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**Regularization of Constrained PDEs of
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REGULARIZATION OF CONSTRAINED PDES OF SEMI-EXPLICIT STRUCTURE

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ABSTRACT. A general framework for the regularization of constrained PDEs, also called operator DAEs, is presented. The given procedure works for semi-explicit operator DAEs of first order which includes the Navier-Stokes and other flow equations. This reformulation is a regularization in the sense that a semi-discretization in space leads to a DAE of lower index, i.e., of differentiation index 1 instead of 2. The regularized operator DAE may help to construct numerically stable discretization schemes and thus, lead to a more efficient simulation.

Key words. PDAE, operator DAE, regularization, index reduction, evolution equations, method of lines, mixed finite elements

AMS subject classifications. 65J08, 65J15, 65M20, 65L80

1. INTRODUCTION

Constrained PDEs arise naturally in the modelling of physical, chemical, and many other real-world phenomena. For example, they occur whenever different PDE models are coupled, e.g., via mutual variables at the interfaces, since the coupling is typically modelled via algebraic constraints. We will consider these couplings of ordinary or partial differential equations (ODEs, PDEs) in line with other constrained PDEs – often referred to as PDAEs – as differential-algebraic equations (DAEs) in function spaces, so-called abstract or operator DAEs.

Examples of abstract DAE models can be found in all kinds of applications. They are widely used in flexible multibody dynamics, e.g., the pantograph and catenary benchmark problem [AS00] or the flexible slider crank mechanism [Sim96, Sim06]. Flow equations such as the Navier-Stokes equations are constrained by the divergence-free condition [Tem77, Wei97]. Further applications can be found in circuit simulation [Tis04], electromagnetics, and chemical engineering [CM99].

Despite the large range of applications and the advantages from the modeling perspective, their mathematical analysis is still not well understood. There is still no common classification like the index concepts for DAEs [LMT13, Ch. 12]. The generalization of the *tractability index* as proposed, e.g., in [Tis04] does not apply for the commonly used formulation by means of *Gelfand triples*.

The very general concept of the *perturbation index*, as it was defined in [RA05] for linear PDAEs, applies under strong regularity conditions but is still ambiguous in the choice of the norm in which one measures the perturbation and their derivatives. Also the *differentiation index* was generalized to PDAEs [MB00] but has difficulties with the agreement of the PDAE index with the index of the semi-discretized DAE. Yet another idea is to classify the index of a PDAE directly by the index that may be determined after

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a spatial discretization. This, however, leads to the similar unclear problem, what a good discretization of a PDAE is.

The aim of this paper is to introduce an index reduction method of PDAEs without introducing an index of such a system. Here, we only use the index of the semi-discretized system after a discretization in the space variable. Thus, we apply a reformulation of the given PDAE system such that a semi-discretization by finite elements leads to a DAE of lower index. The idea is that a transformation on the operator level can be the base for numerically advantageous discretization schemes. The commonly taken approach of first discretizing and then transforming the equations comes with the latent risk that the algebraic manipulation are not valid in infinite dimensions [Hei14]. This may cause instabilities or inconsistencies as the discretization becomes more accurate.

Within this paper, we analyse constrained systems of first order and semi-explicit structure, particularly we consider systems of the form

$$\begin{aligned} \dot{u} + \mathcal{K}u + \mathcal{B}^* \lambda &= \mathcal{F}, \\ \mathcal{B}u &= \mathcal{G}. \end{aligned}$$

In the case of a nonlinear constraint, the place of dual operator \mathcal{B}^* in the first line is taken by the dual of its Fréchet derivative. Throughout this paper, we use the beneficial notion of operators and thus, refer to PDAEs as operator DAEs.

In view of numerical simulations, the incorporation of the constraints via a Lagrange multiplier and a suitable reformulation seem particularly promising when the side condition $\mathcal{B}u = \mathcal{G}$ is nonlinear. The direct approach of resolving the constraint by approximating an implicit function $u_2 = \mathcal{R}(u_1)$ comes with several difficulties. It is known that this approach can cap the convergence of classical Runge-Kutta methods to second order [Arn98a]. The situation is likely to be worse, when the computation of $u_2 = \mathcal{R}(u_1)$ is done with an error. Also, there may be no implicit function for resolving the side conditions a-priori. This is the case if \mathcal{B} is not injective, as in the Stefan problem [Fri68], or if it is nonlocal, e.g. if it contains spatial derivatives as in Robin boundary conditions like the nonlinear Stefan-Boltzmann conditions.

To provide the theoretical framework we proceed as follows. In Section 2 we recall the notion of Gelfand triples and Nemytskii maps, which are basic tools in functional analysis for the formulation of operator differential equations. These tools are then used for the formulation and regularization of the operator DAEs in Section 3. Here we provide a general framework for linear (time-dependent) as well as nonlinear constraints. The advantages of the obtained formulation and the justification of calling this procedure an index reduction on operator level is topic of Section 4. Therein, the spatial discretization by finite elements is discussed. In particular, we discuss the index of the resulting DAEs of the original and regularized operator equations. In Section 5 we provide two examples which fit in the given framework. An example with linear constraints is given by the Navier-Stokes equations. The nonlinear setting is applied to the regularized two-phase Stefan problem. Finally, we summarize and conclude in Section 6.

2. PRELIMINARIES

This section is devoted to the introduction of spaces and operators which are needed for the analysis in Section 3 below. Throughout this paper, we use the standard notion of Sobolev spaces [AF03] and Bochner spaces [Rou05, Ch. 1.5].

2.1. Spaces. To keep the setting as general as possible, we consider a real, separable, and reflexive Banach space \mathcal{V} and a real separable Hilbert space \mathcal{H} . We assume that the spaces

\mathcal{V} , \mathcal{H} , and \mathcal{V}^* form a *Gelfand triple* (also called evolution triple) [Zei90, Ch. 23.4]. This means that \mathcal{V} is densely, continuously embedded in \mathcal{H} and that \mathcal{H} and its dual space \mathcal{H}^* are identified via the *Riesz isomorphism*. Such a triple implies the inclusion $\mathcal{H}^* \hookrightarrow \mathcal{V}^*$ in the sense that for $h \in \mathcal{H} \cong \mathcal{H}^*$ and $v \in \mathcal{V}$ we have

$$\langle h, v \rangle_{\mathcal{V}^*, \mathcal{V}} = (h, v)_{\mathcal{H}}.$$

The space for the constraint is denoted by \mathcal{Q} and is assumed to be a real, separable, and reflexive Banach space. The constraint operator \mathcal{B} then maps from \mathcal{V} to \mathcal{Q}^* . Together with its dual operator \mathcal{B}^* , we obtain the following diagram:

$$\begin{array}{ccccc} \mathcal{V} & \xrightarrow{\mathcal{d}} & \mathcal{H} = \mathcal{H}^* & \xrightarrow{\mathcal{d}} & \mathcal{V}^* \\ & \searrow \mathcal{B} & & \nearrow \mathcal{B}^* & \\ & & \mathcal{Q}^* & & \mathcal{Q} \end{array}$$

Example 2.1. A typical example for a Gelfand triple $\mathcal{V}, \mathcal{H}, \mathcal{V}^*$ is given by the Sobolev spaces $\mathcal{V} := H_0^1(\Omega)$, $\mathcal{H} := L^2(\Omega)$, and $\mathcal{V}^* = H^{-1}(\Omega)$.

We will consider the time derivatives in the generalized sense as defined, e.g., in [Zei90, Ch. 23.5]. We require solutions of system (3.1) to satisfy

$$u \in L^p(0, T; \mathcal{V}) \quad \text{with} \quad \dot{u} \in L^q(0, T; \mathcal{V}^*),$$

where $1 < q \leq p < \infty$. If q is the conjugated exponent, i.e. $1/p + 1/q = 1$, then, by the well-known embedding theorems for Gelfand triples [Zei90, Th. 23.23], it holds that such a solution u is continuous as a function $u: [0, T] \rightarrow \mathcal{H}$, i.e., $u \in C([0, T], \mathcal{H})$. Thus, an initial condition $u(0) = g$ for $g \in \mathcal{H}$ is well-defined.

Remark 2.1. The regularization proposed in Section 3 operates with splittings of the state space \mathcal{V} and is independent of the time regularity of the function u or \dot{u} . Thus, we can also consider less regular systems with $\dot{u} \in L^q(0, T; \mathcal{V}^*)$ with $q \leq 1 - 1/p$, as they may appear in applications. However, we will have to assume the well-posedness of an initial condition.

