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Adaptive multilevel trust-region methods for time-dependent PDE-constrained optimization

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Abstract. We present a class of adaptive multilevel trust-region methods for the efficient solution of optimization problems governed by time-dependent nonlinear partial differential equations with control constraints. The algorithm is based on the ideas of the adaptive multilevel inexact SQP-method from [26], [27]. It is in particular well suited for problems with time-dependent PDE constraints. Instead of the quasi-normal step in a classical SQP method which results in solving the linearized PDE sufficiently well, in this algorithm a (nonlinear) solver is applied to the current discretization of the PDE. Moreover, different discretizations and solvers for the PDE and the adjoint PDE may be applied. The resulting inexactness of the reduced gradient in the current discretization is controlled within the algorithm. Thus, highly efficient PDE solvers can be coupled with the proposed optimization framework. The algorithm starts with a coarse discretization of the underlying optimization problem and provides during the optimization process implementable criteria for an adaptive refinement strategy of the current discretization based on error estimators. We prove global convergence to a stationary point of the infinite-dimensional problem. Moreover, we illustrate how the adaptive refinement strategy of the algorithm can be implemented by using a posteriori error estimators for the state and the adjoint equation. Numerical results for a semilinear parabolic PDE-constrained problem with pointwise control constraints are presented.

Mathematics Subject Classification: 90C55, 49M05, 49M25, 49M37

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1. Introduction

In this paper we introduce and analyze a class of adaptive multilevel trust-region methods for the efficient solution of optimization problems governed by time-dependent nonlinear partial differential equations (PDEs) with control constraints. The resulting method can be considered as an inexact trust-region method applied to the reduced problem, where the state is eliminated by using the discretized state equation on the current grid. One can alternatively also intepret the method as a generalized composite step SQP method, where instead of the quasi-normal step of a classical composite step trust-region SQP method which results from solving the linearized PDE sufficiently well, a (nonlinear) solver is applied to the current discretization of the PDE. The algorithm is based on ideas of the adaptive multilevel inexact SQP-method from [26], [27]. It is inspired by and particularly shaped for optimization problems governed by parabolic PDEs, since solving a linearized parabolic PDE or the nonlinear parabolic PDE itself numerically with linear implicit methods in time, as e.g. Rosenbrock schemes, on a given spatial discretization has about the same computational costs. The adaptive multilevel trust-region method is designed to combine efficient optimization techniques and fast PDE solvers with error estimators in a rigorous way. Therefore, it offers the possibility to use different solvers for the state PDE and the adjoint PDE. The occuring inexactness in the reduced gradient on a fixed discretization level is controlled and modern adaptive discretization techniques for PDEs based on a posteriori error estimators are integrated in this framework. The algorithm starts with a coarse discretization of the underlying optimization problem and provides during the optimization process implementable criteria for an adaptive refinement strategy of the current discretization based on error estimators. This offers the possibility to perform most of the optimization iterations and PDE solves on coarse meshes. Moreover, the optimization problem is always well represented and the infinite-dimensional problem is approached during the optimization in an efficient way.

We consider PDE-constrained optimization problems of the form

$$\min_{y\in Y, u\in U} f(y,u) \qquad \text{s.t.} \qquad C(y,u)=0, \qquad u\in U_{\text{ad}}, \tag{1}$$

where U is the control space, $U_{\text{ad}} \subset U$ a closed and convex subset representing the set of admissible controls, Y is the state space, $f : Y \times U \to \mathbb{R}$ is the objective function. The state equation $C : Y \times U \to \Lambda$, $C(y,u) = 0$ comprises a (system of) partial differential equation(s) with appropriate initial and/or boundary conditions in a variational formulation with V as the set of test functions. V^* denotes the dual space of V and, thus, we have $\Lambda = V^*$. We assume that U are Hilbert spaces and that Y and V are reflexive Banach spaces. Moreover, we will require that f and C are continuously Fréchet differentiable on a subset of $Y \times U$.

As an example we will consider in Section 5 a semilinear parabolic boundary control problem of the form

$$\begin{aligned} \min f(y,u) \qquad \text{s.t.} \qquad y_t + Ly + d(y) &= 0, && \text{on } (0,T)\times\Omega,\\ y_n + b(y) &= u, && \text{on } (0,T)\times\partial\Omega,\\ y(0,\cdot) &= y_0 && \text{on } \Omega,\\ a \le u &\le b && \text{on } (0,T)\times\partial\Omega, \end{aligned} \tag{2}$$

where $\Omega \subset \mathbb{R}^n$ is a bounded Lipschitz domain, $T > 0$, y_n denotes the outer normal derivative, $u : (0, T) \times \partial\Omega \to \mathbb{R}$ is the control and $y_0 : \Omega \to \mathbb{R}$ are given initial data. b and d are monotone increasing C^2-functions. L denotes for each time t a second order elliptic operator

$$Ly := -\sum_{i,j}^{n} \left(a_{ij}(t,x) y_{x_i}\right)_{x_j} + \sum_{i=1}^{n} b_i(t,x) y_{x_i} + c_0(t,x) y,$$

i.e., there exists a constant $\theta > 0$ such that

$$\sum_{i,j=1}^{n} a_{ij}(t,x)\xi_i\xi_j \geq \theta\|\xi\|^2 \qquad \text{for a.a. } (t,x) \in (0,T) \times \Omega \text{ and all } \xi \in \mathbb{R}^n,$$

see for example [10], [15], [20], [23].

The proposed adaptive multilevel trust-region algorithm for (1) generates a hierarchy of finite-dimensional approximations

$$\min_{y^h \in Y_h, u^h \in U_h} f(y^h, u^h) \quad \text{s.t.} \quad C^h(y^h, u^h) = 0, \quad u^h \in U^h_{\text{ad}}, \tag{3}$$

which result from conformal discretizations of (1) on adaptively refined meshes. Our assumptions on the discretization will be made precise in Section 2.

Multilevel optimization techniques for optimal control problems governed by (nonlinear) PDEs are an active research area. There is a variety of literature for optimization problems governed by elliptic PDEs as outlined in [26], [27]. However, only a few publications are concerned with multilevel adaptive solution techniques for optimal control problems governed by (nonlinear) parabolic PDEs. [3], [21] derive error estimates for adaptive mesh refinements and show possibilities for derivative evaluations of the reduced cost functional. The algorithms from [3], [21] for adaptive mesh refinement solve the optimization problem on the current grid and then refine the mesh.

In [12], [13], [18] multilevel trust-region methods are proposed that focus on the efficient use of a hierarchy of discretizations to solve an optimization problem on the finest grid, but the coupling with adaptive mesh refinement is not considered.

In [17] truncated Newton methods with inexact function and gradient evaluations have been studied, but the combination with error estimators was not considered. A general algorithmic framework for dealing with approximate function and gradient evaluations in steepest descent algorithms for optimal control problems has been proposed in [22]. In this approach the accuracy control mechanism requires an error estimator for the function and gradient value depending on a scalar mesh parameter and is quite different from the method proposed in this work.

The rigorous coupling of error estimators with efficient optimization methods in a multilevel optimization framework for parabolic PDE constrained optimization problems (with control constraints) was to the best of our knowledge not considered so far.

In this paper we develop an implementable adaptive refinement strategy based on error estimators and combine it with an efficient inexact trust-region method. The possibility to use different solvers for the PDE and the adjoint PDE is given. The resulting adaptive multilevel trust-region method generates a hierarchy of adaptive discretizations (3), controls the inexactness of the reduced gradient on the current discretization and refines the grid – if necessary – adaptively in an appropriate way based on error estimators, e.g. [1], [2], [8], [9], [21], [24], to ensure convergence to a solution of the original problem (1). We will prove global convergence under standard assumptions to a first-order optimal point of the infinite-dimensional problem (1). Moreover, we illustrate how the adaptive refinement strategy of the algorithm can be implemented by using a posteriori error estimators for the state and the adjoint equation.

The presented method has several advantages. The multilevel approach carries out most optimization iterations on coarse meshes. The accuracy of the optimization result is controlled and the mesh adaptation is tailored to the needs of the optimization method. This offers the possibility to obtain optimization results of high accuracy by an effort of a few simulation runs on the finest grid.

This paper is organized as follows. In Section 2 we formulate our general assumptions that take the nature of nonlinear PDE constraints into account and can easily be verified e.g. for semilinear parabolic problems as well as the Navier–Stokes equations. We derive optimality conditions and formulate our assumptions on the discretization. In Section 3 we develop step by step the adaptive multilevel trust-region method. The convergence analysis is carried out in Section 4. In Section 5 the assumptions are verified for a semilinear parabolic boundary control problem and numerical results are presented.

Notations. For a Gâteaux- or Fréchet-differentiable operator $C : Y \times U \to V^*$, we denote by $C_y(y,u) \in L(Y,V^*)$ and $C_u(y,u) \in L(U,V^*)$ the partial derivative with respect to y and u, respectively. If $f : Y \times U \to \mathbb{R}$ is Gâteaux- or Fréchet-differentiable and U is a Hilbert space then we denote by the gradient $\nabla_u f(y,u) \in U$ the Riesz representation of $f_u(y,u) \in U^*$.

2. Optimality conditions and discretization

We make the following assumptions, which can conveniently be verified, e.g., for semilinear parabolic problems or the unsteady Navier–Stokes equations in 2D and takes care of the fact that for nonlinear problems often additional regularity of the state is necessary to obtain differentiability properties of the control to state mapping $u \in U_{\text{ad}} \mapsto y = S(u) \in Y$.

Assumption 2.1. *U is a Hilbert space, Y, V are reflexive Banach spaces, $U_{\text{ad}} \subset U$ is closed and convex. Moreover, there exists a Banach space $Y^+ \hookrightarrow Y$ and a convex closed subset $D := D_Y \times D_U \subset Y^+ \times U$ with $U_{\text{ad}} \subset D_U$ such that the following holds.*

A1 *$f : Y \times U \to \mathbb{R}$ is continuously Fréchet differentiable and the derivative is Hölder continuous on bounded subsets of $Y^+ \times U$.*

A2 *There exists a unique solution operator $u \in D_U \mapsto S(u) \in D_Y \subset Y^+$ for $C(y, u) = 0$ that is bounded on bounded sets in $(D_U, \|\cdot\|_U)$. Moreover, $u \in (D_U, \|\cdot\|_U) \mapsto S(u) \in Y$ is continuous.*

A3 *$C : Y^+ \times U \to V^*$ is continuously Fréchet differentiable. Moreover, also $C : (D_Y, \|\cdot\|_Y) \times U \to V^*$ is continuously Fréchet differentiable. The partial derivative $C_y(x) \in L(Y^+, V^*)$ admits for all $x \in D$ an extension $C_y(x) \in L(Y, V^*)$ that has a bounded inverse $C_y(x)^{-1} \in L(V^*, Y)$. Moreover, $(y, u) \in (D_Y, \|\cdot\|_Y) \times U \mapsto C_x(y, u) \in L(Y \times U, V^*)$ is Hölder continuous on bounded subsets of $Y^+ \times U$.*

By applying the generalization [11], Thm. 3.1 of the implicit function theorem we obtain the differentiability of the control-to-state map and of the reduced objective funtional.

