Appl. Numer. Math. 223 (2026) 45–75

Contents lists available at ScienceDirect

Applied Numerical Mathematics

journal homepage: www.elsevier.com/locate/apnum

Research Paper

Discrete gradient methods for port-Hamiltonian differential-algebraic equations

Philipp L. Kinon [a,b], Riccardo Morandin [c,*], Philipp Schulze [d,e]

[a] Institute of Mechanics, Karlsruhe Institute of Technology (KIT), Otto-Ammann-Platz 9, Karlsruhe, 76131, Germany
[b] Department of Mechanical Engineering, Eindhoven University of Technology (TU/e), Eindhoven, 5600 MB, The Netherlands
[c] Faculty of Mathematics, OvGU Magdeburg, Universitätsplatz 2, Magdeburg, 39106, Germany
[d] Institute of Mathematics, Technische Universität Berlin, Str. des 17. Juni 136, Berlin, 10587, Germany
[e] Institute of Mathematics, University of Potsdam, Potsdam, 14476, Germany

ARTICLE INFO

2020 MSC:
34A09
65L80
65P10
70E55
93C10

Keywords:
Port-Hamiltonian systems
Differential-algebraic equations
Structure-preserving discretization
Time integration methods
Discrete gradients

ABSTRACT

Discrete gradient methods are a powerful tool for the time discretization of dynamical systems, since they are structure-preserving regardless of the form of the total energy. In this work, we discuss the application of discrete gradient methods to the system class of nonlinear port-Hamiltonian differential-algebraic equations - as they emerge from the port- and energy-based modeling of physical systems in various domains. We introduce a novel numerical scheme tailored for semi-explicit differential-algebraic equations and further address more general settings using the concepts of discrete gradient pairs and Dirac-dissipative structures. Additionally, the behavior under system transformations is investigated and we demonstrate that under suitable assumptions port-Hamiltonian differential-algebraic equations admit a representation which consists of a parametrized port-Hamiltonian semi-explicit system and an unstructured equation. Finally, we present the application to multibody system dynamics and discuss numerical results to demonstrate the capabilities of our approach.

1. Introduction

Port-Hamiltonian (pH) systems have gained significant importance in various research areas, with a particular focus on the modeling, simulation, and control of dynamical systems [1,2]. pH systems offer a valuable framework for analyzing complex problems, where the complexity may arise from multi-physical interactions, non-trivial domains, and various nonlinearities. One of the key advantages of the pH representation is its explicit description of power interfaces, known as ports, which facilitate power-preserving interconnections between submodules. Thus, this approach simplifies the modular composition of models, which often leads to the presence of algebraic constraints. Correspondingly, the governing equations at hand are *differential-algebraic equations* (DAEs), also known as *descriptor systems* in the context of control theory. If the system has in addition a pH structure, we speak of *port-Hamiltonian differential-algebraic equations* (pHDAEs). A definition for linear time-varying pHDAEs was provided in [3] and a full, nonlinear generalization has been provided in [4]. An important subclass consists of semi-explicit pHDAEs, see e.g. [5, Eq. 3.16], where local representations of implicit port-Hamiltonian DAEs are discussed. In [6,7], the Hamiltonian as a backbone of pH systems is replaced by Lagrangian subspaces or submanifolds to define generalized pHDAEs.

* Corresponding author.
E-mail addresses: philipp.kinon@kit.edu (P.L. Kinon), riccardo.morandin@ovgu.de (R. Morandin), pschulze@math.tu-berlin.de (P. Schulze).

https://doi.org/10.1016/j.apnum.2025.12.006
Received 3 June 2025; Received in revised form 19 December 2025; Accepted 23 December 2025
Available online 27 December 2025

In general, discretizing a structured dynamical system, such as a pH system, can result in the loss of its continuous-time properties, potentially leading to numerical solutions that exhibit unphysical behavior (see, for example, [8, Ch. 1]). One way to mitigate this issue is by employing a structure-preserving time discretization scheme, as the system's properties are often embedded in the algebraic or geometric structure of the original continuous-time model. Examples of such systems include gradient [9], Hamiltonian [10], and, particularly relevant to this work, pH systems. Structure-preserving time discretization approaches for Hamiltonian systems have been widely studied, with [8] offering a general overview. Notably, the development of structure-preserving discretization methods has been driven by computational mechanics [11–15], where variational integrators [14,16,17] represent an important discretization approach within the group of symplectic methods [18]. An interesting approach is also given by time finite element methods (see, e.g. [19–23]). Structure-preserving techniques for other system classes are for example explored in [24–27].

Compared to those works, the structure-preserving time discretization of pH systems is still a relatively young field. When performing numerical integration of pH systems, it is essential to account for the energy exchange through the ports resulting in the presence of a power balance equation. The following developments have been made in recent years:

- In [28], the authors show that certain collocation methods can achieve an exact power balance at the discrete level, provided that the total energy function, the *Hamiltonian*, is a quadratic function of the state. This result is further extended to descriptor systems in [4].
- Structure-preserving discretization approaches based on Petrov-Galerkin projections have been proposed in [23,29] and are closely connected to the aforementioned time finite element approaches. Although these methods can provide continuous solutions also between discrete points in time, and one can obtain arbitrarily high convergence rates, they require the numerical approximation of integrals in time. If the integrand is non-polynomial, one may not be able to integrate these formulas sufficiently accurately, which can lead to the loss of the desired convergence and conservation properties [20]. Moreover, this numerical quadrature imposes additional numerical costs for the emanating schemes.
- In several recent works, e.g. [30–32], the authors consider splitting schemes that separate the energy-conserving and dissipative parts of the dynamics. While this approach can achieve high order convergence and seems quite promising, to the best of our knowledge, it has been so far only applied to linear port-Hamiltonian systems with quadratic Hamiltonian.
- Another approach consists in dropping the requirement for an exact time-discrete power balance, while focusing on minimizing its violation, for example by refining adaptively the time grid of the discretization, see e.g. [33].

Contrary to these approaches, the present work pursues a *discrete gradient* approach, which achieves exact time-discrete power balances also for non-quadratic Hamiltonians. Additionally, the implementation of such schemes is comparably simple and straightforward. While most of the known discrete gradient schemes are restricted to second order convergence rates, there are recent developments to obtain higher accuracy as well (see [34] and the references therein). Another notable work [35] deals with DAEs with a gradient structure and constant descriptor matrix.

Most of the approaches in the literature for pH systems [36–42], which achieve an exact power balance at the discrete level for general Hamiltonians, share the characteristic that they focus on *pH ordinary-differential equations*, where the gradient of the Hamiltonian explicitly appears in the system equations. A challenge with applying methods like discrete gradient techniques to more general systems as introduced in [4] lies in the fact that the gradient of the Hamiltonian in general only appears implicitly in the system equations. The development of discrete gradient pairs [43] has recently addressed this issue.