Remark 2.2. Assuming that $q \leq p$ is no restriction for applications, where typically $p \geq 2$ and, thus, the conjugated exponent is smaller than 2. In this case, one can deduce from the boundedness of the set $(0, T)$ and from the continuous embedding $\mathcal{V} \hookrightarrow \mathcal{H} \hookrightarrow \mathcal{V}^*$ that $v \in L^p(0, T; \mathcal{V})$ is also a function in $L^q(0, T; \mathcal{V}^*)$.

2.2. Operator \mathcal{K} . Consider a possibly nonlinear operator $\mathcal{K}(t): \mathcal{V} \rightarrow \mathcal{V}^*$ and let $1 \leq q, p < \infty$. The question arises whether this operator induces a bounded operator of the form

$$\begin{aligned} \mathcal{K}: L^p(0, T; \mathcal{V}) &\rightarrow L^q(0, T; \mathcal{V}^*), \\ (\mathcal{K}u)(t) &:= \mathcal{K}(u(t)). \end{aligned}$$

If such an operator exists, then we do not distinguish between these two notions. We state a well-known result for *Nemytskij* mappings for the considered setup of abstract functions.

Theorem 2.1 (cf. [Rou05, Thm. 1.43]). *If the operator $\mathcal{K}: (0, T) \times \mathcal{V} \rightarrow \mathcal{V}^*$ is such that*

- (a) $\mathcal{K}(t, \cdot): \mathcal{V} \rightarrow \mathcal{V}^*$ is continuous for a.e. $t \in (0, T)$,
- (b) $\mathcal{K}(\cdot, v): (0, T) \rightarrow \mathcal{V}^*$ is measurable for all v , and
- (c) $\|\mathcal{K}(t, v)\|_{\mathcal{V}^*} \leq \gamma(t) + c\|v\|_{\mathcal{V}}^{p/q}$ for some $\gamma \in L^q(0, T)$,

then the mapping defined via

$$(\mathcal{K}v)(t) := \mathcal{K}(t, v(t)),$$

is continuous as a map from $L^p(0, T; V)$ into $L^q(0, T; V^*)$, where $1 \leq p < \infty$ and $1 \leq q \leq \infty$.

The case that the exponents $1 < p, q < \infty$ are conjugated, i.e. $1/p + 1/q = 1$, is often assumed for the analysis of nonlinear evolution equations with monotonicity arguments [Rou05, Ch. 2 and Ch. 8]. However, for nonlinear operators, even if they are bounded as a map $\mathcal{V} \rightarrow \mathcal{V}^*$ (uniformly in t), the conjugacy of the time exponents may not hold a priori [Emm04, Ch. 8.2].

Example 2.2 (Navier-Stokes operator). Consider the nonlinear operator which arises in the weak formulation of the Navier-Stokes equations,

$$\mathcal{K}: \mathcal{V} \rightarrow \mathcal{V}^*, \quad \langle \mathcal{K}u, w \rangle_{\mathcal{V}^*, \mathcal{V}} := \int (u \cdot \nabla) \cdot uw \, dx.$$

Then, $\mathcal{K}: \mathcal{V} \rightarrow \mathcal{V}^*$ is bounded independently of t , cf. [Tem77, Lem. II.1.1], but, in the three-dimensional case, it is only bounded as an operator $\mathcal{K}: L^2(0, T; \mathcal{V}) \cap L^\infty(0, T; \mathcal{H}) \rightarrow L^{4/3}(0, T; \mathcal{V}^*)$, see e.g. [Rou05, Ch. 8.8.4].

Example 2.3 (p -Laplacian). For the p -Laplacian, i.e.,

$$\langle \mathcal{K}u, v \rangle_{\mathcal{V}^*, \mathcal{V}} := \int_{\Omega} |\nabla u|^{p-2} \nabla u \cdot \nabla v \, dx,$$

we take the Sobolev space $\mathcal{V} = W_0^{1,p}(\Omega)$. This then induces an operator $\mathcal{K}: L^p(0, T; \mathcal{V}) \rightarrow L^{p'}(0, T; \mathcal{V}^*)$ with $1/p + 1/p' = 1$, see [Ruž04, Ch. 3.3.6].

For special operators \mathcal{K} , as, e.g., linear operators that are uniformly bounded with respect to time, we state the following result.

Corollary 2.2. Consider $1 \leq p < \infty$ and an operator $\mathcal{K}: (0, T) \times \mathcal{V} \rightarrow \mathcal{V}^*$ which is measurable for fixed $v \in \mathcal{V}$ and uniformly bounded in the sense that there exists a constant $C_{\mathcal{K}}$ such that $\|\mathcal{K}(t)v\|_{\mathcal{V}^*} \leq C_{\mathcal{K}}\|v\|_{\mathcal{V}}$ for all $v \in \mathcal{V}$ and a.e. $t \in (0, T)$. Then, $(\mathcal{K}v)(t) := \mathcal{K}(t, v(t))$ defines a continuous operator from $L^p(0, T; \mathcal{V})$ to $L^p(0, T; \mathcal{V}^*)$.

Proof. The application of Theorem 2.1 with $p = q$ and $\gamma = 0$ yields the result. \square

Example 2.4 (Linear elasticity). In the case of linear isotropic material laws for a d -dimensional domain Ω , i.e.,

$$\langle \mathcal{K}u, v \rangle_{\mathcal{V}^*, \mathcal{V}} := \int_{\Omega} (2\mu\varepsilon(u) + \lambda \operatorname{trace} \varepsilon(u) I_{d \times d}) : \varepsilon(v) \, dx$$

with $\varepsilon(u)$ denoting the symmetric gradient, μ, λ the Lamé constants [BS08, Ch. 11], and $A : B := \sum_{i,j} A_{ij} B_{ij}$, we use as ansatz space $\mathcal{V} = H^1(\Omega)$. This setting then implies an operator $\mathcal{K}: L^2(0, T; \mathcal{V}) \rightarrow L^2(0, T; \mathcal{V}^*)$.

3. REGULARIZATION OF OPERATOR DAEs

In this section, we consider semi-explicit operator equations in a time interval $(0, T)$. Enforcing the given constraint by the Lagrangian method, we obtain a system of the form: find $u: (0, T) \rightarrow \mathcal{V}$ and $\lambda: (0, T) \rightarrow \mathcal{Q}$ such that

$$(3.1a) \quad \dot{u}(t) + \mathcal{K}u(t) + \left(\frac{\partial \mathcal{B}}{\partial u}(u) \right)^* \lambda(t) = \mathcal{F}(t) \quad \text{in } \mathcal{V}^*,$$

$$(3.1b) \quad \mathcal{B}u(t) = \mathcal{G}(t) \quad \text{in } \mathcal{Q}^*$$

for a.e. $t \in (0, T)$ with initial condition

$$(3.1c) \quad u(0) = g \in \mathcal{H}.$$

Therein, we use the dual operator of the Fréchet derivative of \mathcal{B} . The operator differential equation (3.1a) with constraint $\mathcal{B}u(t) = \mathcal{G}(t)$ is a generalization of a semi-explicit DAE since here, $u(t)$ belongs to the infinite-dimensional Banach space \mathcal{V} instead of \mathbb{R}^n . Because of this, we call system (3.1) an *operator DAE*.

Suitable function spaces for the solution (u, λ) will be discussed in Theorem 3.4 below. We will assume $\mathcal{F} \in L^q(0, T; \mathcal{V}^*)$ and $\mathcal{G} \in L^p(0, T; \mathcal{Q}^*)$. The equalities (3.1a) and (3.1b) should be understood pointwise in L^1_{loc} in the corresponding dual product. By the *fundamental theorem of variational calculus* [Emm04, Thm. 8.1.3] and the definition of the weak time derivative, this means, that $\dot{v}(t) = \mathcal{F}(t)$ in \mathcal{V}^* if

$$-\int_0^T \langle v(t), w \rangle_{\mathcal{V}^*, \mathcal{V}} \dot{\phi}(t) dt = \int_0^T \langle \mathcal{F}(t), w \rangle_{\mathcal{V}^*, \mathcal{V}} \phi(t) dt$$

for all $w \in \mathcal{V}$ and $\phi \in C_0^\infty(0, T)$.

Furthermore, we assume that the operator \mathcal{K} is bounded as a map $\mathcal{K}: L^p(0, T; \mathcal{V}) \rightarrow L^q(0, T; \mathcal{V}^*)$, cf. Section 2.2, as is $\mathcal{B}: L^p(0, T; \mathcal{V}) \rightarrow L^p(0, T; \mathcal{Q}^*)$ with $1 < p \leq q < \infty$.

