (5.11).
PRECONDITIONED INEXACT ACTIVE-SET METHOD

- \( \mu \in (-\infty, -\frac{1}{2}(1 + \sqrt{5})) \): As in Thm. 5.2 we have that \( \Psi \) is negative definite, and we also know that \( \frac{1}{\mu} A_3 \) is negative semi-definite. Therefore \( \Psi + \frac{1}{\mu} A_3 \) is negative definite, yielding a contradiction with (5.1).
- \( \mu \in (\frac{1}{2}(1 - \sqrt{5}), 0) \): Here \( \Psi \) is negative definite, \( \frac{1}{\mu} A_3 \) is negative semi-definite.
- \( \mu \in (0, 2\cos(\frac{3\pi}{7})) \): Here \( \Psi \) is positive definite, \( \frac{1}{\mu} A_3 \) is positive semi-definite.
- \( \mu \in (2\cos(\frac{\pi}{7}), +\infty) \): Here \( \Psi \) is positive definite, \( \frac{1}{\mu} A_3 \) is positive semi-definite.

The result is again proved by excluding the remaining intervals by contradiction. \( \square \)

**Remark 1.** We note that the bounds of Thm. 5.3 match those obtained in Thm. 3.4 of the recent preprint [8], using a different structure of proof. In this interesting paper, the authors also demonstrate the effect of approximating the blocks \( A_1, S_1, S_2 \) within the block-diagonal preconditioner, further highlighting the effectiveness of this strategy. We also highlight [8, Thm. 3.3], which analyzes the case \( A_2 = 0 \).

Along with block-diagonal preconditioners for (5.3), we may construct block-triangular preconditioners, stated and analyzed in the simple result below.

**Theorem 5.4.** Let

\[
P_L = \begin{pmatrix} A_1 & 0 & 0 \\ B_1 & -S_1 & 0 \\ 0 & B_2 & S_2 \end{pmatrix}, \quad P_U = \begin{pmatrix} A_1 & B_1^T & 0 \\ 0 & -S_1 & B_2^T \\ 0 & 0 & S_2 \end{pmatrix},
\]

with \( A \) as defined in (5.3), where \( A_1, S_1 = A_2 + B_1 A_1^{-1} B_1^T, S_2 = A_3 + B_2 S_1^{-1} B_2^T \) are assumed to be invertible. Then all eigenvalues of \( P_L^{-1} A \) and \( P_U^{-1} A \) are equal to 1.

**Proof.** It may easily be verified that

\[
P_L^{-1} A = \begin{pmatrix} I & A_1^{-1} B_1^T & 0 \\ 0 & I & -S_1^{-1} B_2^T \\ 0 & 0 & I \end{pmatrix}, \quad A P_U^{-1} = \begin{pmatrix} I & 0 & 0 \\ B_1 A_1^{-1} & I & 0 \\ 0 & -B_2 S_1^{-1} & I \end{pmatrix},
\]

which gives the result (using similarity of the matrices \( P_U^{-1} A \) and \( A P_U^{-1} \)). \( \square \)

We note Thm. 5.4 makes no assumptions on the properties of \( B_2 \), or the positive definiteness of \( A_1, S_1, S_2 \), unlike Thms. 5.2 and 5.3. However, we note the limitations of Thm. 5.4 with a block-triangular preconditioner, diagonalizability of the preconditioned system is not given, and implementing this preconditioner requires a nonsymmetric iterative solver for which the eigenvalue distribution does not guarantee a fixed convergence rate.