In contrast to the works focusing on ordinary differential equations, we want to generalize the application field of discrete gradient methods to pHDAEs with possibly state-dependent descriptor matrices, as introduced in [4]. The primary contributions of this work are outlined in the following:

1. Discussion of discrete gradient pairs for general pHDAEs along with a corresponding time integration approach, see Section 4.1.
2. Development of a tangible discrete gradient method for *semi-explicit* pHDAEs, see Section 4.2. This already covers many application problems.
3. Introduction of discrete gradient methods for general pHDAEs, based on a different modeling approach which emphasizes the underlying Dirac structure, see Section 4.3.
4. In-depth analysis of relations between the proposed methods and their behavior under coordinate transformations, see Section 5.

The remainder of this work is structured as follows: Preliminary basics are recapitualed in Section 2, including the definition of pHDAEs and discrete gradients. In Section 3 we focus on a certain class of pHDAEs, namely semi-explicit pHDAEs. We then introduce new methods for the numerical integration of pHDAEs using discrete gradients in Section 4. We analyze their behavior under system transformations and provide conditions for the existence of a semi-explicit representation in Section 5. Section 6 is entirely devoted to the application of our approaches to multibody systems, including numerical experiments. Conclusions and a brief outlook are given in Section 7.

1.1. Notation

We denote by $\mathbb{N}$ the positive natural numbers and by $\mathbb{N}_0$ the natural numbers including zero. With $I_n \in \mathbb{R}^{n,n}$ or simply I we denote the identity matrix and with 0 the zero matrix or vector. We mostly assume that the dimension should become clear from the context. For every matrix $A \in \mathbb{R}^{n,m}$ or vector $v \in \mathbb{R}^n = \mathbb{R}^{n,1}$ we denote by $A^\top \in \mathbb{R}^{m,n}$ and $v^\top \in \mathbb{R}^{1,n}$ their corresponding transposes. For the sake of readability, we sometimes abbreviate less important, unspecified terms by "$\star$".

We denote by $C(X,Y)$ the continuous functions between two topological spaces X and Y. For $k \in \mathbb{N}_0 \cup \{\infty\}$ we denote by $C^k(\mathcal{X}_1, \mathcal{X}_2)$ the k-times continuously differentiable functions from $\mathcal{X}_1$ to $\mathcal{X}_2$, where typically $\mathcal{X}_1 \subseteq \mathbb{R}^n$ and $\mathcal{X}_2 \subseteq \mathbb{R}^m$ are open subsets for some $n, m \in \mathbb{N}$.

If $f \in C^1(\mathcal{X}, \mathbb{R})$ with $\mathcal{X} \subseteq \mathbb{R}^n$ open, we denote by $\nabla f \in C(\mathcal{X}, \mathbb{R}^n)$ the gradient of f, intended as a column vector function. If $F \in C^1(\mathcal{X}, \mathbb{R}^m)$ with $\mathcal{X} \subseteq \mathbb{R}^n$ open, we denote by $\mathrm{D}F \in C(\mathcal{X}, \mathbb{R}^{m,n})$ the Jacobian of F, intended as a matrix function whose rows transposed are the gradients of the entries of F. Furthermore, given a partition $F = (F_1, \dots, F_m)$ for the function and $x = (x_1, \dots, x_r)$ of the state variable, with $x_i = (x_{i,1}, \dots, x_{i,n_i}) \in \mathbb{R}^{n_i}$ for $i = 1, \dots, r$, we denote the corresponding partial gradients and partial Jacobians as

$$\nabla_{x_i} f = \begin{bmatrix} \frac{\partial f}{\partial x_{i,1}} \\ \vdots \\ \frac{\partial f}{\partial x_{i,n_i}} \end{bmatrix}, \qquad \mathrm{D}_{x_i} F = \begin{bmatrix} \frac{\partial F_1}{\partial x_{i,1}} & \cdots & \frac{\partial F_1}{\partial x_{i,n_i}} \\ \vdots & \ddots & \vdots \\ \frac{\partial F_m}{\partial x_{i,1}} & \cdots & \frac{\partial F_m}{\partial x_{i,n_i}} \end{bmatrix},$$

such that in particular

$$\nabla f = \begin{bmatrix} \nabla_{x_1} f \\ \vdots \\ \nabla_{x_r} f \end{bmatrix}, \qquad \mathrm{D}F = \begin{bmatrix} \mathrm{D}_{x_1} F & \cdots & \mathrm{D}_{x_r} F \end{bmatrix}. \tag{1}$$

Additionally, the derivative with respect to time t deserves its own notation, which is $\dot{x} := \frac{\mathrm{d}x}{\mathrm{d}t}$.

If $f : \mathcal{X} \to \mathcal{Y}$ and $g : \mathcal{Y} \to \mathcal{Z}$ are two maps, we denote as usual with $g \circ f : \mathcal{X} \to \mathcal{Z}$ their composition, i.e., $g \circ f(x) = g(f(x))$. When $\overline{g} : \mathcal{Y} \times \mathcal{Y} \to \mathcal{Z}$, we sometimes abuse the notation and write $\overline{g} \circ f : \mathcal{X} \times \mathcal{X} \to \mathcal{Z}$ to denote the map $\overline{g} \circ f(x, x') = \overline{g}(f(x), f(x'))$.

For every matrix function $A \in C(\mathcal{X}, \mathbb{R}^{m,n})$, we denote by $A^\top \in C(\mathcal{X}, \mathbb{R}^{n,m})$ its pointwise transpose $A^\top(x) = A(x)^\top$. If furthermore $m = n$ and A is pointwise invertible, we usually denote by $A^{-1} \in C(\mathcal{X}, \mathbb{R}^{n,n})$ its pointwise inverse $A^{-1}(x) = A(x)^{-1}$, instead of the inverse map, unless otherwise specified. We also introduce the short notation $A^{-\top}$ for $(A^{-1})^\top = (A^\top)^{-1}$. Given a subset $\mathcal{V} \subseteq \mathbb{R}^n$, we denote by $\mathrm{span}(\mathcal{V}) \subseteq \mathbb{R}^n$ the smallest linear subspace of $\mathbb{R}^n$ containing $\mathcal{V}$, and by

$$\mathcal{V}^\perp = \{v \in \mathbb{R}^n \mid v \perp w \text{ for all } w \in \mathcal{V}\}$$

its orthogonal complement. When $\mathcal{V}$ consists of only one vector $v \in \mathbb{R}^n$, we simply write $\mathrm{span}(v)$ and $v^\perp$ instead of $\mathrm{span}(\{v\})$ and $\{v\}^\perp$. Given a subset $\mathcal{X} \subseteq \mathbb{R}^{n_1} \times \mathbb{R}^{n_2}$, we usually denote by $\pi_1 : \mathcal{X} \to \mathbb{R}^{n_1}$ and $\pi_2 : \mathcal{X} \to \mathbb{R}^{n_2}$ the corresponding orthogonal projections, i.e., $\pi_1(x_1, x_2) = x_1$ and $\pi_2(x_1, x_2) = x_2$ for all $(x_1, x_2) \in \mathcal{X}$.

2. Preliminaries

In this section, we recall some preliminary concepts and definitions that will be useful in the remainder of this work.