3.1. Linear Constraints. In this subsection, we consider the operator DAE (3.1) with a linear constraint operator \mathcal{B} , which may depend on time. In this case, the Fréchet derivative of \mathcal{B} is again \mathcal{B} such that the operator DAE (3.1) simplifies to

$$(3.2a) \quad \dot{u}(t) + \mathcal{K}(t)u(t) + \mathcal{B}(t)^* \lambda(t) = \mathcal{F}(t) \quad \text{in } \mathcal{V}^*,$$

$$(3.2b) \quad \mathcal{B}(t)u(t) = \mathcal{G}(t) \quad \text{in } \mathcal{Q}^*$$

with initial condition as before,

$$(3.2c) \quad u(0) = g \in \mathcal{H}.$$

3.1.1. Assumptions on \mathcal{B} . In this subsection, we summarize the properties of \mathcal{B} which we require for a reformulation of the operator DAE (3.2).

Assumption 3.1 (Properties of \mathcal{B}). The constraint operator $\mathcal{B}(t): \mathcal{V} \rightarrow \mathcal{Q}^*$ satisfies the following conditions:

- (a) $\mathcal{B}(t)$ is linear and uniformly bounded, and $\mathcal{B}(\cdot)v$ is measurable for all $v \in \mathcal{V}$,
- (b) $\mathcal{V}_{\mathcal{B}} := \ker \mathcal{B}(t)$ is independent of time t ,
- (c) there exists a uniformly bounded right inverse of $\mathcal{B}(t)$, i.e., there exists a uniformly bounded operator $\mathcal{E}(t): \mathcal{Q}^* \rightarrow \mathcal{V}$ such that for all $q \in \mathcal{Q}^*$ it holds that

$$\mathcal{B}(t)\mathcal{E}(t)q = q,$$

- (d) the range of the right inverse $\mathcal{V}^c := \text{range } \mathcal{E}(t)$ is independent of time t , and
- (e) there exist continuous time derivatives $\dot{\mathcal{B}}(t): \mathcal{V} \rightarrow \mathcal{Q}$ and $\dot{\mathcal{E}}(t): \mathcal{Q}^* \rightarrow \mathcal{V}$.

Remark 3.1 (Time-independent constraint). If the constraint operator is independent of time, i.e., $\mathcal{B}(t) \equiv \mathcal{B}$, then Assumption 3.1 reduces to the points (a) and (c).

Remark 3.2 (Induced operators). By Corollary 2.2 it follows that $\mathcal{B}(t)$ and $\mathcal{E}(t)$ from Assumption 3.1 induce operators of the form

$$\mathcal{B}: L^p(0, T; \mathcal{V}) \rightarrow L^p(0, T; \mathcal{Q}^*) \quad \text{and} \quad \mathcal{E}: L^p(0, T; \mathcal{Q}^*) \rightarrow L^p(0, T; \mathcal{V}^c).$$

Note that, in general, the choice of the right inverse in Assumption 3.1 is not unique. A special case, for which the existence of a right-inverse follows, is when $\mathcal{B}(t)$ satisfies an inf-sup condition of the form

$$\inf_{q \in \mathcal{Q}} \sup_{v \in \mathcal{V}} \frac{\langle \mathcal{B}(t)v, q \rangle}{\|v\|_{\mathcal{V}} \|q\|_{\mathcal{Q}}} \geq \beta > 0.$$

Nevertheless, this does not imply the time-independence of the range of $\mathcal{E}(t)$. In the next lemma, we summarize several properties of the right inverse $\mathcal{E}(t)$ from Assumption 3.1.

Lemma 3.1 (Properties of \mathcal{E}). *Let $\mathcal{B}(t)$ satisfy Assumption 3.1. Then, the right inverse $\mathcal{E}(t): \mathcal{Q}^* \rightarrow \mathcal{V}^c \subset \mathcal{V}$ is linear and one-to-one. Furthermore, $\mathcal{V}^c = \text{range } \mathcal{E}(t)$ is a subspace of \mathcal{V} and the operator $\mathcal{E}(t)\mathcal{B}(t): \mathcal{V} \rightarrow \mathcal{V}$, restricted to \mathcal{V}^c , equals the identity.*

Proof. The linearity of $\mathcal{E}(t)$ follows from the linearity of the operator $\mathcal{B}(t)$ [RR04, Ch. 8.1.2]. For the one-to-one relation, consider $q_1, q_2 \in \mathcal{Q}^*$ with $\mathcal{E}(t)q_1 = \mathcal{E}(t)q_2$. Then, the application of $\mathcal{B}(t)$ yields $q_1 = \mathcal{B}(t)\mathcal{E}(t)q_1 = \mathcal{B}(t)\mathcal{E}(t)q_2 = q_2$.

The linearity of $\mathcal{E}(t)$ and the continuity of $\mathcal{E}(t)$ and $\mathcal{B}(t)$ imply that \mathcal{V}^c is a (closed) subspace of \mathcal{V} . Finally, for $v \in \mathcal{V}^c$ and fixed $t \in (0, T)$ there exists $q \in \mathcal{Q}^*$ with $\mathcal{E}(t)q = v$. Then, Assumption 3.1 implies

$$v = \mathcal{E}(t)q = \mathcal{E}(t)(\mathcal{B}(t)\mathcal{E}(t)q) = \mathcal{E}(t)\mathcal{B}(t)v.$$

In other words, $\mathcal{E}(t)\mathcal{B}(t): \mathcal{V} \rightarrow \mathcal{V}$ is a projection onto \mathcal{V}^c . \square

An important implication of Assumption 3.1 and Lemma 3.1 is the decomposition of $L^p(0, T; \mathcal{V})$ given in the following lemma. This decomposition will be the basis for the index reduction procedure of Section 3.1.2.

Lemma 3.2 (Decomposition of $L^p(0, T; \mathcal{V})$). *Consider the subspaces $\mathcal{V}_{\mathcal{B}}$ and \mathcal{V}^c of \mathcal{V} from Assumption 3.1. Then, we have the decomposition*

$$L^p(0, T; \mathcal{V}) = L^p(0, T; \mathcal{V}_{\mathcal{B}}) \oplus L^p(0, T; \mathcal{V}^c).$$

Proof. For given $v \in L^p(0, T; \mathcal{V})$, we define $r := \mathcal{B}v \in L^p(0, T; \mathcal{Q}^*)$, cf. Remark 3.2. Then, a decomposition of $v \in L^p(0, T; \mathcal{V})$ is given by

$$(3.3) \quad v = v_0 + v^c := (v - \mathcal{E}r) + \mathcal{E}r.$$

Obviously, $v^c = \mathcal{E}r \in L^p(0, T; \mathcal{V}^c)$ and $v_0 \in L^p(0, T; \mathcal{V}_{\mathcal{B}})$ follows from Assumption 3.1 by $\mathcal{B}v_0 = \mathcal{B}v - \mathcal{B}\mathcal{E}\mathcal{B}v = 0$. We show that the decomposition in (3.3) is unique. For this, consider $v_0, w_0 \in L^p(0, T; \mathcal{V}_{\mathcal{B}})$ and $v^c, w^c \in L^p(0, T; \mathcal{V}^c)$ with $v = v_0 + v^c = w_0 + w^c$. The application of \mathcal{B} yields $\mathcal{B}v^c = \mathcal{B}w^c$. Furthermore, there exist $r_v, r_w \in L^p(0, T; \mathcal{Q}^*)$ such that $v^c = \mathcal{E}r_v$ and $w^c = \mathcal{E}r_w$. By Assumption 3.1 we then obtain

$$r_v - r_w = \mathcal{B}\mathcal{E}r_v - \mathcal{B}\mathcal{E}r_w = \mathcal{B}v^c - \mathcal{B}w^c = 0.$$

Thus, it holds that $v^c = \mathcal{E}r_v = \mathcal{E}r_w = w^c$ and finally also $v_0 = w_0$. \square

The last lemma of this subsection is devoted to time derivatives of functions in $L^p(0, T; \mathcal{V})$.

Lemma 3.3. *Let \mathcal{W} be a subspace of \mathcal{V} such that there is a projection $\mathcal{P}: \mathcal{V} \rightarrow \mathcal{V}$ that maps \mathcal{V} onto \mathcal{W} and let $v \in L^p(0, T; \mathcal{W})$. Then, the existence of a time derivative $\dot{v} \in L^p(0, T; \mathcal{V})$ implies $\dot{v} \in L^p(0, T; \mathcal{W})$.*

Proof. Assume $v \in L^p(0, T; \mathcal{W})$ with $\dot{v} \in L^p(0, T; \mathcal{V})$. Because of the assumption, it holds that $(\text{id} - \mathcal{P})v(t) = 0$ for a.e. $t \in (0, T)$ with id denoting the identity. Since the time

derivative of v exists (at least in a generalized sense [Zei90, Ch. 23.5]), we can write $(\text{id} - \mathcal{P})\dot{v}(t) = 0$, which finally implies for a.e. $t \in (0, T)$,

$$\dot{v}(t) = \mathcal{P}\dot{v}(t) \in \mathcal{W}. \quad \square$$

3.1.2. Reformulation. This subsection is devoted to the reformulation of the operator DAE (3.2). In Section 4, which deals with the semi-discretized equations, we will see that this reformulation is in fact an index reduction on operator level.