Proposition 2.2. *Let Assumption 2.1 hold. Then the mapping $u \in (D_U, \|\cdot\|_U) \mapsto S(u) \in Y$ is continuously Fréchet differentiable with derivative*

$$S'(u) = -C_y\big(S(u), u\big)^{-1} C_u\big(S(u), u\big) \tag{4}$$

that is Hölder continuous on bounded subsets of $(D_U, \|\cdot\|_U)$. Moreover, also the reduced objective functional

$$u \in (D_U, \|\cdot\|_U) \mapsto \hat{f}(u) := f\big(S(u), u\big)$$

is continuously Fréchet differentiable with derivative

$$\hat{f}'(u) = f_y\big(S(u), u\big) S'(u) + f_u\big(S(u), u\big) \in U^* \tag{5}$$

that is Hölder continuous on bounded subsets of $(D_U, \|\cdot\|_U)$. Finally, the solution operator

$$(y, u) \in (D_Y, \|\cdot\|_Y) \times (D_U, \|\cdot\|_U) \mapsto S_{l_y}(y, u) := C_y(y, u)^{-*} f_y(y, u) \in V$$

of the adjoint equation $l_y(y, u, \lambda) = 0$ is continuous.

Proof. The Fréchet differentiability of $u \in (D_U, \|\cdot\|_U) \mapsto S(u) \in Y$ and (4) follow from [11], Thm. 3.1 by setting $Y_1 = Y_2 := Y$, $Z = Z_0 := V^*$ and by using $(D_U, \|\cdot\|_U)$ instead of U. The continuity of $S'(u)$ and boundedness on bounded subsets follows from (4) by A1–A3. The continuity of $S_{l_y}(u)$ is also a consequence of A1–A3. Hence, S is Lipschitz continuous on bounded subsets and from A1–A3 and (4) it follows that S' is Hölder continuous on bounded subsets.

The continuous Fréchet differentiability of $u \in (D_U, \|\cdot\|_U) \mapsto \hat{f}(u) = f(S(u), u)$ is now a consequence of A1 and the chain rule. $\hat{f}'(u) \in U^*$ follows by (4), A1 and A3. Moreover, the Hölder continuity on bounded subsets is a consequence of the Hölder continuity of S'. □

We introduce the Lagrangian function

$$l : Y \times U \times V \to \mathbb{R}, \qquad l(y, u, \lambda) = f(y, u) + \langle \lambda, C(y, u) \rangle_{V, V^*}. \tag{6}$$

By using Proposition 2.2, differentiating $\hat{f}(u) = f(S(u), u) = l(S(u), u, \lambda)$ with respect to u and choosing $\lambda \in V$ as the unique solution of the adjoint equation

$$l_y(S(u), u, \lambda) = 0, \qquad \text{i.e., } C_y(S(u), u)^* \lambda = -f_y(S(u), u),$$

which has a unique solution by A2 and A3, we still obtain the classical adjoint representation

$$\hat{f}'(u) = l_u(S(u), u, \lambda), \qquad \text{where } l_y(S(u), u, \lambda) = 0. \tag{7}$$

We conclude that under Assumption 2.1 the problem (1) can equivelantly be written as the reduced problem

$$\min_{u \in U} \hat{f}(u) := f(S(u), u) \qquad \text{sunject to } u \in U_{\mathrm{ad}}. \tag{8}$$

Moreover, the reduced objective function $u \in (D_U, \|\cdot\|_U) \mapsto f(S(u), u)$ is continuously Fréchet differentiability and its derivative can be computed by the adjoint formula (7).

2.1. Optimality conditions. Let $(\bar{y}, \bar{u}) \in Y \times U_{\mathrm{ad}}$ be a locally optimal solution of problem (1). Then $\bar{y} = S(\bar{u}) \in D_Y \subset Y^+$ by A2 and $\bar{u}$ is a local solution of the reduced problem (8). Hence, Proposition 2.2 yields with the Riesz representation $\nabla\hat{f}(\bar{u}) \in U$ of $\hat{f}'(\bar{u}) \in U^*$) that for the local solution $\bar{u}$ of (8) the optimality condition

$$\bar{u} \in U_{\mathrm{ad}}, \qquad \left(\nabla\hat{f}(\bar{u}), u - \bar{u}\right)_U \geq 0 \qquad \forall u \in U_{\mathrm{ad}}$$

holds. Since $U_{\mathrm{ad}} \subset U$ is closed and convex, it is well known that this variational inequality is equivalent to

$$P_{U_{\mathrm{ad}}}\big(\bar{u} - \nabla \hat{f}(\bar{u})\big) = 0,$$

where $P_{U_{\mathrm{ad}}} : U \to U_{\mathrm{ad}} - \bar{u}$ denotes the projection onto the closed and convex set U_{ad} i.e.

$$P_{U_{\mathrm{ad}}}(u) \in U_{\mathrm{ad}}, \qquad P_{U_{\mathrm{ad}}}(u) = \arg\min_{w \in U_{\mathrm{ad}}} \|w - u\|_U \qquad \forall u \in U,$$

see, e.g., [15], [23]. Using (7) we conclude that under Assumption 2.1 in a local solution $(\bar{y}, \bar{u})$ of (1) the following first-order necessary optimality conditions hold: There exists an adjoint state $\bar{\lambda} \in V$ such that

$$\begin{aligned} C(\bar{y}, \bar{u}) &= 0 \qquad \text{(state equation)}, \\ l_y(\bar{y}, \bar{u}, \bar{\lambda}) &= 0 \qquad \text{(adjoint equation)}, \\ P_{U_{\mathrm{ad}}}\big(\bar{u} - \nabla_u l(\bar{y}, \bar{u}, \bar{\lambda})\big) &= 0 \qquad \text{(stationarity)}, \end{aligned} \tag{9}$$

where $\nabla_u l(\bar{y}, \bar{u}, \bar{\lambda}) \in U$ denotes the Riesz representation of the control gradient $l_u(\bar{y}, \bar{u}, \bar{\lambda})$ of the Lagrangian, cf. [15], [23]. We will call $\big\|P_{U_{\mathrm{ad}}}\big(u - \nabla_u l(y, u, \lambda)\big)\big\|_U$ criticality measure.

2.2. Discretized problem. To allow for a wide variatey of possible PDE solvers within the proposed optimization method, we assume the following framework.

We assume that there is a suitable solver for the state equation $C(y, u) = 0$ available, which generates for simplicity a conformal discretization. More precisely, for a given mesh $\mathscr{T}_h$ corresponding to a state space $Y_h \subset Y$ and $U_h \subset U$ it generates for given $u^h \in U_h$ a unique solution $y^h \in Y_h$ of a discretized state equation $C^h(y^h, u^h) = 0$ leading to a discrete solution operator $S^h : u^h \in U_h \mapsto y^h \in Y_h$. By $h' < h$ we indicate that the mesh $\mathscr{T}_{h'}$ is a refinement of $\mathscr{T}_h$ in the sense that $Y^h \subset Y^{h'}$ and $U^h \subset U^{h'}$. Moreover, we denote by $h_k \searrow 0$ that $\mathscr{T}_{h_k}$ is a sequence of refined meshes, such that 1) the maximal diameter of mesh cells tends to zero, 2) $d_Y(y, Y_{h_k}) + d_U(u, U_{h_k}) \to 0$ for all $(y, u) \in Y \times U$, 3) specific requirements of the solver are satisfied, e.g. ratio between time step and spacial mesh size and regularity properties of the meshes. Here, d_Y and d_U denote the distance with respect to $\|\cdot\|_Y$ and $\|\cdot\|_U$, respectively. Finally, let $U_{\mathrm{ad}}^h \subset U_h$ be an approximation of U_{ad} with $d_U(u, U_{\mathrm{ad}}^{h_k}) \to 0$ for all $u \in U_{\mathrm{ad}}$ as $h_k \searrow 0$. A possible choice is $U_{\mathrm{ad}}^h = U_{\mathrm{ad}} \cap U_h$. This leads for a mesh $\mathscr{T}_h$ to the corresponding discretized problem (3). The reduced objective function for (3) is given by $\hat{f}^h(u^h) = f\big(S^h(u^h), u^h\big)$ and the equivalent reduced problem by

$$\min_{u^h \in U_h} \hat{f}^h(u^h) := f\big(S^h(u^h), u^h\big) \qquad \text{s.t.} \qquad u \in U_{\mathrm{ad}}^h. \tag{10}$$

We do not necessarily require that the exact gradient $\nabla \hat{f}^h(u^h) \in U_h$ is computed by using the discrete adjoint. Instead, we assume that for given $(y^h, u^h) \in Y_h \times U_h$ there is an appropriate conformal solver available for the adjoint PDE $l_y(y^h, u^h, \lambda) = 0$ leading to a discrete solution operator $(y^h, u^h) \in Y_h \times U_h \mapsto \lambda^h = S_{l_y}^h(y^h, u^h) \in V_h$, where $V_h \subset V$. As above, we assume that $h_k \searrow 0$ implies $d_V(\lambda, V_{h_k}) = 0$ for all $\lambda \in V$. For $u^h \in U_h$ we approximate now $\nabla \hat{f}^h(u^h) \in U_h$ (and thus $\nabla \hat{f}^h(u^h) \in U$) by

$$\hat{g}^h := \nabla_{u^h} l(y^h, u^h, \lambda^h) \in U_h, \qquad \lambda^h = S_{l_y}^h(y^h, u^h),$$

where $\nabla_{u^h} l(y^h, u^h, \lambda^h) \in U_h$ is the Riesz representation of $l_u(y^h, u^h, \lambda^h) \in U^* \subset U_h^*$.

We make the following assumptions on the discrete solution operators that are analogous to Assumption 2.1.

Assumption 2.3. *Let Assumption* 2.1 *hold and let $\mathcal{T}_H$ be an initial grid. Then for each refined mesh $\mathcal{T}_h$, $h \le H$ (see above), let $U_h \subset U$, $Y_h \subset Y^+$, $U_{\mathrm{ad}}^h \subset D_U$, $V_h \subset V$. Moreover, the following holds.*

D1 *There exists a unique continuously differentiable solution operator $u^h \in U_h \cap D_U \mapsto S^h(u^h) \in Y_h \cap D_Y \subset Y^+$ for $C^h(y^h, u^h) = 0$ that is bounded on bounded sets of $(D_U, \|\cdot\|_{U_h})$ uniformly in $h \le H$. Moreover, $u^h \in U_h \cap D_U \mapsto (S^h)'(u^h) \in L(U_h, Y_h)$ is Hölder continuous on bounded subset of $(D_U, \|\cdot\|_{U_h})$ uniformly in $h \le H$.*

D2 *The discrete solution operator $(y^h, u^h) \in (Y_h \cap D_Y) \times (U_h \cap D_U) \mapsto S_{l_y}^h(y^h, u^h) \in V_h$ of the adjoint PDE $l_y(y^h, u^h, \lambda) = 0$ is continuous.*

D3 *For any sequence $h_k \searrow 0$ of mesh refinements of the initial mesh $h_0 = H$ and any bounded sequence $(y_k^h, u_k^h) \in (Y_{h_k} \cap D_Y) \cap (U_{h_k} \cap D_U)$ and $v_k^h \in U_{h_k}$ the discrete approximations converge, i.e.,*

$$\lim_{k\to\infty} \|S^{h_k}(u_k^h) - S(u_k^h)\|_Y \to 0,$$

$$\lim_{k\to\infty} \|(S^{h_k})'(u_k^h) - S'(u_k^h)\|_{L(U,Y)} \to 0,$$

$$\lim_{k\to\infty} \|S_{l_y}^{h_k}(y_k^h, u_k^h) - S_{l_y}(y_k^h, u_k^h)\|_V \to 0,$$

$$\lim_{k\to\infty} \|P_{U_{\mathrm{ad}}^{h_k}}(v_k^h) - P_{U_{\mathrm{ad}}}(v_k^h)\|_U \to 0, \qquad U_{\mathrm{ad}}^{h_k} \subset U_{\mathrm{ad}}^{h_{k+1}} \subset U_{\mathrm{ad}}\ \forall k.$$