2.1. Differential-algebraic equations

Differential-algebraic equations are systems of the form

$$F\left(t, x, \frac{\mathrm{d}x}{\mathrm{d}t}, \dots, \frac{\mathrm{d}^k x}{\mathrm{d}t^k}\right) = 0 \tag{2}$$

for some map $F : \mathcal{D}_F \to \mathbb{R}^m$, where $t \in \mathbb{T} \subseteq \mathbb{R}$ denotes the time variable, $x \in \mathcal{X} \subseteq \mathbb{R}^n$ the state variable, and $\mathcal{D}_F \subseteq \mathbb{R}^{1+(k+1)n}$ is the domain of F. Here n is the dimension of the state variable, m the number of equations, and k is the order of the DAE. Typically, the domain of F is of the form $\mathcal{D}_F = \mathbb{T} \times \mathcal{X} \times \mathbb{R}^{kn}$, where $\mathbb{T} \subseteq \mathbb{R}$ is an open (possibly unbounded) interval and $\mathcal{X} \subseteq \mathbb{R}^n$ is an open subset, while the solutions of (2) are to be found in $C^k(\mathbb{T}, \mathcal{X})$.

We are particularly interested in first order quasilinear DAEs, i.e., equations of the form

$$E(t,x)\dot{x} = f(t,x), \tag{3}$$

see e.g. [44,45], for some maps $E : \mathcal{D}_E \to \mathbb{R}^{m,n}$ and $f : \mathcal{D}_f \to \mathbb{R}^m$, where $\mathcal{D}_E, \mathcal{D}_f \subseteq \mathbb{R}^{1+n}$. In particular, if we had $n = m$ and E were pointwise invertible, then (3) would be equivalent to $\dot{x} = E(t,x)^{-1} f(t,x)$, which is a system of first order ordinary differential equations (ODEs). However, when this property is not satisfied, the system might include algebraic constraints and be under- or overdetermined. This presents several challenges, both in the study of the existence and uniqueness of solutions and in the time discretization of the system, see e.g. [46]. In particular, dedicated numerical methods are often necessary.

Enriching a DAE with input and output variables $u \in \mathbb{R}^p$ and $y \in \mathbb{R}^q$ we obtain a *descriptor system*

$$\begin{aligned} E(t,x)\dot{x} &= f(t,x,u), \\ y &= g(t,x,u), \end{aligned} \tag{4}$$

for some maps $E : \mathcal{D}_E \to \mathbb{R}^{m,n}$, $f : \mathcal{D}_f \to \mathbb{R}^m$, and $g : \mathcal{D}_g \to \mathbb{R}^q$, where $\mathcal{D}_E \subseteq \mathbb{R}^{1+n}$ and $\mathcal{D}_f, \mathcal{D}_g \subseteq \mathbb{R}^{1+n+p}$. In applications, the input u is typically a given fixed time-varying function, a state feedback, or an output feedback.

2.2. Port-Hamiltonian descriptor systems

In this paper we focus on time-invariant port-Hamiltonian descriptor systems. We introduce first the concept of gradient pair, which will replace the gradient of the Hamiltonian in the equations.

Definition 1. Let $\mathcal{X} \subseteq \mathbb{R}^n$ be an open set and let $\mathcal{H} \in C^1(\mathcal{X}, \mathbb{R})$, $E \in C(\mathcal{X}, \mathbb{R}^{n,n})$, and $z \in C(\mathcal{X}, \mathbb{R}^n)$. We say that (E, z) is a *gradient pair* for $\mathcal{H}$ if

$$E(x)^\top z(x) = \nabla \mathcal{H}(x) \tag{5}$$

holds for all $x \in \mathcal{X}$.

Port-Hamiltonian descriptor systems are then defined as follows.

Definition 2 (see also [4])**.** Consider a time interval $\mathbb{T} = [0, t_{\text{end}}]$ with $t_{\text{end}} > 0$ and an open state space $\mathcal{X} \subseteq \mathbb{R}^n$. A *time-invariant port-Hamiltonian descriptor system*, in short *pHDAE*, is a descriptor system of the form

$$\begin{aligned} E(x)\dot{x} &= \big(J(x) - R(x)\big)z(x) + B(x)u, \\ y &= B(x)^\top z(x), \end{aligned} \tag{6}$$

together with a *Hamiltonian* $\mathcal{H} \in C^1(\mathcal{X}, \mathbb{R})$, where $E, J, R \in C(\mathcal{X}, \mathbb{R}^{n,n})$, $B \in C(\mathcal{X}, \mathbb{R}^{n,m})$, and $z \in C(\mathcal{X}, \mathbb{R}^n)$ satisfy the properties $J(x) = -J(x)^\top$, $R(x) = R(x)^\top \succeq 0$ for all $x \in \mathcal{X}$, and (E, z) is a gradient pair for $\mathcal{H}$. Here E, J, R are called the *descriptor, structure*, and *dissipation* matrix functions, respectively, and z is called the *costate* function.

Remark 1.

In the context of the modeling of pH systems, the state variables x are also sometimes called *energy variables* (see e.g. [5] and [2, Ch. 11]), since the Hamiltonian $\mathcal{H} : x \mapsto \mathcal{H}(x)$ depends on them. Likewise, the *coenergy variables* e are given as the derivative of the Hamiltonian with respect to the energy variables, i.e., $e = \nabla \mathcal{H}(x)$. While the energy variables can be interpreted as points on a differential manifold $x \in \mathcal{X}$, the coenergy variables are elements of the cotangent bundle $e \in T^*\mathcal{X}$. We have then a natural duality induced by the pair $(T\mathcal{X}, T^*\mathcal{X})$, which yields a power balance equation given as $\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{H}(x(t)) = \langle \dot{x}, e(x)\rangle = \langle \dot{x}, \nabla\mathcal{H}(x)\rangle$. This also corresponds to the duality between flow and effort variables.

In the present case however, the coenergy variables e do not directly correspond to the costate function $x \mapsto z(x)$, but to $x \mapsto e(x) = E(x)^\top z(x) = \nabla \mathcal{H}(x)$ instead. Furthermore, as we will see in more detail in Section 3, the presence of algebraic equations typically induces a partition on both the state and costate of the system, which decouples some of the variables from the energy. Thus, to avoid ambiguity, in the context of pHDAEs we refer to x as the state and to z as the costate, evading the energy/coenergy nomenclature altogether.

Remark 2. In this work we formally consider only systems without a feedthrough term in the output equation. Nevertheless, our results can be easily adapted for systems with feedthrough, i.e., replacing the output equation with $y = C(x)^\top z(x) + D(x)u$ for some matrix functions C, D and requiring some additional dissipative structure involving R, B, C, D, see e.g. definitions in [4,47].

Remark 3. Although the system from Definition 2 could emerge from a change of variables of a pH ODE system with state $\tilde{x}$ and Jacobian $\mathrm{D}\tilde{x}(x) = E(x)$ inducing $z(x) = \nabla\widetilde{\mathcal{H}}(\tilde{x}(x))$, the presented framework additionally covers many more cases.