**6. Implementation Details.** Among all problems of the form (5.1), we focus our attention in the remainder to a family of nonlinear and possibly badly conditioned benchmark problems of the specific form (cf. [30, 18]):

\[
\begin{align*}
\text{min} \quad & \frac{1}{2} \int_\Omega |u - u_d|^2 + \frac{\gamma}{2} \int_\Omega |q|^2 \\
\text{s.t.} \quad & \nabla \cdot \left( [a + b |u|^2] \nabla u \right) = q, \quad q_l \leq q \leq q_u,
\end{align*}
\]

(6.1)

where \( \Omega \subset \mathbb{R}^d, d = 2, 3, \) is a bounded domain with Lipschitz boundary and \( a, b, \gamma > 0 \) with control bounds \( q_l, q_u \in L^r(\Omega), r \in (2, \infty), \) and a tracking target function \( u_d \in L^2(\Omega). \) The difficulty of problem (6.1) can be tuned by the scalar parameters: smaller \( \gamma \) and \( a \) result in worse conditioning of the problem, while larger \( b \) increases the nonlinearity. We caution that the interplay with the objective function is nontrivial: small values of \( a \) in combination with large values of \( b \) might lead to an optimal solution
with small $|u|$ over $\Omega$, eventually resulting in less nonlinearity in the neighborhood of the optimal solution. We focus on $\gamma = 10^{-6}$, $a = 10^{-2}$, $b = 10^2$, which was experienced as the most difficult instance in the numerical results in [48]. All remaining problem data was set to the values in [48]. There is some freedom in choosing $Y$ and formulating the weak form of the PDE either using $Y = H^{-1}(\Omega) = U^*$ and the duality pairing or using $Y = H_0^1(\Omega) = U$ and the inner product. Both approaches lead to the same discretized systems when the Riesz representation operator is used correctly.

Consider the linear system (5.2), with the first block row eliminated. Then, we arrive at a double saddle-point system in the notation of the previous section, with

$$A_1 = \lambda \tilde{M}_Q^h + \tilde{H}_Q, \quad A_2 = \frac{\lambda}{1+\rho \lambda} M_Y^h, \quad A_3 = \lambda M_Y^h + H_U, \quad B_1 = M_Y^h \tilde{G}_Q, \quad B_2 = G_Y^h M_Y^h,$$

$$S_1 = \frac{\lambda}{1+\rho \lambda} M_Y^h + B_1 (\lambda \tilde{M}_Q^h + \tilde{H}_Q)^{-1} B_1^T, \quad S_2 = \lambda M_Y^h + H_U + B_2 S_1^{-1} B_2^T.$$

In order to efficiently apply block preconditioners derived above, we need to approximately apply the inverse operations of $A_1$, $S_1$, $S_2$ to generic vectors, in a computationally efficient way. Numerically, we compare a number of increasingly efficient preconditioner choices, which we elaborate on in more detail below:

1. **Direct** sparse decomposition of $A$ without the use of Krylov space solver, which can be considered as a preconditioner that leads to convergence in one step.
2. **Exact Schur complement** block-diagonal preconditioner with sparse decomposition of the Schur complements $A_1$, $S_1$, $S_2$.
3. **Matching Schur complement** block-diagonal preconditioner with sparse decomposition of $A_1$ and $S_1$ in combination with a matching approach for $S_2$ using sparse decompositions for the factors of the multiplicative approximation of $S_2$.
4. **AMG$[S_1]$ matching Schur complement** block-diagonal preconditioner, which coincides with the matching Schur complement preconditioner, except using an Algebraic Multigrid (AMG) approximation for $S_1^{-1}$ instead of a direct decomposition.
5. **Decomposition-free Schur complement** block-diagonal preconditioner with completely decomposition-free approximations of all Schur complements $A_1$, $S_1$, $S_2$ based on matching for $S_2$. The preconditioner can be implemented using publicly available parallelizable preconditioners.
6. **Block-triangular** decomposition-free Schur complement preconditioner. In contrast to the previous preconditioners, this preconditioner must be used with a nonsymmetric solver such as GMRES instead of MINRES because it is a lower block-triangular and not a symmetric preconditioner.

Each preconditioner in the list above serves as the baseline for the next in terms of number of nonlinear iterations, which are expected to grow from top to bottom, and the resulting computation time. We used FEniCS [15, 35] to discretize problem (6.1) with P1 finite elements and implemented all preconditioners in PETSc [17, 46, 3].