D4 *For the state solver* S^h *and the adjoint solver* $S^h_{l_y}$ *reliable a posteriori estimators* $\eta_y^{h_k}$ *and* $\eta_\lambda^{h_k}$ *are available, i.e. there exist constants* $c_y, c_\lambda > 0$ *such that for all* $h_k \searrow 0$ *and* (y_k^h, u_k^h) *as in* D3 *it holds*

$$\|C(S^{h_k}(u_k^h), u_k^h)\|_{V^*} \le c_y \eta_y^{h_k}(S^{h_k}(u_k^h)) \to 0,$$
$$\|l_y(y_k^h, u_k^h, S_{l_y}^{h_k}(y_k^h, u_k^h))\|_{Y^*} \le c_\lambda \eta_\lambda^{h_k}(S_{l_y}^{h_k}(y_k^h, u_k^h), y_k^h, u_k^h) \to 0,$$

or alternatively

D4′ *Instead of the a posteriori estimators for the residuals there are reliable a posteriori estimators* $\eta_y^{h_k}$ *and* $\eta_\lambda^{h_k}$ *available for the error in state and adjoint, more precisely,*

$$\|S^{h_k}(u_k^h) - S(u_k^h)\|_Y \le c_y \eta_y^{h_k}(S^{h_k}(u_k^h)) \to 0,$$
$$\|S_{l_y}^{h_k}(y_k^h, u_k^h) - S_{l_y}(y_k^h, u_k^h)\|_V \le c_\lambda \eta_\lambda^{h_k}(S_{l_y}^{h_k}(y_k^h, u_k^h), y_k^h, u_k^h) \to 0.$$

For our numerical results we will work with an a posteriori error estimator proposed in [8], but any reliable a posteriori error estimator could be used, see for example [1], [2], [9], [24].

Proposition 2.4. *Under Assumptions* 2.1 *and* 2.3 *the discrete reduced objective function* $\hat{f}^h : U_h \cap D_U \to \mathbb{R}$ *is continuously differentiable and the derivative is Hölder continuous on bounded subsets of* $(D_U, \|\cdot\|_{U_h})$ *uniformly in* $h \le H$.

Proof. By Assumptions 2.1 and D1 this follows analogously as at the end of the proof of Proposition 2.2. □

3. An adaptive multilevel trust-region algorithm

3.1. Main components of the adaptive multilevel trust-region algorithm. In this section we derive and motivate the adaptive multilevel trust-region method.

3.1.1. Basic concept. Consider the reduced problem (8). Let $u_k \in U_{\text{ad}}$ be a current iterate. A trust-region type method for (8) computes a step s_k by (approximately) solving the trust-region problem

$$\min_{s \in U} \hat{q}_k(s) := (\nabla \hat{f}(u_k), s)_U + \frac{1}{2}\langle s, \hat{H}_k s\rangle_{U,U^*} \text{ s.t. } u_k + s \in U_{\text{ad}}, \quad \|s\|_U \le \Delta_k, \quad (11)$$

where $\Delta_k > 0$ is a trust-region radius and $\hat{H}_k \in L(U, U^*)$ is an approximation of the reduced Hessian $\hat{f}''(u_k)$ (if it exists). The step is now evaluated by using the decrease ratio

$$\rho_k := \frac{\mathrm{ared}_k(s_k)}{\mathrm{pred}_k(s_k)}$$

with actual reduction and predicetd reduction

$$\mathrm{ared}_k(s_k) := \hat{f}(u_k) - \hat{f}(u_k + s_k), \qquad \mathrm{pred}_k(s_k) := q_k(0) - q_k(s_k).$$

If ρ_k is large enough, the step is accepted, i.e., $u_{k+1} := u_k + s_k$, $\Delta_{k+1} \geq \Delta_k$ and otherwise rejected, i.e., $u_{k+1} := u_k$, $\Delta_{k+1} < \Delta_k$. See below for the precise update mechanism.

By using (7), we have

$$\hat{q}_k(s) = (\hat{g}_k, s)_U + \frac{1}{2}\langle s, \hat{H}_k s\rangle_{U, U^*},$$

where

$$\hat{g}_k = \nabla_u l(y_k, u_k, \lambda_k), \qquad y_k = S(u_k), \qquad \lambda_k = S_{l_y}(y_k, u_k).$$

Let now $\mathscr{T}_{h_0}$ be an initial mesh that is adaptively refined during the optimization and let h_k with $h_k \leq h_{k-1} \leq \cdots \leq h_0$ be the current grid and $u_k^h \in U_{h_k}$ the current control. We approximate now the trust-region problem (11) by using the solvers S^{h_k} and $S_{l_y}^{h_k}$ for the state equation and the adjoint equation on the current mesh. This leads to the approximation of (11)

$$\min_{s \in U_{h_k}} \hat{q}_k^h(s) := (\hat{g}_k^h, s\rangle_U + \frac{1}{2}\langle s, \hat{H}_k s\rangle_{U, U^*} \text{ s.t. } u_k^h + s \in U_{\mathrm{ad}}^{h_k}, \qquad \|s\|_U \leq \Delta_k, \quad (12)$$

where

$$\hat{g}_k^h := \nabla_{u^{h_k}} l(y_k^h, u_k^h, \lambda_k^h) \in U_{h_k}, \qquad y_k^h = S^{h_k}(u_k^h), \qquad \lambda_k^h = S_{l_y}^{h_k}(y_k^h, u_k^h). \quad (13)$$

The basic idea is now to apply a trust-region method on the current mesh h_k until error control criteria based on error estimators indicate that the mesh should be refined in order to approach the solution of (8) efficiently. Then the mesh is refined accordingly and the trust region method is continued on the new mesh.

To this end, the following errors have to be controlled.

- The error $\hat{f}(u_k^h) - \hat{f}^{h_k}(u_k^h)$ in the reduced objective function can be reduced by choosing an adaptively refined mesh $h_{k+1} < h_k$ for the state solver $S^{h_{k+1}}$.

- The error $\nabla\hat{f}(u_k^h) - \hat{g}_k^h$ in the reduced gradient at the current control u_k^h as well as the inexactness $\nabla\hat{f}^{h_k}(u_k^h) - \hat{g}_k^h$ of the discrete reduced gradient resulting from using independent state and adjoint solvers can be controlled by adaptive mesh refinement for the state solver $S^{h_{k+1}}$ and the adjoint solver $S_{l_y}^{h_{k+1}}$.
- The error in the admissible sets $U_{\rm ad}$ and $U_{\rm ad}^{h_k}$ can be reduced by mesh refinement $h_{k+1} < h_k$ of the control space $U_{h_{k+1}}$.

3.1.2. Sufficient decrease condition for the trust-region step. Let h_k be the current mesh. We compute now an approximate solution s_k^h of the trust-region problem (12) that satisfies the generalized Cauchy decrease condition

$$\begin{aligned} u_k^h + s_k^h \in U_{\rm ad}^{h_k}, \qquad \|s_k^h\|_U \le \Delta_k, \\ \operatorname{pred}_k^h(s_k^h) := \hat{q}_k^h(0) - \hat{q}_k^h(s_k^h) \\ \ge \kappa_1 \|P_{U_{\rm ad}^{h_k}}(u_k^h - \hat{g}_k^h)\|_U \min\{\kappa_2 \|P_{U_{\rm ad}^{h_k}}(u_k^h - \hat{g}_k^h)\|_U, \kappa_3\Delta_k\}, \end{aligned} \tag{14}$$

where κ_1, κ_2, κ_3 are positive constants independent of k and the grid.

If $U_{\rm ad} = U$ then we have $\|P_{U_{\rm ad}^{h_k}}(u_k^h - \hat{g}_k^h)\|_U = \|\hat{g}_k^h\|_U$ and (14) is just the classical Cauchy decrease condition ensuring that s_k^h provides a fraction of the decrease that is possible along the direction of steepest descent inside the trust-region. We refer to [27], §5.3 for several possibilities to compute suitable steps.

If control constraints are considered, the decrease condition is generalized to the projected negative gradient path direction. Possibilities to compute such steps are discussed in [26]. A simple procedere to guarantee the generalized Cauchy decrease condition is to compute the projected negative gradient direction with Armijo or Goldstein type linesearch. If the Hessians are bounded, which will be guaranteed by Assumption 4.1, then one can show that in this way (14) can be ensured, cf. [26].

To invoke second order methods, in the case of simple pointwise bound constraints it is possible to compute a projected inexact Newton step ([4], [16]) and to check if the generalized Cauchy decrease condition (14) is satisfied as described in the fallback projected inexact Newton algorithm in [26], Alg. 5.10. By [26], Rem. 5.11 the step s_k^h computed by Algorithm [26], Alg. 5.10 satisfies the generalized Cauchy decrease condition (14).

3.1.3. Acceptance of steps. As in the standard trust-region method sketched above the decision about the acceptance of the step and the update of the trust-region radius Δ_k is based on the ratio

$$\rho_k^h := \frac{\operatorname{ared}_k^h(s_k^h)}{\operatorname{pred}_k^h(s_k^h)}$$

of the actual reduction

$$\mathrm{ared}_k^h(s_k^h) := \hat{f}^{h_k}(u_k^h) - \hat{f}^{h_k}(u_k^h + s_k^h), \tag{15}$$

and the predicted reduction based on the quadratic model on the current mesh

$$\mathrm{pred}_k^h(s_k^h) = \hat{q}_k^h(0) - \hat{q}_k^h(s_k^h). \tag{16}$$

Note that $\hat{q}_k^h$ is an approximation of the reduced cost functional $\hat{f}^{h_k}$, but the gradient $\hat{g}_k^h$ is in general inexact. This issue will be considered in 3.1.4.

The step s_k^h is accepted if

$$\rho_k^h \geq \eta_1,$$

otherwise s_k^h is rejected and the trust-region is reduced.

We choose the trust-region radius as follows:

For fixed $0 < \alpha_0 \leq \alpha_1 < 1 < \alpha_2$, $0 < \eta_1 < \eta_2 < 1$, and $\Delta_{\min} \geq 0$ set

$$\Delta_{k+1} \in \begin{cases} [\alpha_0 \Delta_k, \alpha_1 \Delta_k], & \text{if } \rho_k^h < \eta_1 \\ [\max\{\Delta_{\min}, \alpha_1 \Delta_k\}, \max\{\Delta_{\min}, \Delta_k\}], & \text{if } \rho_k^h \in [\eta_1, \eta_2) \\ [\max\{\Delta_{\min}, \Delta_k\}, \max\{\Delta_{\min}, \alpha_2 \Delta_k\}], & \text{if } \rho_k^h \geq \eta_2. \end{cases} \tag{17}$$

3.1.4. Accuracy control of the inexact reduced gradient. To control the inexactness of the reduced gradient $\hat{g}_k^h$ we use the following condition, which is a weakened variant of the condition proposed in [14], see also [25–27].

If the step s_k^h was rejected then the gradient accuracy condition

$$\left| \left(\nabla \hat{f}^{h_k}(u_k^h), s_k^h \right)_U - (\hat{g}_k^h, s_k^h)_U \right| \leq \xi_2 \min\{\|P_{U_{\mathrm{ad}}^{h_k}}(u_k^h - \hat{g}_k^h)\|_U, \Delta_k\} \|s_k^h\|_U \tag{18}$$

is checked, where $\xi_2 > 0$ is a fixed constant. Note that the directional derivative $\left(\nabla \hat{f}^{h_k}(u_k^h), s_k^h \right)_U$ can also be computed approximately by a difference quotient using the state solver. If (18) is satisfied, the accuracy of $\hat{g}_k^h$ is sufficient and no mesh refinement is required.