We adapt the technique of minimal extension [KM04], which is an index reduction procedure especially suitable for semi-explicit DAEs. For this, we first add to system (3.2) the time derivative of the constraint,

$$\mathcal{B}\dot{u} + \dot{\mathcal{B}}u = \dot{\mathcal{G}}.$$

Clearly, this requires the right-hand side \mathcal{G} to be differentiable in the generalized sense, i.e., $\mathcal{G} \in W^{1,p}(0, T; \mathcal{Q}^*)$. Note that this assumption is already needed for the existence of a solution of (3.2). This fact comes from the theory of DAEs, see for example [KM06, Th.2.29] which shows that even for the finite dimensional case with constant coefficients higher derivatives of the right-hand side are necessary. At this point, also $\dot{u} \in L^p(0, T; \mathcal{V})$ seems to be a necessary condition. However, as the next paragraph shows, this requirement applies only to a part of \dot{u} .

Second, we use the decomposition from Lemma 3.2 to split u into $u_1 \in L^p(0, T; \mathcal{V}_{\mathcal{B}})$ and $u_2 \in L^p(0, T; \mathcal{V}^c)$. Therewith, the two constraints reduce to

$$\mathcal{B}u_2 = \mathcal{G} \quad \text{and} \quad \mathcal{B}\dot{u}_2 + \dot{\mathcal{B}}u_2 = \dot{\mathcal{G}}.$$

Thus, it is sufficient that the derivative of u_2 is an element of \mathcal{V} . For u in general, we only need that $\dot{u} \in L^q(0, T; \mathcal{V}^*)$. The assumed regularity of \mathcal{G} implies with Assumption 3.1, Lemma 3.1, and equation (3.2b) that $u_2 \in W^{1,p}(0, T; \mathcal{V}^c)$.

Having added one equation, we introduce in a third step a new variable $v_2 := \dot{u}_2 \in L^p(0, T; \mathcal{V}^c)$. Note that \mathcal{V}^c is a subspaces of \mathcal{V} for which there exists a projection, cf. Lemma 3.1. Thus, we can apply Lemma 3.3 at this point. The addition of a new variable compensates the redundancy of the two constraints. Note that in the reformulated system the variable u_2 is not differentiated anymore such that we only need an initial condition for u_1 . The initial condition for u_2 in the original formulation is just the consistency condition of the constraint, which typically appears for DAEs [KM06, Ch. 1]. In the sequel, we neglect the time-dependency of the operators \mathcal{K} and \mathcal{B} . The overall system then reads: for data $\mathcal{F} \in L^q(0, T; \mathcal{V}^*)$ and $\mathcal{G} \in W^{1,p}(0, T; \mathcal{Q}^*)$ find functions $u_1 \in L^p(0, T; \mathcal{V}_{\mathcal{B}})$ with $\dot{u}_1 \in L^q(0, T; \mathcal{V}^*)$, $u_2, v_2 \in L^p(0, T; \mathcal{V}^c)$, and $\lambda \in L^{p'}(0, T; \mathcal{Q})$ such that

$$(3.4a) \quad \dot{u}_1(t) + v_2(t) + \mathcal{K}(u_1(t) + u_2(t)) + \mathcal{B}^*\lambda(t) = \mathcal{F}(t) \quad \text{in } \mathcal{V}^*,$$

$$(3.4b) \quad \mathcal{B}u_2(t) = \mathcal{G}(t) \quad \text{in } \mathcal{Q}^*,$$

$$(3.4c) \quad \mathcal{B}v_2(t) + \dot{\mathcal{B}}u_2(t) = \dot{\mathcal{G}}(t) \quad \text{in } \mathcal{Q}^*$$

holds a.e. in $(0, T)$ with initial condition

$$(3.4d) \quad u_1(0) = g - \mathcal{E}\mathcal{G}(0) \in \mathcal{H}.$$

The initial condition is well-posed for time differentiable \mathcal{G} since $W^{1,p}(0, T; \mathcal{Q}^*)$ is continuously embedded in the space of continuous functions with values in \mathcal{Q}^* , namely $C([0, T], \mathcal{Q}^*)$ [Rou05, Lem. 7.1]. In the following theorem, we discuss the connection of the original system (3.2) and the regularized formulation (3.4).

Theorem 3.4 (Equivalence of reformulation). *Consider exponents $1 < q \leq p < \infty$, and p' with $1/p' + 1/p = 1$. Assume that $\mathcal{F} \in L^q(0, T; \mathcal{V}^*)$, $\mathcal{G} \in W^{1,p}(0, T; \mathcal{Q}^*)$, and $g \in \mathcal{H}$ as well as the operator \mathcal{B} satisfying Assumption 3.1. Then, the operator DAE (3.2) has a solution (u, λ) with $u \in L^p(0, T; \mathcal{V})$, $\dot{u} \in L^q(0, T; \mathcal{V}^*)$, and $\lambda \in L^{p'}(0, T; \mathcal{Q})$ if and only if system (3.4) has a solution (u_1, u_2, v_2, λ) with $u_1 \in L^p(0, T; \mathcal{V}_\mathcal{B})$, $\dot{u}_1 \in L^q(0, T; \mathcal{V}^*)$, $u_2, v_2 \in L^p(0, T; \mathcal{V}^c)$, and $\lambda \in L^{p'}(0, T; \mathcal{Q})$. Furthermore, it holds that $u = u_1 + u_2$ and $\dot{u}_2 = v_2$.*

Proof. By Proposition 1.38 in [Rou05], for a separable Banach space \mathcal{Q}^* , the dual space $[L^{p'}(0, T; \mathcal{Q})]^*$ can be identified with $L^p(0, T; \mathcal{Q}^*)$ since $1/p' + 1/p = 1$. Thus, $L^{p'}(0, T; \mathcal{Q})$ is the right space for the multiplier λ .

Let (u, λ) be a solution of (3.2). We define

$$u_1 := u - \mathcal{E}\mathcal{B}u \in L^p(0, T; \mathcal{V}_\mathcal{B}) \quad \text{and} \quad u_2 := \mathcal{E}\mathcal{B}u \in L^p(0, T; \mathcal{V}^c).$$

With equation (3.2b), we obtain $u_2 = \mathcal{E}\mathcal{G}$ and thus, by the regularity of \mathcal{G} and Assumption 3.1, $\dot{u}_2 \in L^p(0, T; \mathcal{V}^c)$. With $v_2 := \dot{u}_2$ the quadruple (u_1, u_2, v_2, λ) satisfies equations (3.4a-c). The initial condition (3.4d) is satisfied because of

$$u_1(0) = u(0) - u_2(0) = g - \mathcal{E}\mathcal{G}(0).$$

For the reverse direction consider a solution of (3.4), namely (u_1, u_2, v_2, λ) . Then, $u := u_1 + u_2 \in L^p(0, T; \mathcal{V})$ and because of the regularity of \mathcal{G} and equation (3.4b), by Remark 2.2, it holds that $\dot{u} = \dot{u}_1 + \dot{u}_2 \in L^q(0, T; \mathcal{V}^*)$. We show that $\dot{u}_2 = v_2$. Equation (3.4c) and the time derivative of equation (3.4b) yield

$$\mathcal{B}v_2 + \dot{\mathcal{B}}u_2 = \dot{\mathcal{G}} = \frac{d}{dt}(\mathcal{B}u_2) = \mathcal{B}\dot{u}_2 + \dot{\mathcal{B}}u_2.$$

Note that $\dot{u}_2 \in L^p(0, T; \mathcal{V}^c)$, as shown in the first part of the proof. The invertibility of \mathcal{B} on \mathcal{V}^c (see Lemma 3.1) then gives $\dot{u}_2 = v_2$. Thus, the pair (u, λ) satisfies equations (3.2a) and (3.2b). For the initial condition (3.2c), we obtain

$$u(0) = u_1(0) + u_2(0) = g - \mathcal{E}\mathcal{G}(0) + \mathcal{E}\mathcal{G}(0) = g. \quad \square$$

From the solution representation given in Theorem 3.4 we deduce that not every initial condition $g \in \mathcal{H}$ admits a solution to (3.2).