Note that in Definition 2 the input and output variables, usually taken as functions in $C(\mathbb{T}, \mathbb{R}^m)$, have the same size. In fact, the product $y^\top u$ typically has the same physical dimension as power. In particular, one can easily verify (see e.g. [4]) that every pHDAE of the form (6) satisfies the *power balance equation* (PBE)

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{H}\big(x(t)\big) = -z\big(x(t)\big)^\top R\big(x(t)\big)z\big(x(t)\big) + y(t)^\top u(t) \tag{7}$$

and the dissipation inequality

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{H}\big(x(t)\big) \le y(t)^\top u(t), \tag{8}$$

along every solution (x, u, y) of (6), for all $t \in \mathbb{T}$. Note that the PBE and the dissipation inequality can be reinterpreted in integral form as

$$\mathcal{H}\big(x(t_1)\big) - \mathcal{H}\big(x(t_0)\big) = \int_{t_0}^{t_1} \big(-z(x(t))^\top R(x(t))z(x(t)) + y(t)^\top u(t)\big)\mathrm{d}t \tag{9}$$

and

$$\mathcal{H}\big(x(t_1)\big) - \mathcal{H}\big(x(t_0)\big) \le \int_{t_0}^{t_1} y(t)^\top u(t)\,\mathrm{d}t \tag{10}$$

respectively, for every $t_0, t_1 \in \mathbb{T},\ t_0 \le t_1$.

Let us now briefly introduce another equivalent representation of pHDAEs, which will be used throughout this work. Similarly as introduced in [48], by defining a new variable $f = z(x)$ representing the costate, and adding the gradient pair condition $E(x)^\top f = \nabla\mathcal{H}(x)$ explicitly to the pHDAE Eqs. (6), we obtain an equivalent system defined as follows.

Definition 3 (Dirac-dissipative representation). Consider a pHDAE (6), then

$$\begin{bmatrix} \nabla \mathcal{H}(x) \\ 0 \\ y \end{bmatrix} + \begin{bmatrix} 0 & -E(x)^\top & 0 \\ E(x) & J(x) - R(x) & B(x) \\ 0 & -B(x)^\top & 0 \end{bmatrix} \begin{bmatrix} -\dot{x} \\ f \\ u \end{bmatrix} = 0, \tag{11a}$$

$$f = z(x), \tag{11b}$$

is referred to as the *Dirac-dissipative representation* related to (6). Shorthand we can call it *DDR*-pHDAE.

Note that we use a different letter to denote the costate as a variable, to avoid ambiguity with the costate function and its discrete approximations that will be introduced in the following sections. Moreover, it should be highlighted that the pH structure is entirely encoded in (11a). In fact, this equation corresponds to the intersection of the Dirac structure and the dissipative relation of the pH system, and has the form $\mathfrak{e} + (\mathfrak{J}(x) - \mathfrak{R}(x))\mathfrak{f} = 0$, where $\mathfrak{f} = (-\dot{x}, f, u)$ and $\mathfrak{e} = (\nabla \mathcal{H}(x), 0, y)$ are the flow and effort vectors, and $\mathfrak{J} = -\mathfrak{J}^\top$ and $\mathfrak{R} = \mathfrak{R} \succeq 0$ hold pointwise, see [48] for further details.

As we will discuss in Section 4.3, similarly as in [48], the Dirac-dissipative representation can be particularly useful for the structure-preserving discretization of pHDAEs. This can be deducted particularly due to its structure yielding the following result.

Theorem 1. *Every solution* (x, f, u, y) *of* (11a) *satisfies the PBE and dissipation inequality, since*

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{H}\big(x(t)\big) - y(t)^\top u(t) = -\mathfrak{f}^\top \mathfrak{e} = \mathfrak{f}^\top \big(\mathfrak{J}(x) - \mathfrak{R}(x)\big)\mathfrak{f} = -\mathfrak{f}^\top \mathfrak{R}(x)\mathfrak{f} = -f^\top R(x) f \leq 0.$$

Remark 4. The reader should not confuse the acronym *DDR* with the notion of *difference and differential representations*, which has been coined in, e.g. [49]. While both concepts are related to pH systems and both can be combined with discrete gradient methods, the works related to the difference and differential representation propose a hybrid approach combining discrete-time equations with differential equations. Contrarily, the DDR in the present work lives in continuous time and highlights the underlying geometric structure.

Since the PBE (7) and dissipation inequality (8) are fundamental properties satisfied by every pH system, there is much effort in the literature [4,23,28,29,40,41,43] in developing time-discretization schemes to preserve them on a discrete level. This is also the focus of this paper.

2.3. Discrete gradients

Discrete gradients are a popular tool for generating structure-preserving integration methods for dynamical systems [8,50,51]. A general definition is as follows.

Definition 4 (Discrete gradients, see [8]). Given a function $f \in C^1(\mathcal{X}, \mathbb{R})$ with $\mathcal{X} \subseteq \mathbb{R}^n$ open, a *discrete gradient* for f is any vector function $\overline{\nabla} f \in C(\mathcal{X} \times \mathcal{X}, \mathbb{R}^n)$ that satisfies the properties

1. $\overline{\nabla} f(x, x')^\top (x' - x) = f(x') - f(x)$ for all $x, x' \in \mathcal{X}$,
2. $\overline{\nabla} f(x, x) = \nabla f(x)$ for all $x \in \mathcal{X}$,

where (i) is referred to as *directionality* and (ii) as *consistency* condition.

Especially the directionality property will be handy later on for the design of structure-preserving discretizations. The following definition provides an example for a discrete gradient, which can yield a symmetric method of second order accuracy, as it represents a second-order approximation to the exact gradients.

Definition 5 (Gonzalez discrete gradient, see [51]). For a given function $f \in C^1(\mathcal{X}, \mathbb{R})$ with $\mathcal{X} \subseteq \mathbb{R}^n$ convex open subset, its Gonzalez (or midpoint) discrete gradient $\overline{\nabla} f \in C(\mathcal{X} \times \mathcal{X}, \mathbb{R}^n)$ is defined by

$$\overline{\nabla} f(x, x') = \begin{cases} \nabla f\left(\frac{x+x'}{2}\right) + \dfrac{f(x') - f(x) - \nabla f\left(\frac{x+x'}{2}\right)^\top (x' - x)}{||x' - x||^2} (x' - x) & \text{if } x' \neq x, \\ \nabla f(x) & \text{otherwise.} \end{cases} \tag{12}$$

Notably, the Gonzalez discrete gradient is determined by the directionality condition together with its action on the orthogonal complement $(x' - x)^\perp$, that is, $\overline{\nabla} f(x, x')^\top z = \nabla f(\frac{x+x'}{2})^\top z$ for all $x, x' \in \mathcal{X}$ and $z \in (x' - x)^\perp$.

Note that for the special case of polynomial functions with degree of at most two, the Gonzalez discrete gradient is equivalent to a midpoint evaluation of the analytical gradient. Next, the concept of discrete gradients may also be generalized to vector-valued functions.