If (18) fails, then the discretization is refined and the iteration is recomputed until either the stopping criterion of the algorithm is satisfied or the trial step is accepted or the gradient accuracy condition (18) is satisfied. The latter can be achieved by sufficient refinement as shown in the convergence analysis.

Remark 3.1. *If $\hat{g}_k^h$ is the exact discrete reduced gradient, i.e., $\hat{g}_k^h = \nabla \hat{f}^{h_k}(u_k^h)$ then* (18) *is always satisfied, since the left hand side vanishes.*

3.1.5. Refinement criteria. So far only the gradient accuracy condition (18) may require a mesh refinement. As we will see, the trust-region method together with the accuracy condition (18) ensures that the criticality measure satisfies $\liminf_{k\to\infty} \|P_{U_{\mathrm{ad}}^{h_k}}(u_k^h - \hat{g}_k^h)\|_U = 0$ under weak additional assumptions.

To ensure that for the generated iterates $(y_k^h, u_k^h, \lambda_k^h)$ the residual of the optimality system (9) for the infinite dimensional optimization problem (1) is driven to zero, we have to refine the meshes accordingly during the optimization.

The main idea for refinement is to control the residuals in the infinite dimensional optimality system (9) with the discrete criticality measure $\|P_{U_{\mathrm{ad}}^{h_k}}(u_k^h - \hat{g}_k^h)\|_U$. As long as the criticality measure is large enough compared to the residuals $\|C(y_k^h, u_k^h)\|_{V^*}$ of the state equation and $\|l_y(y_k^h, u_k^h, \lambda_k^h)\|_{Y^*}$ of the adjoint equation, the current discretization can be considered as sufficiently accurate to compute productive steps. On the other hand, if the norm of the discrete criticality measure on the current grid is small compared to the residuals of state and adjoint equation then one has to ensure by refinement of the discretizations that the infinite dimensional problem and, in particular, the infinite dimensional reduced gradient and its projection are well represented in the current discretization such that reasonable steps can be computed. Observe that the inexact reduced gradient $\hat{g}_k^h$ depends on the (inexact) state $y_k^h = S^{h_k}(u_k^h)$ and the (inexact) adjoint $\lambda_k^h = S_{l_y}^{h_k}(y_k^h, u_k^h)$. Therefore, the residual norms of the infinite dimensional state- and adjoint equation must be controlled. Since these residual norms cannot be computed directly, we will use reliable error estimators instead.

Hence, we would like to ensure the following inequalities

$$
\begin{aligned}
\|C(y_k^h, u_k^h)\|_{V^*} &\le K_y \|P_{U_{\mathrm{ad}}^{h_k}}(u_k^h - \hat{g}_k^h)\|_U \\
\|l_y(y_k^h, u_k^h, \lambda_k^h)\|_{Y^*} &\le K_\lambda \|P_{U_{\mathrm{ad}}^{h_k}}(u_k^h - \hat{g}_k^h)\|_U \\
\|P_{U_{\mathrm{ad}}}(u_k^h - \hat{g}_k^h) - P_{U_{\mathrm{ad}}^{h_k}}(u_k^h - \hat{g}_k^h)\|_U &\le K_u \|P_{U_{\mathrm{ad}}^{h_k}}(u_k^h - \hat{g}_k^h)\|_U
\end{aligned}
\tag{19}
$$

with fixed constants $K_y, K_\lambda, K_u > 0$, where

$$
y_k^h = S^{h_k}(u_k^h), \qquad \lambda_k^h = S_{l_y}^{h_k}(y_k^h, u_k^h).
$$

The third inequality in (19) results from the difference of the (infinite dimensional) projection onto U_{ad} and the discrete projection onto $U_{\mathrm{ad}}^{h_k}$. Note that it implies

$$
\|P_{U_{\mathrm{ad}}}(u_k^h - \hat{g}_k^{h(k)})\|_U \le (K_u + 1)\|P_{U_{\mathrm{ad}}^{h_k}}(u_k^h - \hat{g}_k^h)\|_U \tag{20}
$$

Since a direct computation of the residual norms of the state and adjoint PDE is too expensive to compute, we use the reliable error estimators in Assumption

2.3, D4. Then instead of (19) we check the condition

$$\eta_y^{h_k}(y_k^h) \le \tilde{c}_y \|P_{U_{\mathrm{ad}}^{h_k}}(u_k^h - \hat{g}_k^h)\|_U \tag{21a}$$

$$\eta_\lambda^{h_k}(\lambda_k^h, y_k^h, u_k^h) \le \tilde{c}_\lambda \|P_{U_{\mathrm{ad}}^{h_k}}(u_k^h - \hat{g}_k^h)\|_U \tag{21b}$$

$$\|P_{U_{\mathrm{ad}}}(u_k^h - \hat{g}_k^h) - P_{U_{\mathrm{ad}}^{h_k}}(u_k^h - \hat{g}_k^h)\|_U \le \tilde{c}_u \|P_{U_{\mathrm{ad}}^{h_k}}(u_k^h - \hat{g}_k^h)\|_U \tag{21c}$$

with fixed (arbitrary) constants $\tilde{c}_y, \tilde{c}_\lambda, \tilde{c}_u > 0$. By D4 this implies (19) with $K_y = c_y\tilde{c}_y$, $K_\lambda = c_\lambda\tilde{c}_\lambda$ and $K_u = \tilde{c}_u$.

Remark 3.2. In the important case $U = L^2\big((0,T)\times\Omega_c\big)$ and $U_{\mathrm{ad}} = \{u \in U : a \le u \le b\}$ with $a, b \in L^\infty\big((0,T)\times\Omega_c\big)$ the left hand side of (21c) can usually be estimated directly as long as a, b are not too complicated.

If according to D4′ a posteriori estimators for the error in state and adjoint are available then one can use the fact that by A1 and A3 the mapping $C : (D_Y, \|\cdot\|_Y) \times U \to V^*$ is Lipschitz continuous on bounded subsets of $Y^+ \times U$ and $l_y(y,u,\cdot) \in L(V, Y^*)$ is bounded on bounded subsets of $Y^+ \times U$. If D_U in Assumptions 2.1 and 2.3 are bounded in U then by A2 and D1 we can choose $D_Y \subset Y^+$ bounded and have $S(u_j^h) \in D_Y$ and $S^{h_k}(u_j^h) \in D_Y$ for all $u_j^h \in U_{\mathrm{ad}}^{h_j} \subset D_U$. Now let L_y and L_λ be the corresponding local Lischitz constants of C and $l_y(y,u,\cdot)$ on $D_Y \times D_U$. Under assumption D4′ we obtain with $x_k^h = (y_k^h, u_k^h)$

$$\begin{aligned} \|C(x_k^h)\|_{V^*} &= \big\|C(y_k^h, u_k^h) - C\big(S(u_k^h), u_k^h\big)\big\|_{V^*} \le L_y \|y_k^h - S(u_k^h)\|_Y, \\ \|l_y(x_k^h, \lambda_k^h)\|_{Y^*} &= \big\|l_y(x_k^h, \lambda_k^h) - l_y\big(x_k^h, S_{l_y}(x_k^h)\big)\big\|_{Y^*} \le L_\lambda \|\lambda_k^h - S_{l_y}(x_k^h)\|_V. \end{aligned} \tag{22}$$

If we use now (21) with the a posteriori error estimators in D4′ then (22) yields that again (19) holds with constants $K_y = L_y c_y \tilde{c}_y$, $K_\lambda = L_\lambda c_\lambda \tilde{c}_\lambda$, and $K_u = \tilde{c}_u$.

3.1.6. Sufficient mesh refinement. After the computation of a successful step on the current grid we need (at least after some iteration K) that the decrease produced for $\hat{f}^{h_k}$ on the current grid ensures also decrease for the exact objective function $\hat{f}^{h_k}$. To this end, we impose the following condition for sufficient refinement

$$\begin{aligned} \mathrm{ared}_k^h(s_k^h) \ge (1+\delta)\Big(&\big(\hat{f}(u_k^h + s_k^h) - \hat{f}^{h_k}(u_k^h + s_k^h)\big) \\ &- \big(\hat{f}(u_k^h) - \hat{f}^{h_k}(u_k^h)\big)\Big) \qquad \forall k \ge K, \end{aligned} \tag{23}$$

with $0 < \delta < 1$. If criterion (23) is not satisfied the Y-grid is refined properly and the step is recomputed until (23) holds.

To implement condition (23) assume that the algorithm generates a sequence $h_k \searrow 0$. If $u_k^h, u_k^h + s_k^h \subset D_U$ remain bounded, D3 and A1 yield

$$\begin{aligned} \alpha(u_k^h) &:= \hat{f}(u_k^h) - \hat{f}^{h_k}(u_k^h) =\longrightarrow 0 \\ \alpha(u_k^h + s_k^h) &:= \hat{f}(u_k^h + s_k^h) - \hat{f}^{h_k}(u_k^h + s_k^h) \to 0. \end{aligned} \tag{24}$$

Assume now that we have a realible estimator $\beta^{h_k}(u_k^h, s_k^h) > 0$, which can be contructed from the error estimator $\eta_y^{h_k}$ in D4 or D4′, such that

$$\alpha(u_k^h + s_k^h) - \alpha(u_k^h) \leq K\beta^{h_k}(u_k^h, s_k^h) \to 0 \qquad \text{for } k \to \infty \tag{25}$$

with some fixed possibly unkown $K > 0$.

Then to ensure (23) it suffices to verify the following sufficient refinement condition

$$\text{ared}_k^h(s_k^h) \geq \xi\beta^{h_k}(u_k^h, s_k^h)^{\omega} \tag{26}$$

for fixed $\omega \in (0, 1)$ and $\xi > 0$. In fact, having (26), assumption (24) yields with (25)

$$(1+\delta)\big(\alpha(u_k^h + s_k^h) - \alpha(u_k^h)\big) \leq (1+\delta)K\beta^{h_k}(u_k^h, s_k^h) \leq \xi\beta^{h_k}(u_k^h, s_k^h)^{\omega} \qquad \forall k \geq K$$

with K large enough and consequently (23).

An alternative criterion to (23) is the sufficient refinement condition

$$\sum_{k=0}^{\infty} f\big(S^{h_{k+1}}(u_{k+1}^h), u_{k+1}^h\big) - f\big(S^{h_k}(u_{k+1}^h), u_{k+1}^h\big) < \infty \tag{27}$$

that originates from the jumps in the differences of the cost functional due to refinement of the meshes which shall be summable.

Our convergence proof is given for criterion (26) which implies (23) after finitely many iterations if the algorithm refines infinitely many times. A convergence proof using condition (27) instead of (23) or (26) in the algorithm is very similar. Only a few details in the proof of Theorem 4.5 need to be adapted.

3.2. Statement of the adaptive multilevel trust-region algorithm. We now state the complete algorithm.

Algorithm 3.3. Adaptive multilevel trust-region algorithm

S0 *Initialization: Choose* $\varepsilon_{\text{tol}} > 0$, $0 < \alpha_0 \leq \alpha_1 < 1 < \alpha_2$, $0 < \eta_1 < \eta_2 < 1$, $\Delta_{\min} \geq 0$, $\xi_2 > 0$, $\delta > 0$, $\tilde{c}_y, \tilde{c}_\lambda, \tilde{c}_u > 0$, *an initial mesh* $\mathscr{T}_{h_0}$, $u_0^h \in U_{\text{ad}}^{h_0}$ *and* $\Delta_0 > 0$ *with* $\Delta_0 \geq \Delta_{\min}$. *Set* $k := 0$.