### 6.1. Exact Schur complement preconditioner.

The matrix $A_1$ is a scaled finite element (FE) mass matrix and can easily be assembled. The first term in $S_1$ is a scaled FE stiffness matrix. For the second term in $S_1$, we first note that $B_1$ is a FE mass matrix, so that the second term simplifies to a scaled FE mass matrix. We remark that the stiffness term dominates $S_1$ for large $\lambda$, while the mass matrix term dominates for small $\lambda$. We can use direct sparse decompositions of $A_1$ and $S_1$ to compute the action of their inverses to high accuracy. Regarding $S_2$, we first note that $B_2$ is a nonsymmetric FE matrix for the linearized elliptic PDE operator with respect to the state. The direct assembly of $S_2$ is prohibitive because $S_2$ is a
dense matrix. However, the action of $S_2^{-1}$ can be computed by unrolling the Schur complement through a direct sparse decomposition of the sparse block matrix

$$
\begin{pmatrix}
\lambda M_U^h + H_U & B_2 \\
B_2^T & -S_1
\end{pmatrix}.
$$

We investigate this preconditioner purely to assess the quality of the Schur complement approach in general and as a baseline for the following Schur complement approximations. We discourage the use of the exact Schur complement preconditioner for the solution of (6.1).

6.2. Matching Schur complement preconditioner. We now address the approximation of the most delicate Schur complement $S_2$ by a matching strategy, which has found considerable utility for PDE-constrained optimization problems [12, 44], including those with additional bound constraints [40, 13]. A key challenge is that inverses of matrix sums are much harder to apply than inverses of matrix products.

For the problem at hand, the second Schur complement has the explicit form

$$S_2 = \lambda M_U^h + H_U + B_2 S_1^{-1} B_2^T = \lambda M_U^h + H_U + B_2 \left[(1 + \rho \lambda)^{-1} \lambda M_U^h + (\lambda + \gamma)^{-1} M_Q^h\right]^{-1} B_2^T,$$

with $M_Q^h$ a FE mass matrix. We now approximate $S_2$ by a product $DS_1^{-1}D^T$, where

$$D = \alpha_Y M_U^h + \alpha_Q M_Q^h + B_2 \text{ s.t. } \left(\alpha_Y M_Y^h + \alpha_Q M_Q^h\right) S_1^{-1} \left(\alpha_Y M_Y^h + \alpha_Q M_Q^h\right) \approx \lambda M_U^h + H_U,$$

and we wish to match the factors $\alpha_Y, \alpha_Q > 0$. As $M_U^h = M_V^h$ and $H_U = M_Q^h + N^h$, where $N^h$ contains nonlinear terms from the PDE operators, a computationally efficient choice is to neglect the effect of $N^h$, and match the terms in $M_V^h, M_Q^h$ separately. This heuristic strategy means we wish to select

$$\left(\alpha_Y M_Y^h\right) \left[(1 + \rho \lambda)^{-1} \lambda M_Y^h\right]^{-1} \left(\alpha_Y M_Y^h\right) = \lambda M_Y^h \quad \Rightarrow \quad \alpha_Y = \frac{\lambda}{\sqrt{1+\rho \lambda}};$$

$$\left(\alpha_Q M_Q^h\right) \left[(\lambda + \gamma)^{-1} M_Q^h\right]^{-1} \left(\alpha_Q M_Q^h\right) = M_Q^h \quad \Rightarrow \quad \alpha_Q = \frac{1}{\sqrt{\lambda + \gamma}}.$$

Note that we can readily assemble $D = \lambda(1 + \rho \lambda)^{-1/2} M_U^h + (\lambda + \gamma)^{-1/2} M_Q^h + B_2$ and use a direct sparse decomposition of $D$ to approximate $S_2^{-1}$ with $S_2^{-1} = D^{-T} S_Y D^{-1}$.