Definition 6 (Discrete Jacobians, see [50, Def. 3.3]). Given a vector-valued function $F \in C^1(\mathcal{X}, \mathbb{R}^m)$ with $\mathcal{X} \subseteq \mathbb{R}^n$ open, a *discrete Jacobian* for F is any matrix function $\overline{\mathrm{D}} F \in C(\mathcal{X} \times \mathcal{X}, \mathbb{R}^{m,n})$ that satisfies the directionality and consistency properties

1. $\overline{\mathrm{D}} F(x, x')(x' - x) = F(x') - F(x)$ for all $x, x' \in \mathcal{X}$,

2. $\overline{\mathrm{D}}F(x,x) = \mathrm{D}F(x)$ for all $x \in \mathcal{X}$.

As pointed out in [50], a discrete Jacobian $\overline{\mathrm{D}}F$ may be equivalently characterized by the fact that all of its rows are discrete gradients of the corresponding component functions of F. In a similar notation as in (1), we write

$$\overline{\nabla}F = \begin{bmatrix} \overline{\nabla}_{x_1} F \\ \vdots \\ \overline{\nabla}_{x_r} F \end{bmatrix}, \qquad \overline{\mathrm{D}}F = \begin{bmatrix} \overline{\mathrm{D}}_{x_1} F & \cdots & \overline{\mathrm{D}}_{x_r} F \end{bmatrix}$$

for partial discrete derivatives and a partition $x = (x_1, \dots, x_r)$ of the state variable. In particular, as long as $\mathcal{X} \subseteq \mathbb{R}^n$ is convex, we define the *Gonzalez discrete Jacobian* of a differentiable vector field $F \in C^1(\mathcal{X}, \mathbb{R}^m)$ as

$$\overline{\mathrm{D}}F(x,x') = \begin{cases} \mathrm{D}F\left(\frac{x+x'}{2}\right) + \dfrac{F(x') - F(x) - \mathrm{D}F\left(\frac{x+x'}{2}\right)(x'-x)}{\|x'-x\|^2}(x'-x)^\top & \text{if } x' \neq x, \\ \mathrm{D}F(x) & \text{otherwise,} \end{cases}$$

which is again determined by the directionality condition together with $\overline{\mathrm{D}}F(x,x')w = \mathrm{D}F(\frac{x+x'}{2})w$ for all $x, x' \in \mathcal{X}$ and $w \in (x'-x)^\perp$.

Remark 5. For the construction of classical discrete gradients or discrete Jacobians, some assumptions on the state space $\mathcal{X}$, like its convexity, are usually necessary. However, in general the existence of discrete gradients is actually independent from the structure of $\mathcal{X}$. For example, replacing $\nabla f(\frac{x+x'}{2})$ by $\nabla f(x)$ or $\nabla f(x')$ in (12) yields a discrete gradient regardless of the structure of $\mathcal{X}$, although its usefulness for discretization is unclear.

Let us focus again on discrete gradients and observe the following property.

Lemma 1. *Let $f \in C^1(\mathcal{X}, \mathbb{R})$ with $\mathcal{X} = \mathcal{X}_1 \times \mathcal{X}_2$, where $\mathcal{X}_1 \subseteq \mathbb{R}^{n_1}$ and $\mathcal{X}_2 \subseteq \mathbb{R}^{n_2}$ are open and $\mathcal{X}_2$ is convex, let us partition $x = (x_1, x_2) \in \mathbb{R}^{n_1} \times \mathbb{R}^{n_2}$, and suppose that $\nabla_{x_2} f = 0$ holds everywhere in $\mathcal{X}$. Then there is $f_1 \in C^1(\mathcal{X}_1, \mathbb{R})$ such that $f_1(x_1) = f(x_1, x_2)$ and $\nabla f_1(x_1) = \nabla_{x_1} f(x_1, x_2)$ for every $(x_1, x_2) \in \mathcal{X}$, or in short $f_1 \circ \pi_1 = f$ and $\nabla f_1 \circ \pi_1 = \nabla_{x_1} f$. Let now $\overline{\nabla} f_1$ be a discrete gradient for f_1 and $\overline{\nabla} f = (\overline{\nabla} f_1 \circ \pi_1, 0) : \mathcal{X} \times \mathcal{X} \to \mathbb{R}^{n_1} \times \mathbb{R}^{n_2}$, i.e.,*

$$\overline{\nabla} f(x,x') = \begin{bmatrix} \overline{\nabla} f_1(x_1, x_1') \\ 0 \end{bmatrix}$$

for every $x = (x_1, x_2), x' = (x_1', x_2') \in \mathcal{X}$. Then $\overline{\nabla} f$ is a discrete gradient for f.

Proof. The interested reader is referred to Appendix A for some detailed lines showing that there is $f_1 \in C^1(\mathcal{X}_1, \mathbb{R})$ such that $f_1(x_1) = f(x_1, x_2)$ and $\nabla f_1(x_1) = \nabla_{x_1} f(x_1, x_2)$ for every $(x_1, x_2) \in \mathcal{X}$. We now show that $\overline{\nabla} f$ is a discrete gradient for f. In fact, for every $x = (x_1, x_2), x' = (x_1', x_2') \in \mathcal{X}$ it holds that

$$\overline{\nabla} f(x,x) = \begin{bmatrix} \overline{\nabla} f_1(x_1, x_1) \\ 0 \end{bmatrix} = \begin{bmatrix} \nabla f_1(x_1) \\ 0 \end{bmatrix} = \begin{bmatrix} \nabla_{x_1} f(x) \\ \nabla_{x_2} f(x) \end{bmatrix} = \nabla f(x)$$

and

$$\overline{\nabla} f(x,x')^\top (x'-x) = \begin{bmatrix} \overline{\nabla} f_1(x_1, x_1') \\ 0 \end{bmatrix}^\top \begin{bmatrix} x_1' - x_1 \\ x_2' - x_2 \end{bmatrix} = \overline{\nabla} f_1(x_1, x_1')^\top (x_1' - x_1) = f_1(x_1') - f_1(x_1) = f(x') - f(x),$$

which concludes the proof. □

Remark 6. We note that the previous lemma is still true when replacing the assumption that $\mathcal{X}$ has the form $\mathcal{X}_1 \times \mathcal{X}_2$ with convex $\mathcal{X}_2$ by the weaker assumption that there exist an open set $\widetilde{\mathcal{X}} \subseteq \mathbb{R}^{n_1} \times \mathbb{R}^{n_2}$ and a diffeomorphism $\varphi = (\varphi_1, \varphi_2) : \widetilde{\mathcal{X}} \to \mathcal{X}$ such that $\pi_2(\widetilde{\mathcal{X}})$ is convex and $\varphi_1 : \pi_1(\widetilde{\mathcal{X}}) \to \pi_1(\mathcal{X})$ is well-defined. However, in order to keep the setting simple, in this paper we will focus on the case where $\mathcal{X} = \mathcal{X}_1 \times \mathcal{X}_2$ with convex $\mathcal{X}_2$, with the awareness that this setting can be extended.