For $k = 0, 1, 2, \ldots$

S1 *Compute* $y_k^h = S^{h_k}(u_k^h)$ *as solution of the discretized state equation and the error estimator* $\eta_y^{h_k}(y_k^h)$ *for the state as in* D4 *or* D4′ (*if not already done*).

S2 *Compute the discretized adjoint state* $\lambda_k^h = S_{l_y}^{h_k}(y_k^h, u_k^h)$ *and the error estimator* $\eta_\lambda^{h_k}(\lambda_k^h, y_k^h, u_k^h)$ *for the adjoint as in* D4 *or* D4′. *Determine the inexact reduced gradient* $\hat{g}_k^h$ *by* (13) *and the criticality measure* $\|P_{U_{\text{ad}}^{h_k}}(u_k^h - \hat{g}_k^h)\|_U$.

S3 *If the refinement condition* (21) *holds then goto* S5.

S4 *If the refinement condition* (21a) *fails then refine the* Y*-grid adaptively. If* (21b) *or* (21c) *is violated then refine the* V*- or* U*-grid, respectively. Goto* S1.

S5 *If* $\eta_y^{h_k}(y_k^h) + \eta_\lambda(\lambda_k^h, y_k^h, u_k^h) + \|P_{U_{\text{ad}}^{h_k}}(u_k^h - \hat{g}_k^h)\|_U \le \varepsilon_{\text{tol}}$ *holds in* S5 *or during the refinement in* S4 *then stop and return* (y_k^h, u_k^h) *as approximate solution for problem* (1).

S6 *Compute* s_k^h *as inexact solution of* (12) *satisfying* (14) *and compute* $\text{pred}_k^h(s_k^h)$ *in* (16).

S7 *Compute a discrete state* $y_{k+1}^h = S^{h_k}(u_k^h + s_k^h)$ *and* $\text{ared}_k^h(s_k^h)$ *as in* (15).

S8 *If* $\rho_k^h = \text{ared}_k^h(s_k^h)/\text{pred}_k^h(s_k^h) \ge \eta_1$, *then provisionally accept* s_k^h, *update the trust-region radius according to* (17) *and goto* S9.
If the gradient accuracy condition (18) *is violated then refine the* Y*- and* V*-grid properly leading to a new mesh* h_k *and go back to* S1 *with* u_k^h.
Otherwise reject the step s_k^h *and reduce the trust-region radius according to* (17).
Set $(y_{k+1}^h, u_{k+1}^h) := (y_k^h, u_k^h)$, $k := k + 1$ *and goto* S6.

S9 *If* (26) *is satisfied* (*or* (23)) *then accept* s_k^h, *set* $(y_{k+1}^h, u_{k+1}^h) := (y_{k+1}^h, u_k^h + s_k^h)$, $k := k + 1$ *and goto* S2. *Otherwise reject* s_k^h, *refine the* Y*-grid properly leading to a new mesh* h_k *and go back to* S1 *with* u_k^h.

4. Convergence analysis

We make the following assumption.

Assumption 4.1. *The iterates* $u_k^h, u_k^h + s_k^h$ *remain in a bounded closed convex set* $D_U \subset U$ *with* $U_{\text{ad}} \subset D_U$ *and Assumptions* 2.1 *and* 2.3 *hold. By* A2 *and* D1 *we can choose* $D_Y \subset Y^+$ *bounded and* $S(u_k^h), S(u_k^h + s_k^h), S^{h_k}(u_k^h), S^{h_k}(u_k^h + s_k^h) \in D_Y$ *holds for all* k. *Finally, there exists* $M_H > 0$ *with*

$$\|\hat{H}_k\|_{L^2(U,U^*)} \le M_H \qquad \forall k.$$

Throughout this section we assume that Assumption 4.1 holds.

4.1. Well definedness of refinement conditions. First we will show that the gradient accuracy condition (18) can always be satisfied by sufficient refinement.

Lemma 4.2. *Let Assumption* 4.1 *hold. If* $\left\|P_{U_{\mathrm{ad}}}\big(u_k^h - \nabla\hat{f}(u_k^h)\big)\right\|_U > 0$ *then a new iteration* $k := k+1$ *is generated after finitely many grid refinements.*

Proof. As long as the algorithm stays in iteration k, the control u_k^h remains unchanged.

By Assumption 2.3, D3 and D4 or D4′ the refinement $(h_{k,j})_j \searrow 0$ within iteration k ensures together with the continuity properties in Assumption 2.1 that the left hand side of (21) tends to zero for $j \to \infty$. Moreover, by D3 we have with $y_{k,j}^h := S^{h_{k,j}}(u_k^h)$ and $\lambda_{k,j}^h := S_{l_y}^{h_{k,j}}(y_{k,j}^h, u_k^h)$

$$\hat{g}_k^{h_{k,j}}(u_k^h) = l_u(y_{k,j}^h, u_k^h, \lambda_{k,j}^h) \to l_u\big(S(u_k^h), u_k^h, S_{l_y}\big(S(u_k^h), u_k^h\big)\big) = \nabla\hat{f}(u_k^h). \quad (28)$$

Hence, the right hand side of (21) satisfies

$$\left\|P_{U_{\mathrm{ad}}^{h_k^j}}\big(u_k^h - \hat{g}_k^{h_{k,j}}(u_k^h)\big)\right\|_U \to \left\|P_{U_{\mathrm{ad}}}\big(u_k^h - \nabla\hat{f}(u_k^h)\big)\right\|_U =: \varepsilon > 0 \quad (29)$$

and thus (21) holds after finitely many refinements and S5 ist reached.

We show that after finitely many refinements also the gradient accuracy condition (18) in S8 is satisfied if it is checked. In fact, by D3 we have

$$\begin{aligned}(\hat{f}^{h_{k,j}})'(u_k^h) &= f_y(y_{k,j}^h, u_k^h)(S^{h_{k,j}})'(u_k^h) + f_u(y_{k,j}^h, u_k^h)\\ &\to f_y\big(S(u_k^h), u_k^h\big)S'(u_k^h) + f_u\big(S(u_k^h), u_k^h\big) = \hat{f}'(u_k^h).\end{aligned}$$

Hence, together with (28) we see that (18) eventually holds, since by (29) the right hand side of (18) is eventually $> \xi_2/2\min\{\left\|P_{U_{\mathrm{ad}}}\big(u_k^h - \nabla\hat{f}(u_k^h)\big)\right\|_U, \Delta_k\}\|s_{k,j}^h\|_U \geq$ const. $\|s_{k,j}^h\|_U$.

Finally, also the sufficient refinement criterion (26) in step S9 is satisfied after finitely many refinements. In fact, u_k^h and Δ_k remain unchanged and thus (29) yields after finitely many refinements $\|P_{U_{\mathrm{ad}}^{h_k}}(u_k^h - \hat{g}_k^h)\|_U \geq \varepsilon/2$. Since S9 is only reached if $\mathrm{ared}_k^h(s_{k,j}^h) \geq \eta_1\, \mathrm{pred}_k^h(s_{k,j}^h)$, the decrease condition (14) yields

$$\mathrm{ared}_k^h(s_{k,j}^h) \geq \eta_1\, \mathrm{pred}_k^h(s_{k,j}^h) \geq \frac{1}{2}\eta_1\kappa_1\varepsilon\min\left\{\kappa_2\frac{1}{2}\varepsilon, \kappa_3\Delta_k\right\} \geq \varepsilon' > 0.$$

Since $\beta^{h_{k,j}}(u_k^h, s_{k,j}^h) \to 0$ as $j \to 0$ by (25), the sufficient refinement criterion (26) is satisfied after finitely many iterations. □

4.2. Acceptance of steps. We start by estimating the difference of actual and predicted reduction.

Lemma 4.3. *Let Assumption* 4.1 *hold and let* $0 < \gamma \le 1$ *be such that* $\hat{f}^{h_k}$ *is* γ*-Hölder continuously differentiable, which is ensured Proposition* 2.4*. Then there exists* $C_{\mathrm{red}} > 0$ *such that for any inexact reduced gradient* $\hat{g}_k^h$ *satisfying the gradient accuracy condition* (18) *and any step* s_k^h *computed by the Algorithm* 3.3 *the inequality*

$$|\mathrm{ared}_k^h(s_k^h) - \mathrm{pred}_k^h(s_k^h)| \le C_{\mathrm{red}}(\Delta_k^{1+\gamma} + \Delta_k^2)$$

holds.

Proof. By the definition of actual and predicted reduction we have by using the γ-Hölder continuous differentiability of $\hat{f}^{h_k}$ on bounded sets, see Proposition 2.4, and the mean value theorem with a $\tau \in [0, 1]$

$$\begin{aligned}|\mathrm{ared}_h(s_k^h) - \mathrm{pred}_k^h(s_k^h)| \le{}& \left|\left(\nabla\hat{f}^{h_k}(u_k^h + \tau s_k^h) - \nabla\hat{f}^{h_k}(u_k^h), s_k^h\right)_U\right| \\ &+ \left|\left(\nabla\hat{f}^{h_k}(u_k^h) - \hat{g}_k^h, s_k^h\right)_U\right| + \frac{1}{2}\langle s_k^h, \hat{H}_k s_k^h\rangle_{U,U*} \\ \le{}& L_g\Delta_k^{1+\gamma} + \xi_2\Delta_k^2 + \frac{1}{2}M_H\Delta_k^2.\end{aligned}$$

Here, L_g denotes the uniform local Hölder constant of $\nabla\hat{f}^{h_k}$ and we have used (18), the boundedness of $\hat{H}_k$ and $\|s_k^h\|_U \le \Delta_k$. □

We next show that after finitely many trial iterations with possible refinements and reductions of the trust-region radius there will be a successful step. In particular, there is a lower bound for the trust-region radius if the criticality measure is bounded from below.

Lemma 4.4. *Let Assumption* 4.1 *hold. Let* $\varepsilon > 0$*, then there exists a constant* $\Delta' > 0$ *depending on* ε *such that if* $\|P_{U_{\mathrm{ad}}^{h_k}}(u_k^h - \hat{g}_k^h)\|_U > \varepsilon$ *and the gradient accuracy condition* (18) *holds then*

$$\mathrm{ared}_h(s_k^h) \ge \eta_1\,\mathrm{pred}_k^h(s_k^h)$$

for $\Delta_k \le \Delta'$*. In particular the step* s_k^h *will be eventually accepted in* S8 *and* $\Delta_{k+1} \ge \Delta_k$.

Proof. By Lemma 4.3 we have

$$|\mathrm{ared}_k^h(s_k^h) - \mathrm{pred}_k^h(s_k^h)| \le C_{\mathrm{red}}(\Delta_k^{1+\gamma} + \Delta_k^2).$$

On the other hand the decrease condition (14) yields

$$\begin{aligned}\mathrm{pred}_k^h(s_k^h) :=\geq \kappa_1 \|P_{U_{\mathrm{ad}}^{h_k}}(u_k^h - \hat{g}_k^h)\|_U \min\{\kappa_2 \|P_{U_{\mathrm{ad}}^{h_k}}(u_k^h - \hat{g}_k^h)\|_U, \kappa_3\Delta_k\} \\ \geq \kappa_1 \varepsilon \min\{\kappa_2\varepsilon, \kappa_3\Delta_k\}.\end{aligned}$$

Hence, there exists $\Delta' = \Delta'(\varepsilon) > 0$ such that

$$\frac{\mathrm{ared}_k^h(s_k^h)}{\mathrm{pred}_k^h(s_k^h)} - 1 \geq -\frac{|\mathrm{ared}_k^h(s_k^h) - \mathrm{pred}_k^h(s_k^h)|}{\mathrm{pred}_k^h(s_k^h)} \geq \eta_1 - 1 \qquad \forall 0 < \Delta_k \leq \Delta'.$$

This proves the first assertion.