6.3. AMG[$S_1$] matching Schur complement preconditioner. This approach extends the matching Schur complement preconditioner by using an AMG preconditioner to approximate $S_1$. We use hypre/BoomerAMG [18, 27] with two sweeps of a V-cycle and one Jacobi iteration for each pre- and post-smoothing step.

6.4. Decomposition-free Schur complement preconditioner. This preconditioner further extends the AMG[$S_1$] matching Schur complement preconditioner. The matrix $A_1$ is a scaled FE mass matrix, so may be well approximated by its diagonal [57]. The use of a nested CG solver for $A_1$ would require the use of a flexible outer Krylov space solver such as Flexible GMRES [51] due to the nonlinearity of CG. Instead, we apply a fixed number of 15 linear Chebyshev semi-iterations (see [24]) on the diagonally scaled $A_1$ with the optimal spectral bounds $[\frac{1}{2}, 2]$ (2D) and $[\frac{1}{2}, 2]$ (3D) from [57], which are independent of the value of $\lambda$. Finally we also employ an AMG preconditioner for approximating the inverses of $D$ and $D^T$. We use hypre/BoomerAMG again with 4 V-cycle sweeps with two Jacobi sweeps for pre- and post-smoothing and a fixed relaxation weight of 0.7. It is crucial to disable CF-relaxation for BoomerAMG to work correctly for application of the transposed preconditioner.
Fig. 7.1. Krylov solver iterations: minres with the exact Schur complement preconditioner. The case $N = 640$ is omitted due to excessive runtime.

Fig. 7.2. Krylov solver iterations: minres with the matching Schur complement preconditioner.

Fig. 7.3. Krylov solver iterations: minres with the decomposition-free Schur complement preconditioner.
Fig. 7.4. *Krylov solver iterations: GMRES with the block-triangular decomposition-free Schur complement preconditioner.*

Fig. 7.5. *Krylov solver iterations: Comparison of different variants for $N = 320$.*

Fig. 7.6. *Krylov solver iterations: Comparison of different variants for $N = 640$.*
**Fig. 7.7.** Comparison of wall clock time vs. iterations of different variants for $N = 640$.

**Fig. 7.8.** Weak scaling results for 2D case using the block-diagonal decomposition free preconditioner and minres. We show the average over the last 10 iterations on the finest grid level.

**Fig. 7.9.** Result for the 3D test case for $N = 160$. The unit cube is cut in half in the $X/Y$ plane. On the left we see isosurfaces of the optimal control and on the right isosurfaces of the optimal state.

| Number of processors | 1 | 4 | 16 | 64 |
|----------------------|---|---|----|----|
| $N$                  | 320 | 640 | 1,280 | 2,560 |
| Degrees of freedom   | 309,123 | 1,232,643 | 4,922,883 | 19,676,163 |

*Table 7.1: Correspondence of number of processors and discretization for the weak scaling experiment.*
7. Numerical Results. We solve problem (6.1) with the sequential homotopy method with the algorithmic parameters from [48], with the changes described above and with the Schur complement approximations of Sec. 6, using block-diagonally preconditioned MINRES and block-lower trianlarly preconditioned GMRES. A maximum number of 100 Krylov method iterations is used. When there is no convergence of within this margin, it is an indication that the current matrix $S_2$ might be indefinite. In this case, the nonlinear step is flagged as failed and the sequential homotopy method increases $\lambda$, which eventually renders $S_2$ positive definite. For the simplified semismooth Newton step, we prescribe the same number of Krylov method iterations that were adaptively determined by the standard termination criterion in the preceding semismooth Newton step. When a sequential homotopy iteration fails due to excess of Krylov method iterations or due to violation of the monotonicity test, we mark the iteration with a black cross in the following figures.

7.1. Preconditioner comparison for the 2D case. We start with the 2D instances. In Fig. 7.1 we see that the number of MINRES iterations per iteration of the sequential homotopy method stays moderately low (20-40 iterations) most of the time. Close to the solution, the number of iterations rises to about 60. This shows that the method saves numerical effort in the linear algebra part when being far away from the solution. The number of nonlinear iterations increases considerably when going from $N = 320$ to $N = 640$, which we attribute to the steep boundary layer of the optimal state, which is not faithfully resolved on meshes smaller than $N \leq 160$.