Remark 7. Moreover, assuming the convexity of $\mathcal{X}$ is in practice not restrictive. Since discrete gradients and other consistent approximations are used for time discretization, it can be usually assumed that they will only be evaluated for arbitrarily close $x, x' \in \mathcal{X}$, up to reducing the time step accordingly. Then, for every $x \in \mathcal{X}$ we can restrict them to $\mathcal{X}_0 \times \mathcal{X}_0$, where $\mathcal{X}_0$ is an appropriate open neighborhood of x, which can be selected to have even stronger structure, like being a ball for the ∞-norm on $\mathbb{R}^n$. This choice in particular ensures that $\mathcal{X}_0$ is convex and can be written in the form $\mathcal{X}_1 \times \mathcal{X}_2$ for every partition of the state variable $x = (x_1, x_2)$.

Discrete gradients have been applied successfully to the time discretization of pH ODEs, see e.g. [39–41]. Here, we want to tackle pHDAEs as described in Definition 2. This brings with it the striking challenge that the gradient of the Hamiltonian, which is supposed to be approximated with a discrete gradient, appears only implicitly within the relation (5) and is not directly part of the DAEs (6), which govern the dynamics of the system. Particularly for singular descriptor matrices, this leads to a non-invertible relation to the costate function. In this context the recent work [43] proposed the notion of *discrete gradient pairs*, which we regard to be helpful throughout the present work.

Definition 7 (Discrete gradient pair, see [43])**.** Let (E, z) be a gradient pair for $\mathcal{H}$. We call $(\overline{E}, \overline{z}) \in C(\mathcal{X} \times \mathcal{X}, \mathbb{R}^{n,n}) \times C(\mathcal{X} \times \mathcal{X}, \mathbb{R}^n)$ a *discrete gradient pair* for $(\mathcal{H}, E, z)$ if the following conditions are satisfied.

1. $\overline{z}(x,x')^\top \overline{E}(x,x')(x'-x) = \mathcal{H}(x') - \mathcal{H}(x)$ for all $(x',x) \in \mathcal{X}\times\mathcal{X}$,
2. $\overline{E}(x,x) = E(x)$ for all $x \in \mathcal{X}$,
3. $\overline{z}(x,x) = z(x)$ for all $x \in \mathcal{X}$.

These conditions essentially yield that $\overline{E}^\top \overline{z}$ is a discrete gradient, see Definition 4. Property (i) can be interpreted as the directionality condition, while conditions (ii) and (iii) ensure the consistency condition for this specific discrete gradient. As it has become obvious from the previous definitions in this section, the property of *consistency* is rather crucial. We therefore make the following statement.

Definition 8. Given two functions $F \in C(\mathcal{X},\mathbb{R}^n)$ and $\overline{F} \in C(\mathcal{X}\times\mathcal{X},\mathbb{R}^n)$, we call $\overline{F}$ a *consistent* approximation or discretization of F if $\overline{F}(x,x) = F(x)$ for all $x \in \mathcal{X}$.

Having discussed basic notions of pHDAEs and discrete gradients, we stress that a special class of pHDAEs is pivotal in this work, see the upcoming section.

3. Semi-explicit port-Hamiltonian descriptor systems

We now specify that the pHDAE under investigation is semi-explicit . This subclass already covers many applications and will be the starting point pivotal for derivations of corresponding time integration methods. We start by introducing the related concept of semi-explicit gradient pairs.

Definition 9. Let (E,z) be a gradient pair for $\mathcal{H}$. We say that (E,z) is a *semi-explicit gradient pair* if $\mathcal{X} = \mathcal{X}_1\times\mathcal{X}_2$ with $\mathcal{X}_1 \subseteq \mathbb{R}^{n_1}$ and $\mathcal{X}_2 \subseteq \mathbb{R}^{n_2}$ open and $\mathcal{X}_2$ convex , and $E = \operatorname{diag}(E_{11},0)$ for some pointwise invertible matrix function $E_{11} \in C(\mathcal{X},\mathbb{R}^{n_1,n_1})$.

Semi-explicit gradient pairs satisfy the following property.

Lemma 2. *Let (E,z) be a semi-explicit gradient pair for $\mathcal{H}$. Then there exists $\mathcal{H}_1 \in C^1(\mathcal{X}_1,\mathbb{R})$ such that $\mathcal{H}_1\circ\pi_1 = \mathcal{H}$ and $\nabla\mathcal{H}_1\circ\pi_1 = \nabla_{x_1}\mathcal{H}$, i.e.,*

$$\mathcal{H}_1(x_1) = \mathcal{H}(x_1,x_2), \qquad \nabla\mathcal{H}_1(x_1) = \nabla_{x_1}\mathcal{H}(x_1,x_2) \tag{13}$$

for all $x_1 \in \mathcal{X}_1,\ x_2 \in \mathcal{X}_2$. In particular, the gradient pair property (5) is determined by

$$\nabla\mathcal{H}_1(x_1) = E_{11}(x_1,x_2)^\top z_1(x_1,x_2), \tag{14}$$

for all $x_1 \in \mathcal{X}_1,\ x_2 \in \mathcal{X}_2$, where $z = (z_1,z_2)$ is the corresponding partition of z.

Proof. Due to the structure of E, the gradient pair property (5) can be written as $\nabla_{x_1}\mathcal{H} = E_{11}^\top z_1,\ \nabla_{x_2}\mathcal{H} = 0$. The latter equation implies with Lemma 1 that there exists $\mathcal{H}_1 \in C^1(\mathcal{X}_1,\mathbb{R})$ satisfying (13), while the former is immediately reinterpreted as (14). □

By abuse of terminology, we will also refer to $\mathcal{H}_1$ as *Hamiltonian* in the remainder of this work, while ensuring that it is clear from the context whether we refer to $\mathcal{H}:\ \mathcal{X}\to\mathbb{R}$ or to $\mathcal{H}_1:\ \mathcal{X}_1\to\mathbb{R}$.

Definition 10. Consider a state space $\mathcal{X} = \mathcal{X}_1\times\mathcal{X}_2 \subseteq \mathbb{R}^n$ with $\mathcal{X}_1 \subseteq \mathbb{R}^{n_1}$ open and $\mathcal{X}_2 \subseteq \mathbb{R}^{n_2}$ open convex, and let us partition the state $x = (x_1,x_2) \in \mathcal{X}$ accordingly. A *semi-explicit pHDAE* is a port-Hamiltonian descriptor system in the sense of Definition 2 with $E = \operatorname{diag}(E_{11},0)$, where $E_{11} \in C(\mathcal{X},\mathbb{R}^{n_1,n_1})$ is pointwise invertible. In particular it admits the form

$$\begin{aligned}\begin{bmatrix} E_{11}(x) & 0\\ 0 & 0\end{bmatrix}\begin{bmatrix}\dot{x}_1\\ \dot{x}_2\end{bmatrix} &= (J(x)-R(x))\begin{bmatrix}z_1(x)\\ z_2(x)\end{bmatrix} + B(x)u,\\ y &= B(x)^\top\begin{bmatrix}z_1(x)\\ z_2(x)\end{bmatrix},\end{aligned} \tag{15}$$

together with a Hamiltonian $\mathcal{H}_1 \in C^1(\mathcal{X}_1,\mathbb{R})$ that satisfies the gradient pair property (14) and conforms with Lemma 2. Since only the time-derivative of x_1 appears in (15), x_1 is termed *differential* state and x_2 is called *algebraic* state. Conforming with Lemma 2, the algebraic state does not contribute to the Hamiltonian of the system.