Now consider step S8. The next iteration $k+1$ is only reached if the step is accepted or if possibly after mesh refinement the gradient accuracy condition (18) is satisfied. Hence, the decrease ratio is tested with (18) holding before a step is rejected and the trust region radius is reduced. After finitely many unsuccessful iterations we have $\Delta_k \leq \Delta'$ and the step is accepted. □

4.3. Global convergence result. We show now global convergence to a stationary point of the infinite dimensional problem (1) if $\varepsilon_{\mathrm{tol}} = 0$ or finite termination if $\varepsilon_{\mathrm{tol}} > 0$, respectively. We start with the following result.

Theorem 4.5. *Let Assumption* 4.1 *hold. If* $\varepsilon_{\mathrm{tol}} > 0$ *then Algorithm* 3.3 *terminates finitely. If* $\varepsilon_{\mathrm{tol}} = 0$ *then Algorithm* 3.3 *terminates finitely or the sequence of iterates generated by Algorithm* 3.3 *satisfies*

$$\liminf_{k\to\infty} \|P_{U_{\mathrm{ad}}^{h_k}}(u_k^h - \hat{g}_k^h)\|_U + \eta_y(y_k^h) + \eta_\lambda(\lambda_k^h, y_k^h, u_k^h) = 0. \tag{30}$$

Proof. Consider first the case $\varepsilon_{\mathrm{tol}} > 0$. Suppose that Algorithm 3.3 runs infinitely. Since $\|P_{U_{\mathrm{ad}}^{h_k}}(u_k^h - \hat{g}_k^h)\|_U + \eta_y(y_k^h) + \eta_\lambda(\lambda_k^h, y_k^h, u_k^h) > \varepsilon_{\mathrm{tol}}$ in S5 and (21) holds by S3, S4, there exists $\varepsilon > 0$ such that

$$\|P_{U_{\mathrm{ad}}^{h_k}}(u_k^h - \hat{g}_k^h)\|_U \geq \varepsilon \qquad \forall k.$$

By Lemma 4.4 there exists $\Delta' > 0$ such that for all accepted steps we obtain by the update rule for the trust-region radius

$$\Delta_k \geq \alpha_0\Delta' =: \Delta_*$$

and there is an infinite sequence of accepted steps. For all eccepted steps we get by the generalized Cauchy decrease condition (14)

$$\mathrm{ared}_k^h(s_k^h) \geq \eta_1\kappa_1\varepsilon \min\{\kappa_2\varepsilon, \kappa_3\Delta_*\} \geq \varepsilon' > 0 \tag{31}$$

for constants $\kappa_1, \kappa_2, \kappa_3 > 0$.

We will distinguish the two different cases where either only finitely many mesh refinements are performed by the algorithm or the algorithm produces infinitely many mesh refinements.

Let us first consider the case where only finitely many mesh refinements are carried out by the algorithm. Then there exists $K \in \mathbb{N}$ such that the mesh is not refined for all iterations with k larger than K. Consequently, condition (26) does not necessarily imply (23). Therefore, we give a separate proof for this case that is similar to the finite dimensional convergence theory.

By Assumption 4.1, u_k^h remains in a bounded set D_U and consequently $y_k^h = S^{h_k}(u_k^h)$ and also $S(u_k^h)$ remain in a bounded subset $D_Y \subset Y^+$. Hence, the sequence $\hat{f}^{h_k}(u_k^h) = f(y_k^h, u_k^h)$ as well as $\hat{f}(u_k^h) = f\big(S(u_k^h), u_k^h\big)$ is bounded below. Summation of the actual reduction in the successful steps gives

$$\begin{aligned}\sum_{k=0}^{\infty} \operatorname{ared}_k^h(s_k^h) &= \sum_{k=0}^{\infty} \big(\hat{f}^{h_k}(u_k^h) - \hat{f}^{h_k}(u_{k+1}^h)\big)\\ &= \sum_{k<K} \operatorname{ared}_k^h(s_k^h) + \sum_{k\geq K}^{\infty} \big(\hat{f}^{h_K}(u_k^h) - \hat{f}^{h_K}(u_{k+1}^h)\big)\\ &= \sum_{k<K} \operatorname{ared}_k^h(s_k^h) + \hat{f}^{h_K}(u_k^h) - \lim_{k\to\infty} \hat{f}^{h_K}(u_k^h) < \infty.\end{aligned}$$

Hence, the summability yields $\operatorname{ared}_h(s_k^h) \to 0$ as $k \to \infty$ bus this contradicts (31).

Let us now consider the case where the algorithm produces infinitely many refinements. Then condition (26) implies condition (23) for all $k \geq K$ with some $K > 0$. We then consider the exact actual reduction

$$\operatorname{ared}(s_k^h) := \hat{f}(u_k^h) - \hat{f}(u_k^h + s_k^h) = f\big(S(u_k^h), u_k^h\big) - f\big(S(u_k^h + s_k^h), u_k^h + s_k^h\big),$$

where S denotes the solution operator of the PDE constraint. Condition (23) then yields

$$\begin{aligned}\operatorname{ared}_k^h(s_k^h) &= \frac{\delta}{1+\delta} \operatorname{ared}_k^h(s_k^h) + \frac{1}{1+\delta} \operatorname{ared}_k^h(s_k^h)\\ &\geq \frac{\delta}{1+\delta} \operatorname{ared}_k^h(s_k^h) + \Big(\big(\hat{f}^{h_k}(u_k^h) - \hat{f}(u_k^h)\big) - \big(\hat{f}^{h_k}(u_{k+1}^h) - \hat{f}(u_{k+1}^h)\big)\Big)\\ &= \frac{\delta}{1+\delta} \operatorname{ared}_k^h(s_k^h) + \operatorname{ared}_k^h(s_k^h) - \operatorname{ared}(s_k^h)\end{aligned}$$

for all $k \geq K$, with some $\delta > 0$. Hence, using this inequality, we obtain

$$\operatorname{ared}(s_k^h) \geq \frac{\delta}{1+\delta} \operatorname{ared}_k^h(s_k^h) \geq \frac{\delta}{1+\delta} \eta_1 \operatorname{pred}_k^h(s_k^h) \geq \frac{\delta}{1+\delta} \eta_1 \varepsilon' \tag{32}$$

for all $k \geq K$. Now, by assumption, $\hat{f}(u_k^h)$ is bounded below. Summation of the infinite dimensional actual reduction in the successful steps gives

$$\sum_{k=0}^{\infty} \mathrm{ared}(s_k^h) = \hat{f}(u_0^h) - \lim_{k\to\infty} \hat{f}(u_k^h) < \infty.$$

Hence, the summability yields $\mathrm{ared}(s_k^h) \to 0$ as $k \to \infty$ which contradicts (32).

Now let $\varepsilon_{\mathrm{tol}} = 0$ and assume that (30) does not hold. Then there exists $\varepsilon'_{\mathrm{tol}} > 0$ small enough such that the algorithm would also not terminate for the stopping tolerance $\varepsilon'_{\mathrm{tol}} > 0$. But this contradicts the finite termination for $\varepsilon_{\mathrm{tol}} > 0$. □

By using the reliability of the error estimators, we obtain the following convergence result.

Corollary 4.6. *Let Assumption* 4.1 *hold. If* $\varepsilon_{\mathrm{tol}} = 0$ *then Algorithm* 3.3 *terminates finitely with a stationary point of problem* (1) *or the sequence of iterates generated by Algorithm* 3.3 *satisfies*

$$\begin{aligned}\liminf_{k\to\infty} \|C(y_k^h, u_k^h)\|_{V^*} + \|l_y(y_k^h, u_k^h, \lambda_k^h)\|_{Y^*} \\ + \left\|P_{U_ad}\left(u_k^h - \nabla_u l(y_k^h, u_k^h, \lambda_k^h)\right)\right\|_U\big) = 0.\end{aligned} \tag{33}$$

Proof. The steps S3 and S4 ensure that (21) holds and we have shown in 3.1.5 that Assumption 2.3, D4 or D4′ ensure (19).

Hence, if the algorithm runs infinitely then (30) implies by (19) the assertion (33).

If the algorithm terminates finitely then $\|P_{U_{\mathrm{ad}}^{h_k}}(u_k^h - \hat{g}_k^h)\|_U = 0$ and (19) shows with $U_{\mathrm{ad}}^{h_k} \subset U_{\mathrm{ad}}$ (see D3) that (y_k^h, u_k^h) satisfies (9). □

5. Numerical results

In this section we present some numerical results for the adaptive multilevel trust-region method. The algorithm has been implemented in MATLAB. We use the method of lines with conformal finite element discretization in space by quadratic finite elements and the 3-stage Rosenbrock method ROS3P from [19] in time. Moreover, our MATLAB implementation uses adaptive refinement in time and uniform refinement in space. We present results for a semilinear parabolic boundary control problem with control constraints of the form (2).

Further results can be found in [25]. Moreover, we have coupled the presented algorithm with the highly efficient PDAE solver KARDOS, which uses adaptive refinements in space and time, and have applied it to a realistic glass cooling problem as well as a thermistor problem, see [5–7].

5.1. An a posteriori error estimator for parabolic PDEs. In our numerical examples we used the error estimator from [8]. We briefly sketch the main ideas of this error estimator. The derivation, proofs and numerical tests can be found in [8].

The error estimator is designed for parabolic initial boundary value problems as the state PDE in (2). The PDE is discretized with the method of lines using for example finite elements in space with a spatial mesh of characteristic mesh size h and an existing time integrator for the resulting system of ordinary diferential equations (ODEs). Let $y_h(t)$ be the unique solution vector of the resulting system of ODEs representing the spatial degrees of freedom. Moreover, let $v_h(t_i)$ denote its approximations in the time grid point t_i on a certain timegrid obtained by applying a numerical integration method of order $p \leq 3$ and denote by $v_h(t)$ an interpolatory polynomial by using Lagrange or Hermite interpolation. The global time error is then defined by $e_h(t) = v_h(t) - y_h(t)$. Let $R_h : y(t, \cdot) \mapsto R_h y(t)$ be the restriction operator which maps $y(t)$ to its spatial degrees of freedom. Then the spatial discretization error is defined by $\eta_h(t) = y_h(t) - R_h y(t)$, where y denotes the solution of the PDE. The overall discretization error $E_h(t) = v_h(t) - R_h y(t)$ is then given as the sum of global time and spatial error, $E_h(t) = e_h(t) + \eta_h(t)$.

Debrabant and Lang approximate these residuals by solving a linear spatial error transport equation and a linear time error transport equation. They involve the spatial truncation error, which is in [8] estimated by Richardson extrapolation, and the residual time error, respectively. The obtained approximations of the global error $\tilde{E}_h(t) = \tilde{e}_h(t) + \tilde{\eta}_h(t)$ can be controlled by spatial and temporal adaptivity. [8] conclude that based on tolerance proportionality, reducing the local error tolerances by a factor will reduce the global error by the same factor. Hence, given a prescribed tolerance for the global error, the local tolerances can be chosen appropriately. If the global error is not below a prescribed tolerance, the state computation is redone with adjusted tolerances and refined spatial resolution, cf. [8].