Compared to Fig. 7.1, we see in Fig. 7.2 that the matching approach slightly increases the required number of MINRES iterations, while the number of nonlinear iterations stays roughly the same. In contrast to the exact Schur complement preconditioner, also the case $N = 640$ can be solved in an acceptable amount of time.

Using the AMG$[S_1]$ and decomposition-free Schur complement preconditioners result in qualitatively very similar behavior, so we just display the latter in Fig. 7.3. This exhibits the efficiency and robustness of the solver for a range of problem sizes.

Using the block-triangular version of the decomposition-free Schur complement preconditioner seems to deliver a more robust preconditioner with fewer fluctuations in the number of iterations. In particular, the required iterations in the last few iterations is almost cut in half (see Fig. 7.4).

When it comes to runtime, there is a clear benefit of using the decomposition-free Schur complement preconditioners, which somewhat surprisingly even outperform the use of direct linear algebra even for the 2D problem on a reasonably fine grid (see Fig. 7.7), even though it requires more outer nonlinear iterations. This feature can be attributed to the fact that while the linear systems of the simplified semismooth Newton step must be decomposed again if the active set changes, we do not apply such changes to the matching matrix $D$ and can thus reuse already set up AMG preconditioners from the previous semismooth Newton step. The Chebyshev semi-iteration preconditioner for the control block, where the active set changes occur, has a negligible setup cost.

7.2. Parallelization for the 2D case. We report weak scaling results of the decomposition-free Schur complement preconditioner in Fig. 7.8 for up to 64 processors. The number of degrees of freedom for each run is provided in Tab. 7.1. The runtime is dominated by the cost to solve the linear systems with the decomposition-

\footnote{All results were computed on a 2×32-core AMD EPYC 7452 workstation with 256 GB RAM running GNU/Linux.}
free Schur complement solver. There is a noticeable drop in parallel efficiency from 16 up to 64 processors. However, this drop goes in conjunction with a drop in parallel efficiency also for the Riesz solver, which is simply AMG-preconditioned CG for the Poisson equation. We conjecture that further tuning of the AMG preconditioner or switching to a parallel geometric multigrid method would improve the parallel efficiency.

7.3. 3D case. In Fig. 7.9 we show the optimal solution of the model problem (6.1) on the unit cube on a regular tetrahedral grid with $N = 160$ element edges per edge of the unit cube and control bounds of $\pm50$. The final discretization has $3 \cdot 161^3 = 12,519,843$ degrees of freedom. Similar to the optimal solutions in 2D, the optimal controls and optimal states exhibit very steep slopes. Altogether the proposed inexact sequential homotopy method with the suggested preconditioners can reliably and efficiently solve large-scale, highly nonlinear, badly conditioned problems.

8. Conclusion. We have extended a sequential homotopy method to allow the use of inexact solvers for the linearized subsystems, and provided sufficient conditions that permit a proof of convergence to the solution determined by the projected gradient/antigradient flow. For a prominent class of nonlinear PDE-constrained optimization problems, we provided analysis for symmetric positive-definite block-diagonal Schur complement preconditioners for double saddle point systems. For a challenging model problem, we provided approximations of the Schur complements for the efficient and parallel application of approximated double saddle-point preconditioners. The implicit regularization feature of the sequential homotopy method was beneficial for the solution of the linearized subproblems with preconditioned MINRES and GMRES. We provided numerical results for a hierarchy of Schur complement approximations, which shed light on the consequences of each approximation step on the way to the eventual fast, effective, and parallelizable, decomposition-free preconditioner. The preconditioners allowed us to solve even the 2D model problem faster than using direct sparse linear algebra. We provided a weak scaling analysis for the 2D case and efficiently solved a large 3D problem instance with 12 million degrees of freedom.

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