Note that systems of the form (15) have also been considered in [48], where the application of partitioned Runge-Kutta schemes for their time discretization was considered. We now illustrate Lemma 2 and Definition 10 by exploring some examples.

Example 1. *Consider the simple linear semi-explicit pHDAE of index 1 with $x = (x_1,x_2)$ governed by*

$$\begin{bmatrix}1 & 0\\ 0 & 0\end{bmatrix}\begin{bmatrix}\dot{x}_1\\ \dot{x}_2\end{bmatrix} = \begin{bmatrix}0 & 1\\ -1 & -1\end{bmatrix}\begin{bmatrix}x_1\\ x_2\end{bmatrix}, \tag{16}$$

together with its Hamiltonian $\mathcal{H}_1(x_1) = \frac{1}{2}x_1^2$. Conforming with Definition 10, x_1 is the differential state, x_2 is the algebraic state, and the Hamiltonian only depends on x_1. Moreover, the gradient pair property (14) is satisfied with $E_{11} = 1$ and $z_1(x_1,x_2) = x_1$. ◊

Example 2 (Constrained input-output pH systems in classical form). *The above framework naturally includes all systems which are covered by the standard notion of pH systems in* constrained input-output representation *(see e.g. [1, Eq. 2.154] or [5, Eq. 4.44]) described by local coordinates $\tilde{x}$ satisfying*

$$\begin{aligned}\dot{\tilde{x}} &= \left(\widetilde{J}(\tilde{x}) - \widetilde{R}(\tilde{x})\right)\nabla\widetilde{\mathcal{H}}(\tilde{x}) + g(\tilde{x})u + b(\tilde{x})\lambda,\\ y &= g(\tilde{x})^\top \nabla\widetilde{\mathcal{H}}(\tilde{x}),\\ 0 &= b(\tilde{x})^\top \nabla\widetilde{\mathcal{H}}(\tilde{x}),\end{aligned}$$

with $x = (x_1, x_2) = (\tilde{x}, \lambda)$, $\mathcal{H}_1(x_1) = \widetilde{\mathcal{H}}(\tilde{x})$, $E_{11} = I$, $z_1 = \nabla\widetilde{\mathcal{H}}(\tilde{x})$, $z_2 = \lambda$, $B(x)^\top = [g(\tilde{x})^\top, 0]$ and

$$J(x) - R(x) = \begin{bmatrix} \widetilde{J}(\tilde{x}) - \widetilde{R}(\tilde{x}) & b(\tilde{x}) \\ -b(\tilde{x})^\top & 0 \end{bmatrix}.$$

Note that the Lagrange multipliers $x_2 = \lambda$ are here algebraic state variables. ◊

Example 3 (Nonlinear multibody systems). *It can be shown that the governing equations for nonlinear multibody systems fit well into the above framework of semi-explicit pHDAEs. The equations of motion are given as*

$$\begin{bmatrix} I & 0 & 0 \\ 0 & M & 0 \\ 0 & 0 & 0 \end{bmatrix}\begin{bmatrix} \dot{q} \\ \dot{v} \\ \dot{\lambda} \end{bmatrix} = \left(\begin{bmatrix} 0 & I & 0 \\ -I & -R_{\mathrm{R}}(q) & -\mathrm{D}g(q)^\top \\ 0 & \mathrm{D}g(q) & 0 \end{bmatrix}\right)\begin{bmatrix} \nabla V(q) \\ v \\ \lambda \end{bmatrix} + \begin{bmatrix} 0 \\ I \\ 0 \end{bmatrix}u,$$

$$y = \begin{bmatrix} 0 & I & 0 \end{bmatrix}\begin{bmatrix} \nabla V(q) \\ v \\ \lambda \end{bmatrix}.$$

The Hamiltonian

$$\mathcal{H}(x) = \frac{1}{2}v^\top M v + V(q) = T(v) + V(q)$$

denotes the total energy. Verifying that $E^\top z(x) = \nabla\mathcal{H}(x)$ holds true is straightforward. In this example, the Lagrange multipliers λ appear as algebraic states, that do not appear in the Hamiltonian. For more details, especially concerning an introduction of the unknowns, see Section 6.1. ◊

Example 4 (Synchronous machine). *Let us consider a synchronous machine, modeled as described e.g. in [52], and interpreted as a pH system like in [53]. After a change of variables, which is detailed in Appendix B, such that we obtain $x = (I, p, \theta) \in \mathbb{R}^8$, the governing equations can be found in a suitable representation*

$$\begin{bmatrix} L(\theta) & 0 & L'(\theta)I \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}\begin{bmatrix} \dot{I} \\ \dot{p} \\ \dot{\theta} \end{bmatrix} = \begin{bmatrix} -R_{s,r} & 0 & 0 \\ 0 & -d & -1 \\ 0 & 1 & 0 \end{bmatrix}\begin{bmatrix} I \\ J_r^{-1}p \\ -\frac{1}{2}I^\top L'(\theta)I \end{bmatrix} + \begin{bmatrix} I_3 & 0 & 0 \\ 0 & e_1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{bmatrix}\begin{bmatrix} V_s \\ V_f \\ \tau \end{bmatrix}, \tag{17a}$$

$$\begin{bmatrix} I_s \\ I_f \\ \omega \end{bmatrix} = \begin{bmatrix} I_3 & 0 & 0 & 0 \\ 0 & e_1^\top & 0 & 0 \\ 0 & 0 & 1 & 0 \end{bmatrix}\begin{bmatrix} I \\ J_r^{-1}p \\ -\frac{1}{2}I^\top L'(\theta)I \end{bmatrix}. \tag{17b}$$

Here $e_1 \in \mathbb{R}^3$ denotes the first vector of the standard basis of $\mathbb{R}^3$, $I \in \mathbb{R}^6$ contains the currents in the stator and rotor, $p \in \mathbb{R}$ represents the angular momentum of the rotor, $\theta \in \mathbb{R}$ the angle of the rotor, and $R_{s,r} := \mathrm{diag}(R_s, R_r) \succ 0$, where $R_s, R_r \in \mathbb{R}^{3,3}$ are positive diagonal matrices representing the stator and rotor resistances. Additionally, $d > 0$ is the mechanical friction, $V_s, I_s \in \mathbb{R}^3$ are the three-phase stator terminal voltages and currents, $V_f, I_f \in \mathbb{R}$ are the rotor field winding voltage and current, $\tau, \omega \in \mathbb{R}$ are the mechanical torque and angular velocity, $J_r > 0$ is the rotational inertia of the rotor, $L : \mathbb{R} \to \mathbb{R}^{6,6}$ is the inductance matrix, usually assumed to be C^∞, pointwise symmetric positive definite, and periodic of period 2π, and L' denotes its first derivative. Note that V_s, V_f, τ are interpreted as the input variables of the system, while I_s, I_f, ω as the corresponding output variables. The system is completed by the Hamiltonian

$$\mathcal{H}(I, p, \theta) = \frac{1}{2}I^\top L(\theta)I + \frac{1}{2J_r}p^2,$$

which verifies $E(x)^\top z(x) = \nabla\mathcal{H}(x)$, see Appendix B for further details.