Corollary 3.5. *Let the assumptions of Theorem 3.4 hold. For the existence of a solution to (3.2) it is necessary that the initial data g can be decomposed as $g = g_0 - \mathcal{E}\mathcal{G}(0)$, where $\mathcal{E}\mathcal{G}(0) \in \mathcal{V}$ and g_0 is in the closure of $\mathcal{V}_\mathcal{B}$ in \mathcal{H} .*

3.2. Nonlinear Constraints. After studying the operator DAE (3.1) with linear constraints, we now consider a nonlinear constraint operator \mathcal{B} . For this, let $\mathcal{B}: \mathcal{V} \rightarrow \mathcal{Q}^*$ be a time-independent nonlinear operator with Fréchet derivative

$$\mathcal{C}_v := \frac{\partial \mathcal{B}}{\partial u}(v): \mathcal{V} \rightarrow \mathcal{Q}^*$$

at some point $v \in \mathcal{V}$. Recall that for linear operators it holds that $\mathcal{C}_v = \mathcal{B}$ for all $v \in \mathcal{V}$. As already seen in system (3.1), in the nonlinear case, the operator DAE has the form

$$(3.5a) \quad \dot{u}(t) + \mathcal{K}u(t) + \mathcal{C}_u^* \lambda(t) = \mathcal{F}(t) \quad \text{in } \mathcal{V}^*,$$

$$(3.5b) \quad \mathcal{B}u(t) = \mathcal{G}(t) \quad \text{in } \mathcal{Q}^*$$

with an initial condition as given in (3.1c). In the following, we assume that there exists a solution (u, λ) of system (3.5) with $u \in L^p(0, T; \mathcal{V})$, $\dot{u} \in L^q(0, T; \mathcal{V}^*)$, and $\lambda \in L^{p'}(0, T; \mathcal{Q})$. Note that for the formulation of system (3.5) it is sufficient that the Fréchet derivative \mathcal{C}_u exists along the solution u .

3.2.1. *Assumptions on \mathcal{B} .* To define the manifold described by the nonlinear constraints we have to assume the existence of an implicit function that resolves the constraint. Additionally, we require a certain smoothness of the solution manifold.

Assumption 3.2 (Properties of \mathcal{B}). Consider a function $u \in L^p(0, T; \mathcal{V})$ that satisfies $\mathcal{B}u = \mathcal{G}$ in \mathcal{Q}^* for a.e. $t \in (0, T)$. Then, there exists a splitting of \mathcal{V} into subspaces \mathcal{V}_1 and \mathcal{V}_2 , i.e., $\mathcal{V} = \mathcal{V}_1 \oplus \mathcal{V}_2$, and a neighborhood $\mathcal{U}(t) \subseteq \mathcal{V}$ around $u(t)$ such that

- (a) $u = u_1 + u_2$ with $u_1 \in L^p(0, T; \mathcal{V}_1)$, $u_2 \in L^p(0, T; \mathcal{V}_2)$,
- (b) the Fréchet derivative $\frac{\partial \mathcal{B}}{\partial u}$ exists in $\mathcal{U}(t)$,
- (c) $\mathcal{C}_{2,u} := \frac{\partial \mathcal{B}}{\partial u_2}(u): \mathcal{V}_2 \rightarrow \mathcal{Q}^*$ is a homeomorphism, and
- (d) $\frac{\partial \mathcal{B}}{\partial u_2}(\cdot)$ is continuous in u .

Remark 3.3 (Splitting). The splitting of \mathcal{V} into \mathcal{V}_1 and \mathcal{V}_2 is independent of the right-hand side \mathcal{G} and independent of time.

Remark 3.4 (Implicit function theorem). From the implicit function theorem for operators [Ruž04, Ch. 2.2] it follows that if \mathcal{B} satisfies Assumption 3.2 for a function $u = u_1 + u_2$, then there exists a map $\eta(t): \mathcal{V}_1 \rightarrow \mathcal{V}_2$ such that for all $v_1 \in \mathcal{V}_1$ 'close enough' to u_1 it holds that

$$\mathcal{B}(v_1 + \eta(v_1)) = \mathcal{G}.$$

Furthermore, the assumed regularity of \mathcal{B} in point (b) of Assumption 3.2 implies that η is Fréchet differentiable in a neighborhood of u_1 , cf. [Ruž04, Cor. 2.15].

As seen in Remark 3.4, Assumption 3.2 allows to solve the constraint (3.5b) for some variable u_2 . Before we use this result for the reformulation of system (3.5), we state another property of the implicit function η .

Lemma 3.6 (Time derivative of η). *Let $\eta(t): \mathcal{V}_1 \rightarrow \mathcal{V}_2$ be the mapping given by the implicit function theorem in Remark 3.4. Then, the derivative $\partial \eta / \partial t$ exists in a neighbourhood around u_1 , if u_1 and \mathcal{G} are itself differentiable in time.*

Proof. The claim follows by the implicit function theorem applied to the operator

$$\mathcal{D}(u_1, u_2, \mathcal{G}) := \mathcal{B}(u_1 + u_2) - \mathcal{G}. \quad \square$$

3.2.2. *Reformulation.* Similar to the linear case in Section 3.1.2, we need the first time-derivative of the constraint (3.5b). Here, it reads

$$\dot{\mathcal{G}}(t) = \frac{d}{dt}(\mathcal{B}u(t)) = \frac{\partial \mathcal{B}}{\partial u}(u)\dot{u}(t) = \mathcal{C}_u \dot{u}(t).$$

As it is the Fréchet derivative of \mathcal{B} , the operator \mathcal{C}_u is linear [Zei86, Ch. 4.2]. Consider the decomposition of \mathcal{V} into $\mathcal{V}_1 \oplus \mathcal{V}_2$ from Assumption 3.2. Then, assuming sufficient regularity of the solution u of the form $\dot{u}_1, \dot{u}_2 \in L^p(0, T; \mathcal{V})$, we obtain

$$\mathcal{C}_u \dot{u} = \mathcal{C}_u \dot{u}_1 + \mathcal{C}_{2,u} \dot{u}_2 = \dot{\mathcal{G}}(t).$$

Using Lemma 3.3, we introduce the variable $v_2 := \dot{u}_2 \in L^p(0, T; \mathcal{V}_2)$. Then, the extended operator DAE has the form: find $u_1 \in W^{1,p}(0, T; \mathcal{V}_1)$, $u_2, v_2 \in L^p(0, T; \mathcal{V}_2)$, and $\lambda \in L^{p'}(0, T; \mathcal{Q})$ such that

$$(3.6a) \quad \dot{u}_1(t) + v_2(t) + \mathcal{K}(u_1(t) + u_2(t)) + \mathcal{C}_u^* \lambda(t) = \mathcal{F}(t) \quad \text{in } \mathcal{V}^*,$$

$$(3.6b) \quad \mathcal{B}(u_1(t) + u_2(t)) = \mathcal{G}(t) \quad \text{in } \mathcal{Q}^*,$$

$$(3.6c) \quad \mathcal{C}_u \dot{u}_1(t) + \mathcal{C}_{2,u} v_2(t) = \dot{\mathcal{G}}(t) \quad \text{in } \mathcal{Q}^*$$

for a.e. $t \in (0, T)$ with the nonlinear initial condition

$$(3.6d) \quad u_1(0) = g - \eta(u_1(0)) \in \mathcal{H}.$$

Remark 3.5 (Regularity). In some applications the regularity assumption on \dot{u}_1 may be weakened. This is possible if the operator \mathcal{B} can be defined in a weaker sense, e.g., for functions in \mathcal{H} , as it is the case for the divergence operator for the Stokes equation [Hei14]. Note that in this case equation (3.6c) is stated in a weaker topology.

As for the linear case, we have to analyse the connection between the original system (3.5) and the reformulated equations (3.6). We have the following result.