In the context of our adaptive multilevel trust-region algorithm global error estimators for the difference between the solution y_h of the discretized PDE and the infinite dimensional solution y of the original PDE are required. With the global estimates of the space and time error from [8], we obtain the error estimate

$$\|v_h - R_h y\|^2_{L^2(0,T;\mathrm{H}^1(\Omega))} \approx \int_0^T \|\tilde{E}_h(t)\|^2_{\mathrm{H}^1(\Omega)}\, dt. \tag{34}$$

Numerical tests show that the approach yields accurate estimates of global space and time error [8].

5.2. Local refinement and its implementation. The error estimator of Debrabant and Lang [8] provides an estimate of the global space and time error. Moreover, since the error estimator is computed while solving the discretized PDE, the timestep size can be adjusted adaptively such that the local time residual estimation is a suitable portion of a predefined tolerance for the global time error. Thus, a time refinement results in a change of the predefined tolerance for the local time residual, a solve of the discretized PDE including the residual estimation and the possible insertion of additional timepoints.

Thus, since the error estimator provides a global time and space error estimation, we implement the refinement criteria (21) by first checking the refinement condition just for the global time error, here given exemplarily for the state equation

$$\eta_{y,t}(y_k^h) \le c_{y,t} \| P_{U_{\mathrm{ad}}^{h_k}}(u_k^h - \hat{g}_k^h) \|_U, \tag{35}$$

where $\eta_{y,t}$ denotes the error estimator for the time error and $c_{y,t} > 0$ is the (appropriately chosen) constant for the time refinement in the state. For the adjoint state the equation looks the same with λ instead of y. After having checked the refinement condition for the state in time, the refinement condition (21) with the estimation of the global space-time error is tested.

To prevent too much spatial refinements if the stationary measure becomes very small on the current grid, we modify the spatial refinement condition (21) with an additional space residual tolerance $\varepsilon_x > 0$ of the form

$$\eta_{y,x}(y_k^h) \le \max\{\tilde{c}_y \| P_{U_{\mathrm{ad}}^{h_k}}(u_k^h - \hat{g}_k^h) \|_U, \varepsilon_x\} \tag{36}$$

and analogously for the adjoint with y replaced by λ. By choosing the space residual tolerance for example as $\varepsilon_x = \min\{\tilde{c}_y, 1/3\}\varepsilon_{\mathrm{tol}}$, an additional refinement when the criticality measure drops below the stop tolerance can be prohibited. Nevertheless, space refinements are still possible through the gradient condition (18) such that convergence of the criticality measure to the prescribed tolerance $\varepsilon_{\mathrm{tol}}$ can still be guaranteed.

We describe the adaptive refinement strategy. If a time refinement is triggered by the state error estimation we do not only compute the state on an adaptively refined timegrid but also perform an adaptive solve of the discretized adjoint PDE with the same predefinded tolerance for the global time residual estimation in the adjoint state as before and possibly additional timepoints due to the (slightly) different state. If a time refinement is necessary by the adjoint error estimate it is done vice versa. After such a refinement the timegrid is fixed. In our implementation a spatial refinement is performed as a uniform refinement of the space grid followed by an adaptive time refinement during the state and adjoint computation as described above. For numerical results with the fully space-time adaptive solver Kardos, we refer to [5–7].

Let $\mathrm{Tol}_{A,y}, \mathrm{Tol}_{R,y} > 0$ denote the tolerances for the control of the adaptive stepsize choice for the state computation as described in [8] and $\mathrm{Tol}_{A,\lambda}, \mathrm{Tol}_{R,\lambda} > 0$ the corresponding ones for the adjoint state computation. Let $\eta_{y,t}$ denote the estimator for the time error in the state computation. Let $c_{y,t} > 0$ denote the refinement constant in (21a) for the time error. We then implemented the following refinement procedere for the state in time:

While $\eta_{y,t} > c_{y,t} \| P_{U_{\mathrm{ad}}^{h_k}}(u_k^h - \hat{g}_k^h)\|_U$, do

1. Set $\varepsilon = \big(c_{y,t}\|P_{U_{\mathrm{ad}}^{h_k}}(u_k^h - \hat{g}_k^h)\|_U\big)/(1.2 \cdot \eta_{y,t})$.
   Set $\mathrm{Tol}_{A,y} = \max\big(0.2, \min(\varepsilon, 0.9)\big) \cdot \mathrm{Tol}_{A,y}$.
   Set $\mathrm{Tol}_{R,y} = \max\big(0.2, \min(\varepsilon, 0.9)\big) \cdot \mathrm{Tol}_{R,y}$.
2. Recompute the state with $\mathrm{Tol}_{A,y}$, $\mathrm{Tol}_{R,y}$ and insert additional timepoints when necessary.
3. Recompute the adjoint state with $\mathrm{Tol}_{A,\lambda}$, $\mathrm{Tol}_{R,\lambda}$ and insert additional timepoints when necessary.
4. Recompute $\hat{g}_k^h$ and $\|P_{U_{\mathrm{ad}}^{h_k}}(u_k^h - \hat{g}_k^h)\|_U$.

The refinement procedere for the adjoint state in time is the same as for the state with changed roles of y and λ. In our examples, the refinement procedures both in time or in space and time usually needed only one refinement iteration.

5.3. A semilinear parabolic optimal boundary control problem. We consider the following semilinear parabolic boundary control problem of the form (2).

Let $\Omega = (0,1) \times (0,1) \subset \mathbb{R}^2$, $T = 1$, $\Sigma_T := (0,T) \times \partial\Omega$, $\alpha > 0$, $a, b \in L^\infty(\Sigma_T)$ and set $U = L^2(\Sigma_T)$, $H = L^2\big((0,T)\times\Omega\big)$, and $Q = H^1\big((0,T)\times\Omega\big)$. With the Gelfand triple $Q \hookrightarrow H = H^* \hookrightarrow Q^*$ we set

$$Y = W(0,T) = \{y \in L^2(0,T;Q) : y_t \in L^2(0,T;Q^*)\},$$
$$V = V_1 \times V_2 = L^2(0,T;Q) \times H.$$

Moreover, let $y_0 \equiv 1$ in $\overline{\Omega}$, $y_d \equiv 0.2$ in $\overline{\Omega}$ and let $y_Q(t,x) = 1 - 0.8t$, $(t,x) \in [0,1] \times \overline{\Omega}$. Then the problem is given by

$$\begin{aligned}
&\min_{y \in Y, u \in U} f(y,u) := \frac{1}{2}\|y(T) - y_d\|^2_{L^2(\Omega)} + \frac{1}{2}\|y - y_Q\|^2_{L^2((0,T)\times\Omega)} + \frac{\alpha}{2}\|u\|_U^2 \\
&\text{s.t.} \quad y_t - \Delta y = 0 \qquad \text{in } (0,T)\times\Omega, \\
&\qquad\quad y_n = u - y^3|y| \qquad \text{on } (0,T)\times\partial\Omega =: \Sigma_T, \\
&\qquad\quad y(0,\cdot) = y_0 \qquad \text{in } \Omega, \\
&\qquad\quad a \le u \le b,
\end{aligned} \tag{37}$$

where y_n denotes the outer normal derivative and the state equation has to be understood in the weak sense.

Hence, $U_{\rm ad} = \{u \in U : a \le u \le b\}$ is a bounded, convex and closed subset of $L^\infty(\Sigma_T)$ and of U.

5.3.1. Verification of Assumption 2.1. We now verify Assumption 2.1 with $Y^+ := Y \cap C([0,T] \times \overline{\Omega})$ and $D_U := U_{\rm ad}$. A1 is obvious.

Since $U_{\rm ad}$ is bounded in $L^\infty(\Sigma_T)$, the state PDE admits for all $u \in U_{\rm ad}$ a unique weak solution $y \in Y \cap C([0,T] \times \overline{\Omega})$, see [23], Thm. 5.5 and the solution remains in a convex bounded closed set $D_Y \subset Y^+$. Moreover, by [23], Thm. 5.8 the solution mapping $S : u \in L^s(\Sigma_T) \to S(u) \in Y^+$ is Lipschitz continuous for $s > 3$. Since $D_U = U_{\rm ad}$ is bounded in $L^\infty(\Sigma_T)$ and by interpolation $\|u\|_{L^s} \le \|u\|_U^{2/s} \|u\|_{L^\infty}^{1-1/s}$, we conclude that $S : (D_U, \|\cdot\|_U) \to Y^+$ is Hölder continuous. This proves A2.

To verify A3 we note that the weak solution of the state equation is the unique solution of the operator equation $C(y,u) = 0$, where

$$C : Y^+ \times U \mapsto \begin{pmatrix} L^2(0,T;Q^*) \\ H \end{pmatrix} = V_1^* \times V_2^* = V^*$$

$$C(y,u) := \begin{pmatrix} y_t + (\nabla y, \nabla \cdot)_{L^2((0,T)\times\Omega)} + (y^3|y| - u, \cdot)_{L^2(\Sigma_T)} \\ y(0,\cdot) - y_0 \end{pmatrix}.$$

From standard parabolic theory it is obvious that the linear part of $C(y,u)$ is in $L(Y \times U, V^*)$. We study now the differentiability properties of the nonlinear term

$$B : y \in Y^+ \mapsto (y^3|y|, \cdot)_{L^2(\Sigma_T)} \in L^2(0,T;Q^*) = V_1^*.$$

It is obvious that $B : Y^+ \to V_1^*$ is continuously Fréchet differentiable with derivative

$$B'(y)v = (4|y|^3 v, \cdot)_{L^2(\Sigma_T)} \in V_1^*.$$

Since $D_Y \subset Y^+$ is bounded, also the operator $B : (D_Y, \|\cdot\|_Y) \to V_1^*$ is well defined. Moreover, for all $y \in D_Y$ the operator $B'(y)$ admits an extension $B'(y) \in L(Y, V_1^*)$. In fact, we have $Y \hookrightarrow V_1 \hookrightarrow L^2\big(0,T;L^p(\partial\Omega)\big)$ for all $1 \le p < \infty$ and thus

$$\begin{aligned} \langle B'(y)v, w\rangle_{V_1^*,V_1} &= (4|y|^3 v, w)_{L^2(\Sigma_T)} \le 4\|y\|_{Y^+}^3 \|v\|_{L^2(\Sigma_T)} \|w\|_{L^2(\Sigma_T)} \\ &\le c\|y\|_{Y^+}^3 \|v\|_Y \|w\|_{V_1}. \end{aligned}$$

Finally, we show that also $B : (D_Y, \|\cdot\|_Y) \to V_1^*$ is continuously Fréchet differentiable with γ-Hölder continuous derivative for all $0 < \gamma < 1$.