Theorem 3.7 (Equivalence of reformulation). *Consider right-hand sides $\mathcal{F} \in L^q(0, T; \mathcal{V}^*)$, $\mathcal{G} \in W^{1,p}(0, T; \mathcal{Q}^*)$ and let \mathcal{B} satisfy Assumption 3.2 for all $u \in L^p(0, T; \mathcal{V})$ with $\mathcal{B}u = \mathcal{G}$ in \mathcal{Q}^* . Then, there exists a solution $(u, \lambda) \in L^p(0, T; \mathcal{V}) \times L^{p'}(0, T; \mathcal{Q})$ of (3.5) with initial condition (3.1c) and additional smoothness $\dot{u} \in L^p(0, T; \mathcal{V})$ if and only if (3.6) has a solution (u_1, u_2, v_2, λ) with $u_1 \in W^{1,p}(0, T; \mathcal{V}_1)$, $u_2, v_2 \in L^p(0, T; \mathcal{V}_2)$, and $\lambda \in L^{p'}(0, T; \mathcal{Q})$. Also, it holds that $u = u_1 + u_2$ and $\dot{u}_2 = v_2$.*

Proof. Let (u, λ) be a solution of system (3.5) with initial condition (3.1c). Assumption 3.2, Lemma 3.3, and the additional regularity of u allow for a decomposition $u = u_1 + u_2$ with $u_1 \in W^{1,p}(0, T; \mathcal{V}_1)$ and $u_2 \in W^{1,p}(0, T; \mathcal{V}_2)$. Then, by construction, the quadruple (u_1, u_2, v_2, λ) from this subsection with $v_2 := \dot{u}_2$ satisfies equations (3.6a)-(3.6c). Because of the assumed smoothness of u and \mathcal{G} , by Lemma 3.6, the implicit function η is well-defined for $t = 0$. Thus, we may write $u_1(0) + \eta(u_1(0)) = u_1(0) + u_2(0) = u(0) = g$, which is the initial condition in (3.6d).

On the other hand, if (u_1, u_2, v_2, λ) is a solution of (3.6), we first define $u := u_1 + u_2 \in L^p(0, T; \mathcal{V})$. Because of (3.6b), Assumption 3.2 holds for \mathcal{B} along this function u . From the construction of u_1, u_2 in this subsection, we see that $u = u_1 + u_2$ is exactly the decomposition given by point (a) of Assumption 3.2. It remains to show that u_2 is time differentiable and $v_2 = \dot{u}_2$. This then implies $u_1, u_2 \in W^{1,p}(0, T; \mathcal{V})$ and thus, the pair (u, λ) solves (3.5) with initial condition (3.1c).

By the implicit function theorem, we may write $u_2 = \eta(u_1)$, cf. Remark 3.4. Since η is differentiable in time, by Lemma 3.6, we obtain $\dot{u}_2 \in L^p(0, T; \mathcal{V}_2)$. Equation (3.6c) and the time derivative of (3.6b) yield

$$\mathcal{C}_u \dot{u}_1 + \mathcal{C}_{2,u} \dot{u}_2 = \mathcal{C}_u \dot{u}_1 + \mathcal{C}_{2,u} v_2.$$

Since $\dot{u}_2(t), v_2(t) \in \mathcal{V}_2$, part (c) of Assumption 3.2 implies $\dot{u}_2 = v_2$. \square

Remark 3.6. As in the linear case, the initial condition has to satisfy a consistency condition, cf. Corollary 3.5.

4. DISCRETIZATION

For the discretization of the operator equations (3.1), (3.4), and (3.6), we follow the method of lines [Hol07, Ch. 3.4], i.e., we discretize in space first. This then leads to DAEs, for which the differentiation index concept is well-defined [BCP96, KM06]. The index characterizes the necessary number of differentiation steps, in order to obtain an ODE. The index also quantifies to which degree the solution depends on derivatives of the involved quantities which may lead to instabilities within the numerical simulation. For a precise definition, we refer to [HW96, Def. VII.1.2]. Recall that we do not use any index definition of PDAEs but instead analyse the index of the semi-discretized system. Within this paper, we will always write *index*, meaning the differentiation index.

In this section, we show that the DAE corresponding to the original system (3.1) is of index 2 whereas the DAEs resulting from the reformulated systems are of index 1. For this, standard assumptions on the used finite element schemes will be considered.

4.1. Finite Element Discretization. For the spatial discretization, we consider finite dimensional approximations of the spaces \mathcal{V}_1 , \mathcal{V}_2 , and \mathcal{Q} . In the setting of Section 3.1, i.e., in the linear case, we have $\mathcal{V}_1 = \mathcal{V}_{\mathcal{B}}$ and $\mathcal{V}_2 = \mathcal{V}^c$. We denote the approximation spaces by V_{1h} , V_{2h} , and Q_h , respectively. Furthermore, we define $V_h = V_{1h} \oplus V_{2h}$ as finite dimensional approximation of \mathcal{V} .

Thinking of finite elements on a regular mesh \mathcal{T} [Cia78, Bra07] of the domain Ω , we consider basis functions $\{\varphi_i\}_{1,\dots,n_1}$ of V_{1h} , $\{\varphi_i\}_{n_1+1,\dots,n}$ of V_{2h} , and $\{\psi_i\}_{1,\dots,m}$ of Q_h with $m = n - n_1$. Hence, we assume that $\dim V_{2h} = \dim Q_h$. The finite dimensional approximations of u_1, u_2, v_2 , and λ are then represented by the coefficient vectors q_1, q_2, p_2 , and μ , respectively. By $q \in \mathbb{R}^n$ we denote the vector $q = [q_1^T, q_2^T]^T$. Based on this discretization scheme, we define the mass matrix $M \in \mathbb{R}^{n,n}$, which is assumed to be positive definite, by $M_{i,j} := (\varphi_i, \varphi_j)_{\mathcal{H}}$. The discrete version B of the constraint operator \mathcal{B} is defined by

$$(4.1) \quad B: \mathbb{R}^n \rightarrow \mathbb{R}^m, \quad \langle B(q), e_j \rangle := \langle \mathcal{B}(\sum_{i=1}^n q_i \varphi_i), \psi_j \rangle.$$

Therein, $e_j \in \mathbb{R}^m$ denotes the j -th unit vector. In the linear case, we may express B as a (time-dependent) $m \times n$ matrix. Note that, according to Assumption 3.1, it is natural to assume that B is continuously differentiable w.r.t. time.

Remark 4.1 (Nonconforming discretization). In order that B is well-defined, the operator \mathcal{B} has to be defined for the given basis functions. Since nonconforming finite elements are not excluded [BS08, Ch. 10], the application of \mathcal{B} may be generalized to a piecewise (w.r.t. the triangulation \mathcal{T}) application of the operator.

For the discretization B of the operator \mathcal{B} (or the Jacobian in the nonlinear case) we assume that it has full rank.

Remark 4.2 (Inf-sup stability). For the unique solvability of the semi-discrete systems resulting from the finite element discretization it is only necessary that the constraint matrix B is of full rank. For a stable approximation of the Lagrange multiplier λ , with respect to the discretization parameter h , one may use the stronger inf-sup condition, namely there exists a constant $\beta_{\text{disc}} > 0$, independent of h and the time t , such that

$$\inf_{\gamma_h \in Q_h} \sup_{v_h \in V_h} \frac{\langle \mathcal{B}(t)v_h, \gamma_h \rangle}{\|v_h\|_{\mathcal{V}} \|\gamma_h\|_{\mathcal{Q}}} \geq \beta_{\text{disc}},$$

cf., e.g., [Bra07, Ch. III.4].

Finally, we define the discrete version of the operator \mathcal{K} by

$$K: \mathbb{R}^n \rightarrow \mathbb{R}^n, \quad \langle K(q), e_k \rangle := \langle \mathcal{K}(\sum_{i=1}^n q_i \varphi_i), \varphi_k \rangle.$$

Here, e_k denotes the k -th unit vector in \mathbb{R}^n . As before, K can be written as a $n \times n$ matrix if \mathcal{K} is linear. As mentioned in Remark 4.1, we assume that the operator \mathcal{K} is defined for functions in V_h .

4.2. Linear Constraints. Within this section, we assume that the mass matrix M is positive definite and that B is of full rank for all time t . First, we consider the index of

the DAE which results from a spatial discretization of the original system (3.2). With the notation of the previous subsection, the DAE has the form

$$(4.2a) \quad M\dot{q} + K(q) + B^T(t)\mu = f,$$

$$(4.2b) \quad B(t)q = g.$$

It is shown in [HW96, Ch. VII.1] that such a system has index 2 if $BM^{-1}B^T$ is invertible. This condition is satisfied because of the full rank property of B .

The index-2 structure can also be made visible through a differentiation of the constraint (4.2b). This then leads to the (analytically) equivalent DAE

$$\begin{bmatrix} M & B^T(t) \\ B(t) & 0 \end{bmatrix} \begin{bmatrix} \dot{q} \\ \mu \end{bmatrix} = \begin{bmatrix} f - K(q) \\ \dot{g} - \dot{B}(t)q \end{bmatrix}.$$

Again the assumptions on M and B imply that the matrix on the left-hand side is invertible. Thus, a single differentiation leads to an ODE for q and an algebraic equation for the Lagrange multiplier μ .

The remaining part of this subsection is devoted to the analysis of the index of the DAE resulting from the extended system (3.4).

4.2.1. Conforming Discretization. In the case of a conforming discretization, i.e., $V_{1h} \subset \mathcal{V}_1$, $V_{2h} \subset \mathcal{V}_2$, and $Q_h \subset \mathcal{Q}$, the matrix $B(t)$ has the special structure $B(t) = [0 \ B_2(t)]$. Therein, the matrix $B_2(t)$ is square and non-singular. In this case, the semi-discrete version of (3.4) has the form

$$(4.3a) \quad M \begin{bmatrix} \dot{q}_1 \\ p_2 \end{bmatrix} + K(q_1, q_2) + \begin{bmatrix} 0 \\ B_2^T(t) \end{bmatrix} \mu = f,$$

$$(4.3b) \quad B_2(t)q_2 = g,$$

$$(4.3c) \quad B_2(t)p_2 = \dot{g} - \dot{B}_2(t)q_2.$$

At this point we only mention that this system forms a DAE of index 1. We give the proof in Lemma 4.1 below for the more general case.

Remark 4.3 (Index reduction). The index of the DAE (4.3) is, compared to the DAE (4.2), reduced by one. This justifies to call the procedure from Section 3.1 an index reduction on operator level.

4.2.2. Nonconforming Discretization. In many cases one uses a nonconforming spatial discretization [BS08, Ch. 10], i.e., the discrete ansatz spaces are no subspaces of the original search spaces. One simple example is the Crouzeix-Raviart element [CR73], a lowest order piecewise linear but discontinuous discretization scheme. Since we cannot assume $V_{1h} \subset \mathcal{V}_1$ in this case, we lose the special structure of $B(t)$. Furthermore, it is difficult to construct finite elements as subspaces of the constraint spaces and for general mixed finite element discretizations one has that $\ker B \not\subset \ker \mathcal{B}$, cf. [GR86, Ch. 3].

Thus, in general, we have $B(t) = [B_1(t) \ B_2(t)]$ and simply assume that the block B_2 is non-singular. The latter assumption is no restriction, since one can always permute the columns of B such that the B_2 block is regular. Then, the semi-discretized system reads

$$(4.4a) \quad M \begin{bmatrix} \dot{q}_1 \\ p_2 \end{bmatrix} + K(q_1, q_2) + B^T(t)\mu = f,$$

$$(4.4b) \quad B_2(t)q_2 = g - B_1(t)q_1,$$

$$(4.4c) \quad B_2(t)p_2 = \dot{g} - B_1(t)\dot{q}_1 - \dot{B}_1(t)q_1 - \dot{B}_2(t)q_2.$$

Lemma 4.1 (Index-1 DAE). *For a positive definite mass matrix M and a continuously differentiable constraint matrix B with a non-singular block B_2 , the DAEs (4.3) and (4.4) are of index 1.*

Proof. Similar to the proof of [KM06, Th. 6.12], we show that (4.4) is of index 1. The property then follows for system (4.3) as well because it is a special case.

Since the matrix $B_2(t)$ is of full rank, equations (4.4b) and (4.4c) yield direct expressions of q_2 and p_2 in terms of q_1, \dot{q}_1 . Furthermore, a multiplication of (4.4a) from the left by BM^{-1} provides a formula for μ in terms of q_1 . Here we use the assumptions on M and B which imply that the matrix $BM^{-1}B^T$ is invertible. Finally, inserting all these expressions into equation (4.4a), we obtain an ODE in q_1 . Thus, we can solve system (4.4) without any further differentiation steps. \square

4.3. Nonlinear Constraints. In the linear case we have assumed that B has a block structure with a non-singular $m \times m$ block. In the nonlinear case we require this block structure from the Jacobian. As an alternative to (4.1), we work here with an equivalent description of the discrete constraint operator B , namely

$$B: V_h \rightarrow Q_h^*$$

$$\langle B(u_h), \psi_j \rangle := \langle \mathcal{B}(u_h), \psi_j \rangle.$$

Thus, for $u_h = \sum_{i=1}^n q_i \varphi_i$ it follows that $\langle B(u_h), \psi_j \rangle = \langle B(q), e_j \rangle$. Before formulating the sufficient assumptions on B , we comment on the order of discretization and differentiation.

Remark 4.4 (Commutativity). Consider the constraint operator $\mathcal{B}: \mathcal{V} \rightarrow \mathcal{Q}^*$. Then, the discretization with the scheme V_h, Q_h of the Fréchet derivative $\partial \mathcal{B} / \partial u(\cdot): \mathcal{V} \rightarrow (\mathcal{V} \rightarrow \mathcal{Q}^*)$ equals the Fréchet derivative of the discrete operator B .

Assumption 4.1 (Properties of B). Consider $q \in \mathbb{R}^n$ and $u_h = \sum_{i=1}^n q_i \varphi_i$ such that $\langle B(q), e_j \rangle = \langle \mathcal{G}, \psi_j \rangle = \langle g, e_j \rangle$ for $j = 1, \dots, m$. We assume that

- (a) there exist subspaces V_{1h}, V_{2h} with $V_h = V_{1h} \oplus V_{2h}$, $u_h = u_{h,1} + u_{h,2}$,
- (b) B is continuously differentiable in a neighborhood of q (respectively u_h),
- (c) the matrix $\partial B / \partial u_{h,2}(u_h)$ is invertible.

Remark 4.5. With an appropriate basis $\{\varphi_1, \dots, \varphi_n\}$ of V_h , the splitting $V_h = V_{1h} \oplus V_{2h}$ from Assumption 4.1 implies a decomposition of the coefficient vector q . Thus, we may assume that $q \in \mathbb{R}^n$ decomposes into $q = [q_1^T, q_2^T]^T$ such that $u_{h,1} = \sum_{i=1}^{n_1} q_{1i} \varphi_i \in V_{1h}$ and $u_{h,2} = \sum_{i=1}^{n-n_1} q_{2i} \varphi_{n_1+i} \in V_{2h}$.

Let $C := \partial B / \partial u_h(u_h)$ denote the Jacobian of B . The spatial discretization of the operator DAE (3.5) then leads to the system

$$(4.5a) \quad M\dot{q} + K(q) + C^T \mu = f,$$

$$(4.5b) \quad B(q) = g.$$

If the Jacobian C is of full rank, then $CM^{-1}C^T$ is invertible and the DAE (4.5) is of index 2 [HW96, Ch. VII.1]. Similar to the linear case, one differentiation of the constraint is necessary to get an explicit expression for the Lagrange multiplier μ .

Using the spaces V_{1h}, V_{2h} from Assumption 4.1 and appropriate basis functions, according to Remark 4.5, we obtain a spatial discretization of system (3.6):

$$(4.6a) \quad M \begin{bmatrix} \dot{q}_1 \\ p_2 \end{bmatrix} + K(q_1, q_2) + C^T \mu = f,$$

$$(4.6b) \quad B(q_1, q_2) = g,$$

$$(4.6c) \quad C \begin{bmatrix} \dot{q}_1 \\ p_2 \end{bmatrix} = \dot{g}.$$

The following lemma states that this DAE is of index 1.

Lemma 4.2 (Index-1 DAE). *Let M be positive definite and the nonlinear function B satisfy Assumption 4.1 along the solution q . Then, the DAE (4.6) is of index 1.*

Proof. Assumption 4.1 implies that the Jacobian C has the block structure

$$C = \begin{bmatrix} C_1 & C_2 \end{bmatrix}$$

with an invertible matrix C_2 . Because of the implicit function theorem, locally we obtain from (4.6b-c) expressions for q_2 and p_2 in terms of q_1 and \dot{q}_1 . Furthermore, a multiplication of CM^{-1} from the left to (4.6a) yields an equation for μ in terms of q_1 and the right-hand side \dot{g} . Here we use the full rank property of C which implies that $CM^{-1}C^T$ is non-singular. Finally, we have algebraic equations for q_2, p_2 , and μ and an ODE for q_1 without any differentiation steps. \square

5. EXAMPLES

This section is devoted to the application of the framework developed in Section 3 to real-world examples. First, we consider the Navier-Stokes equations as example of a PDAE with linear constraints. Second, we analyse the regularized Stefan problem in terms of Section 3.2.

5.1. Navier-Stokes Equations. We consider the standard formulation of the Navier-Stokes equations [Tem77] for an incompressible flow in a domain $\Omega \subset \mathbb{R}^d$,

$$(5.1) \quad \dot{u} + (u \cdot \nabla)u - \nu \Delta u + \nabla p = f, \quad \nabla \cdot u = 0.$$

We interpret the pressure p as Lagrange multiplier, coupling the incompressibility constraint $\nabla \cdot u = 0$ to the state equations. Then, equation (5.1) takes the form of system (3.2), with the spaces chosen as $\mathcal{V} = [H_0^1(\Omega)]^d$, $\mathcal{H} = [L^2(\Omega)]^d$, and $\mathcal{Q} = L^2(\Omega)/\mathbb{R}$.