We start by showing that $B' : (D_Y, \|\cdot\|_Y) \to L(Y, V_1^*)$ is γ-Hölder continuous for all $0 < \gamma < 1$. We will need the embedding $Y \hookrightarrow L^{2/s}\big(0, T; L^{1/(1-s)}(\partial\Omega)\big)$ for all $1/2 < s < 1$. In fact, the embedding can be proven as follows. The trace theorem and interpolation yields for $1/2 < s < 1$

$$\|\cdot\|_{H^{s-1/2}(\partial\Omega)} \le c\|\cdot\|_{H^s(\Omega)} \le c\|\cdot\|_Q^s \|\cdot\|_H^{1-s}$$

and thus, since $Y = W(0,T) \hookrightarrow C([0,T]; H)$ and $H^{s-1/2}(\partial\Omega) \hookrightarrow L^{1/(1-s)}(\partial\Omega)$

$$\|\cdot\|_{L^{2/s}(0,T;L^{1/(1-s)}(\partial\Omega))} \le c\|\cdot\|_{L^{2/s}(0,T;H^{s-1/2}(\partial\Omega))} \le c\|\cdot\|_{L^\infty(0,T;H)}^{1-s}\|\cdot\|_{L^2(0,T;Q)}^{s} \le c\|\cdot\|_Y.$$

There exists a constant $R > 0$ such that

$$\|y\|_{Y^+}, \|y+h\|_{Y^+} \le R \qquad \forall y, y+h \in D_Y.$$

For all $y, y+h \in D_Y$ Taylor expansion yields with $r := \int_0^1 12(y+\tau h)|y+\tau h|\, d\tau$

$$\big\langle \big(B'(y+h) - B'(y)\big)v, w\big\rangle_{V_1^*, V_1} = (rhv, w)_{L^2(\Sigma_T)}.$$

We have the embedding $V_1 \hookrightarrow L^2\big(0, T; H^{1/2}(\partial\Omega)\big) \hookrightarrow L^2\big(0, T; L^p(\partial\Omega)\big)$ for all $1 \le p < \infty$. Let now $p \ge 2$ (will be adjusted later depending on γ) and let p' be the dual index with $1/p + 1/p' = 1$. Then

$$(rhv, w)_{L^2(\Sigma_T)} \le 12R^2 c\|hv\|_{L^2(0,T;L^{p'}(\partial\Omega))}\|w\|_{V_1}.$$

Fix an arbitrary $0 < \gamma < 1$ and set $q = 2\gamma + 2$. Moreover, choose $1/2 < s < 1$ with $2/s = q$ and $1 < p' < 2$ with $2p' \le \frac{1}{1-s}$. Then $Y \hookrightarrow L^q\big(0, T; L^{2p'}(\partial\Omega)\big)$, $1/2 = 1/q + \gamma/q$ and thus

$$\|hv\|_{L^2(0,T;L^{p'}(\partial\Omega))} \le \|h\|_{L^{q/\gamma}(0,T;L^{2p'}(\partial\Omega))}\|v\|_{L^q(0,T;L^{2p'}(\partial\Omega))} \le cR^{1-\gamma}\|h\|_Y^\gamma \|v\|_Y.$$

Thus, $B' : (D_Y, \|\cdot\|_Y) \to L(Y, V_1^*)$ is γ-Hölder continuous for all $0 < \gamma < 1$.

Now the Fréchet-differentiability of $B : (D_Y, \|\cdot\|_Y) \to V_1^*$ follows easily. Pointwise Taylor expansion with integral remainder term yields with the γ-Hölder continuity of B'

$$\begin{aligned}&\langle B(y+h) - B(y) - B'(y)h, w\rangle_{V_1^*, V_1}\\ &\qquad \le \int_0^1 \|B'(y+\tau h) - B'(y)\|_{L(Y, V_1^*)}\, d\tau \|h\|_Y \|w\|_{V_1} \le c\|h\|_Y^{1+\gamma}\|w\|_{V_1}.\end{aligned}$$

Using the properties of B we have shown that $C : (D_Y, \|\cdot\|_Y) \times U \mapsto V^*$ is Fréchet-differentiable with γ-Hölder continuous derivative for all $0 < \gamma < 1$. To conclude the verification of A3 we note that for $(y,u) \in D_Y \times D_U$ the linear parabolic operator $C_y(y,u) \in L(Y,V^*)$ has a bounded inverse by standard parabolic theory, since the nonlinear term $(4|y|^3\cdot,\cdot)_{L^2(\Sigma_T)}$ is continuous and nonnegative on $L^2(\Sigma_T) \times L^2(\Sigma_T)$.

Finally, it can be shown that the problem (37) has at least one optimal solution, cf. [23], Thm. 5.7.

5.3.2. Numerical results. We present now numerical results for problem (37). We use the method of lines with quadratic finite elements in space and the 3-stage Rosenbrock method ROS3P from [19] in time. For the discretization of the adjoint equation we use also quadratic finite elements in space and ROS3P in time. For the mesh refinement we apply the a posteriori time and space error estimator of [8] and adaptive time refinement as described in 5.2 as well as uniform refinement in space.

For the approximate solution of the trust-region problem we use the projected cg-Newton algorithm [26], Alg. 5.10 with at most 10 cg iterations, where we compute $\hat{H}_k v$ by the discretized version of the exact evaluation of the Hessian vector product based on the standard adjoint formula, see [15], §1.6.5.

For the particular instance of (37) we set $a = -0.2$, $b = 0.3$, and $\alpha = 1\mathrm{e}-2$. In Algorithm 3.3 with the implementation details of 5.2 we have chosen $\varepsilon_{\mathrm{tol}} = 5\mathrm{e}-5$, $\varepsilon_x = 8\mathrm{e}-4$, $c_{y,t} = 0.5$, $\tilde{c}_y = 10$, $c_{\lambda,t} = 0.5$, $\tilde{c}_\lambda = 10$, $\tilde{c}_u = 0.25$, and $\xi_2 = 1.5$. The starting control was $u_0^h \equiv 0$.

Table 1 depicts the iteration history. The first column shows the iteration number, the second column the type of refinement. *cm* is the discrete criticality measure, η_u is the error in the discrete criticality measure (left hand side of (21c)), $\eta_{y,t}/\eta_{\lambda,t}$ and $\eta_{y,x}/\eta_{\lambda,x}$ denote the time and space error of state/adjoint according to 5.2 and the last column shows the size of the (x,t)-grid.

Figure 1 shows the computed optimal state at end time T with two different scalings of the y-axis. One sees that the desired state $y_d \equiv 0.2$ is reached quite accurately. Moreover, the adaptive time grid of the final discretization is shown. The bound constraints become sigificantly active for the computed optimal control u_k^h.

It can be seen that the algorithm requires several refinements for the state and the adjoint in time and two times also in space to achieve the prescribed spatial tolerance. Particularly, the refinement for the adjoint in time in iteration 2 shows that the current discretization was not suitable to compute a sufficiently accurate adjoint state, implying that the gradient could not be resolved adequately. All residuals are driven to zero by suitable refinement. Thus, the residuals in the optimality system are reduced efficiently to the desired tolerance and most of the optimization iterations are carried out on coarser grids, only the last few iterations require execution on the finest mesh.

Table 1. Iteration history for problem 37

It.	Refine	cm	η_u	$\eta_{y,t}$	$\eta_{y,x}$	$\eta_{\lambda,t}$	$\eta_{\lambda,x}$	(x,t)-grid
0		2.7e − 1	0.0e0	1.8e − 4	4.6e − 3	5.3e − 3	7.7e − 2	289 × 32
1		4.4e − 2	0.0e0	2.8e − 4	9.6e − 3	1.3e − 2	2.1e − 2	289 × 32
2	 adjoint t	1.4e − 2 1.4e − 2	 1.9e − 4	8.6e − 4 5.2e − 4	1.6e − 2 7.6e − 3	8.0e − 3 3.6e − 4	1.4e − 2 7.5e − 3	289 × 32 289 × 57
3		8.4e − 3	8.5e − 4	2.4e − 4	9.4e − 3	1.6e − 4	3.7e − 3	289 × 57
4		3.2e − 3	7.2e − 4	5.3e − 4	1.1e − 2	8.8e − 5	1.8e − 3	289 × 57
5		1.2e − 3	2.2e − 4	3.2e − 4	1.0e − 2	4.6e − 5	9.9e − 4	289 × 57
6		1.5e − 3	1.6e − 4	4.9e − 4	9.5e − 3	7.6e − 5	1.5e − 3	289 × 57
7		1.5e − 3	2.0e − 4	4.4e − 4	1.0e − 2	6.7e − 5	1.3e − 3	289 × 57
8	 state x,t	4.0e − 4 4.8e − 3	 1.6e − 5	4.1e − 4 2.0e − 4	1.0e − 2 2.9e − 3	6.1e − 5 7.2e − 5	1.2e − 3 1.1e − 3	289 × 57 1089 × 113
9		2.1e − 3	2.2e − 6	2.0e − 4	2.8e − 3	6.8e − 5	1.0e − 3	1089 × 113
10		1.8e − 3	1.2e − 4	9.8e − 5	2.7e − 3	7.4e − 5	1.1e − 3	1089 × 113
11		7.8e − 4	1.2e − 5	9.8e − 5	2.8e − 3	4.9e − 5	4.5e − 4	1089 × 113
12		4.5e − 4	3.3e − 5	4.5e − 5	2.8e − 3	5.7e − 5	7.4e − 4	1089 × 113
13	 state x,t	1.1e − 4 8.0e − 5	 1.0e − 5	3.9e − 5 1.3e − 5	2.8e − 3 7.2e − 4	4.6e − 5 1.8e − 5	6.3e − 4 3.1e − 4	1089 × 113 4225 × 228
14		1.1e − 4	1.2e − 5	9.8e − 6	7.3e − 4	1.9e − 5	3.2e − 4	4225 × 228
15		1.2e − 4	9.5e − 6	5.4e − 6	7.6e − 4	2.0e − 5	3.3e − 4	4225 × 228
16		1.1e − 4	9.0e − 6	5.4e − 6	7.6e − 4	2.0e − 5	3.3e − 4	4225 × 228
17	 adjoint t	2.1e − 5 2.3e − 5	 5.0e − 6	5.4e − 6 3.0e − 6	7.6e − 4 3.9e − 4	1.9e − 5 9.0e − 6	3.1e − 4 1.8e − 4	4225 × 228 4225 × 306

6. Conclusions

In this paper we have presented an adaptive multilevel trust-region algorithm for optimization problems governed by nonlinear PDEs with control constraints. The algorithm starts on a coarse discretization of the problem and combines an efficient trust-region method with an implementable adaptive refinement strategy for the current discretization based on a posteriori error estimators. The refinements are controlled by a criticality measure which we choose as the norm of the projected gradient step. The optimization method can be used with any given

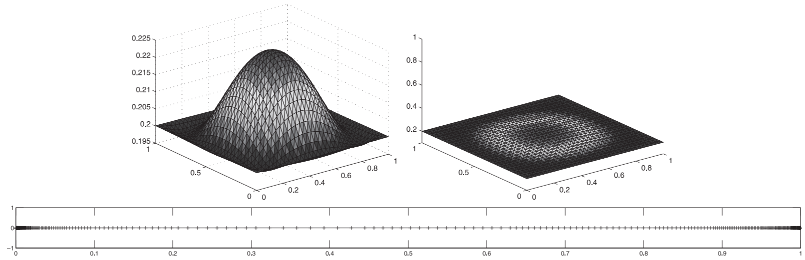

Figure 1. Optimal state of problem (37) at time T in two scalings of the y-axis (top) and adaptive time grid of the last discretization (bottom).

adaptive state and adjoint solvers. In particular, highly efficient solvers for unsteady PDEs can be coupled with the optimization framework. The resulting inexactness of the reduced gradient in the discretizations is controlled by the algorithm. The presented numerical example shows that the algorithm carries out most optimization iterations on relatively coarse discretizations. The error estimators for the state and the adjoint equation as well as the criticality measure are efficiently driven to zero. Thus, the algorithm is a promising rigorous framework for a globally convergent adaptive multilevel method for PDE constrained optimization problems with control constraints that can be used with PDE solvers provided by the user. The approach presented in this paper has several advantages: 1) Different solvers for the state and the adjoint PDE can be used within this optimization framework. 2) The mesh is refined as needed during the optimization algorithm to approach the solution of the PDE constrained problem with control constraints efficiently. 3) (First order) convergence of the proposed multilevel algorithm for nonlinear, non-convex, PDE constrained optimization problems with control constraints is proven.

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