The operator $\mathcal{B}: \mathcal{V} \rightarrow \mathcal{Q}^*$ is defined as the divergence and $\mathcal{K}: \mathcal{V} \rightarrow \mathcal{V}^*$ is the operator representing convection and diffusion. Without further assumptions, the nonlinearity \mathcal{K} only extends to $\mathcal{K}: L^2(0, T; \mathcal{V}) \rightarrow L^1(0, T; \mathcal{V}^*)$, cf. [Tem77, Lem. III.3.1]. This causes the main difficulties in the existence theory for the Navier-Stokes equations. However, this lower regularity does not affect the splitting as proposed in Section 3.1. In particular, Assumption 3.1 is fulfilled. The weak divergence operator is linear and bounded and the existence of a continuous right inverse is shown in, e.g., [Tar06, Lem. I.4.1]. The splitting $\mathcal{V} = \mathcal{V}_{\mathcal{B}} \oplus \mathcal{V}^c$ is then given by the space of divergence-free functions and its (orthogonal) complement. Note that our approach is different from [EM13] where the splitting of V is used to eliminate the constraints rather than to augment the system.

The reformulation introduced in Section 3.1 allows for semi-explicit time integration schemes as shown in [AH13]. For this, one has to split the finite element spaces used in

computational fluid dynamics as described in Section 4.2. This leads to stable approximations of the pressure as shown in the numerical example in [AH13].

5.2. Stefan Problem. The theory of PDAEs with nonlinear constraints from Section 3.2 can be applied to the Stefan problem which models a change of phase. The governing equations which include a condition at the free boundary can be found in [Fri68], see also [And04] for an introduction. We consider the enthalpy formulation as stated in [DPVY13] with regularized enthalpy-temperature function β . For this, assume $\beta: \mathbb{R} \rightarrow \mathbb{R}$ is strictly monotonically increasing and continuously differentiable with $\beta' \geq \varepsilon > 0$. As in [DPVY13] we assume that there exist constants $c, C > 0$ such that $\text{sign}(s)\beta(s) \geq c|s| - C$. We then search for $u \in L^2(0, T; \mathcal{V})$ with $\dot{u} \in L^2(0, T; \mathcal{V}^*)$ satisfying a.e. in time

$$(5.2a) \quad \dot{u} - \nabla \cdot (\nabla \beta(u)) = f \quad \text{in } \Omega,$$

$$(5.2b) \quad \beta(u) = g \quad \text{on } \partial\Omega$$

with initial condition

$$(5.2c) \quad u(0) = u_0.$$

Since β is bijective, we can rewrite the nonlinear equation (5.2b) in the form $u = \beta^{-1}(g)$ on $\partial\Omega$. Then, the boundary constraint is linear. In the case where β^{-1} is not given in explicit form, one has to use some kind of Newton method to obtain the boundary values. It is well-known from DAE theory that small errors in the constraints may lead to instabilities in the solution, see the discussion in [Arn98b, Ch. 2.1]. Alternatively, system (5.2) can be reformulated as a constrained operator equation which fits in the framework of Section 3.2.

Consider the spaces $\mathcal{V} := H^1(\Omega)$, $\mathcal{V}_B := H_0^1(\Omega)$, $\mathcal{V}^c := [H_0^1(\Omega)]^{\perp \nu}$, and $\mathcal{Q}^* := H^{1/2}(\partial\Omega)$. In order to write system (5.2) in form of an operator DAE, we need a constraint operator and its Fréchet derivative. We define the operator $\mathcal{B}: \mathcal{V} \rightarrow \mathcal{Q}^*$ by $\mathcal{B}u := \beta(\text{trace } u)$, i.e.,

$$\langle \mathcal{B}u, q \rangle_{\mathcal{Q}^*, \mathcal{Q}} := \int_{\partial\Omega} \beta(u)q \, dx.$$

The constraint (5.2b) in weak form reads $\mathcal{B}u = \mathcal{G}$ in \mathcal{Q}^* with right-hand side $\mathcal{G} \in L^2(0, T; \mathcal{Q}^*)$ densely defined by

$$\langle \mathcal{G}(t), q \rangle_{\mathcal{Q}^*, \mathcal{Q}} := \int_{\partial\Omega} g(t)q \, dx$$

for all test functions $q \in L^2(\partial\Omega)$. The Fréchet derivative of \mathcal{B} at some point $\bar{u} \in \mathcal{V}$ is given by the linear map

$$\begin{aligned} \frac{\partial \mathcal{B}}{\partial u}(\bar{u}): \mathcal{V} &\rightarrow \mathcal{Q}^* \\ v &\mapsto \beta'(\text{trace } \bar{u}) \cdot \text{trace } v \end{aligned}$$

Let $\mathcal{C}_{\bar{u}}$ denote this Fréchet derivative at point \bar{u} . With \mathcal{B} and its Fréchet derivative $\mathcal{C}_{\bar{u}}$ in hand, we obtain the operator DAE

$$(5.3a) \quad \dot{u} - \mathcal{K}u + \mathcal{C}_{\bar{u}}^* \lambda = \mathcal{F} \quad \text{in } \mathcal{V}^*,$$

$$(5.3b) \quad \mathcal{B}u = \mathcal{G} \quad \text{in } \mathcal{Q}^*$$

with initial condition as in (5.2c).

To show that system (5.3) fits the above framework, we need to check whether Assumption 3.2 is satisfied. The required splitting is given by the set of trace-free functions \mathcal{V}_B and its orthogonal complement \mathcal{V}^c . This implies the decomposition of $u \in \mathcal{V}$ into $u = u_1 + u_2$ with $u_1 \in \mathcal{V}_B$ and $u_2 \in \mathcal{V}^c$.

Lemma 5.1. Consider $\bar{u} \in \mathcal{V}$ that is bounded from above along the trace $\partial\Omega$. Then, the Fréchet derivative w.r.t. the space \mathcal{V}^c ,

$$\frac{\partial \mathcal{B}}{\partial u_2}(\bar{u}): \mathcal{V}^c \rightarrow \mathcal{Q}^*, \quad v \mapsto \beta'(\text{trace } \bar{u}) \cdot \text{trace } v$$

defines a homeomorphism.

Proof. The proof is based on the fact that the trace operator, mapping from \mathcal{V}^c to \mathcal{Q}^* , is a homeomorphism, see [Bra07, Lem. 4.2] combined with [Ste08, Ch. 2.5]. This implies, together with the bound for β' , the bijectivity of the operator. Since the trace of \bar{u} is bounded, we obtain the continuity by

$$\|\beta'(\text{trace } \bar{u}) \cdot \text{trace } v\|_{\mathcal{Q}^*} \leq C_{\beta'} |\text{trace } \bar{u}|_{\infty} \|\text{trace } v\|_{\mathcal{Q}^*} \leq C_{\beta'} C_{\bar{u}} C_{\text{tr}} \|v\|_{\mathcal{V}}.$$

The boundedness of the inverse operator follows from the inverse trace theorem [Ste08, Th. 2.22] and $\beta' \geq \varepsilon > 0$. \square

For Assumption 3.2 it remains to show the continuity of $\partial \mathcal{B} / \partial u_2$. This follows from the fact that β is continuously differentiable and thus, $\beta'(\text{trace } \cdot)$ is continuous. Hence, we have shown that the regularized Stefan problem (5.2) can be reformulated as an operator DAE with nonlinear constraints for which the index reduction procedure of Section 3.2 is applicable.

6. CONCLUSION

Within this paper, we have introduced a reformulation of a special class of semi-explicit operator DAEs such that a spatial discretization by finite elements leads to a DAE of index 1. Since the original operator DAE would yield a DAE of index 2, this procedure can be seen as an index reduction for operator DAEs. The paper provides conditions for linear and nonlinear constraint operators which permit the desired regularization.

At this point we want to emphasize that the procedure can be applied similarly to operator DAEs of second order. For an example from elastodynamics, where the constraints may be given by boundary conditions, we refer to [Alt13].

Another advantage of the presented reformulation on operator level is the ability to apply the Rothe method [Rou05, Ch. 8.2]. The application of the Rothe method to the original constrained system involves instabilities as expected from a DAE point of view. These instabilities do not occur for the index reduced operator formulation. The analysis of the Rothe method for constrained PDEs is part of ongoing research.

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