While one might argue that (17a) is not really a DAE, since E is pointwise invertible, it still fits into Definition 10 for semi-explicit pHDAEs as a special case without algebraic states.This representation has potential advantages compared to the original example from Appendix B. For example, the inductance matrix $L(\theta)$ does not appear under inversion anymore. Furthermore, synchronous machines can be components in complex interconnected systems, e.g. in the modeling of power networks, typically resulting in actual semi-explicit pHDAEs anyway due to the application of Kirchhoff's laws. ◊

In the upcoming section we focus on the discretization of pHDAEs - as discussed both in Definitions 2 and 10.

4. Structure-preserving time discretization

We start by discussing integration methods for general pHDAEs of the form (6) in Section 4.1. Here the concept of discrete gradient pairs will be of central importance. We continue with the discretization of semi-explicit pHDAEs of the form (15) in Section 4.2, yielding a tangible time stepping method. Then, in Section 4.3 we discuss an alternative approach, based on the Dirac-dissipative representation associated to the pHDAE, that does not require the semi-explicit structure. Lastly, in Section 4.4 we investigate how the three different approaches are connected, when a semi-explicit representation is available.

4.1. Discrete gradient pair methods for general pHDAEs

Consider a pHDAE of the form (6) and a temporal grid $0 = t^0 < t^1 < \ldots < t^N = t_{\text{end}}$ with N time intervals of constant time step size $h = t^{k+1} - t^k$ for $k = 0, \ldots, N-1$. We consider uniform time grids for the sake of brevity and propose the scheme

$$\begin{aligned} \overline{E}(x^k, x^{k+1})(x^{k+1} - x^k) &= h\big(\overline{J}(x^k, x^{k+1}) - \overline{R}(x^k, x^{k+1})\big)\overline{z}(x^k, x^{k+1}) + h\overline{B}(x^k, x^{k+1})u^{k,k+1}, \\ y^{k,k+1} &= \overline{B}(x^k, x^{k+1})^\top \overline{z}(x^k, x^{k+1}). \end{aligned} \tag{18}$$

for $k = 0, \ldots, N-1$.

In (18), we define discrete approximations of the state $x^k \approx x(t^k)$ assuming that also $x^k \in \mathcal{X}$ for sufficiently small time steps. The matrices $\overline{E}, \overline{J}, \overline{R}, \overline{B}$ are arbitrary consistent approximations of the matrix functions (see Definition 8), still satisfying $\overline{J} = -\overline{J}^\top$ and $\overline{R} = \overline{R}^\top \geq 0$ pointwise. Moreover, $u^{k,k+1}$ is not necessarily the evaluation of the (possibly discontinuous) input function at t^k, but at some point within the time interval of interest or an average value of it. Correspondingly, the discrete-time output $y^{k,k+1}$ is an approximation for $y(t)$ for the whole time step interval.

Most importantly, we require that $(\overline{E}, \overline{z})$ is a discrete gradient pair for $(\mathcal{H}, E, z)$ in the sense of Definition 7. Finding such a discrete gradient pair is not trivial, but we will study how to construct one in certain special cases in Section 5. For self-containedness of this work, we show that the usage of discrete gradient pairs yields an energy-consistent time integration.

Theorem 2. *Scheme (18) yields an energy-consistent approximation of the time-continuous power balance (7) given by*

$$\mathcal{H}(x^{k+1}) - \mathcal{H}(x^k) = -h\overline{z}(x^k, x^{k+1})^\top \overline{R}(x^k, x^{k+1})\overline{z}(x^k, x^{k+1}) + h(y^{k,k+1})^\top u^{k,k+1} \leq h(y^{k,k+1})^\top u^{k,k+1}. \tag{19}$$

Proof. Combining the directionality property (i) of the discrete gradient pair with (18) one obtains

$$\begin{aligned} \mathcal{H}(x^{k+1}) - \mathcal{H}(x^k) &= \overline{z}(x^k, x^{k+1})^\top \overline{E}(x^k, x^{k+1})(x^{k+1} - x^k) \\ &= h\overline{z}(x^k, x^{k+1})^\top \big(\overline{J}(x^k, x^{k+1}) - \overline{R}(x^k, x^{k+1})\big)\overline{z}(x^k, x^{k+1}) + h\overline{z}(x^k, x^{k+1})^\top \overline{B}(x^k, x^{k+1})u^{k,k+1} \\ &= -h\overline{z}(x^k, x^{k+1})^\top \overline{R}(x^k, x^{k+1})\overline{z}(x^k, x^{k+1}) + h(y^{k,k+1})^\top u^{k,k+1} \leq h(y^{k,k+1})^\top u^{k,k+1}, \end{aligned}$$

which is the desired result. □

4.2. Discrete gradient methods for semi-explicit pHDAEs

In the following we consider the special case of a semi-explicit pHDAE of the form (15) for which we present a concrete time discretization scheme. The scheme itself is outlined in Section 4.2.1 whereas a corresponding convergence analysis is presented in Section 4.2.2.

4.2.1. Time discretization scheme for semi-explicit pHDAEs

For a semi-explicit pHDAE of the form (15), the partitioning of the state and the block matrix structure allow for a straightforward approach using discrete gradients, which leads to a concrete time stepping method outlined in the following. Particularly, the semi-explicit gradient pair property (14) allows for a direct approximation of z_1 in terms of the Hamiltonian $\mathcal{H}_1$. Essentially, the proposed method can be written just like Eqs. (18), which have to be completed by the additional constraint

$$\overline{E}_{11}(x^k, x^{k+1})^\top \overline{z}_1(x^k, x^{k+1}) = \overline{\nabla}\mathcal{H}_1(x^k, x^{k+1}). \tag{20}$$

We now choose $\overline{\nabla}\mathcal{H}_1 \in C(\mathcal{X}_1 \times \mathcal{X}_1, \mathbb{R}^{n_1})$ to be a discrete gradient of $\mathcal{H}_1$ and $\overline{E}_{11} \in C(\mathcal{X} \times \mathcal{X}, \mathbb{R}^{n_1, n_1})$ to be a consistent discretization of E_{11}. This allows to determine uniquely $\overline{z}_1$ as a function of x^k, x^{k+1}, as long $\overline{E}_{11}$ is ensured to be invertible within our search scope.

This is for example the case if we choose the midpoint approximation $\overline{E}_{11}(x, x') := E_{11}(\frac{x+x'}{2})$, since E_{11} is invertible in the convex space $\mathcal{X}$. More in general, any consistent approximation $\overline{E}_{11}$ will be invertible for sufficiently close x^k, x^{k+1}.

While there is in general no guarantee that a discrete matrix function is pointwise invertible, cf. Example 9 in the appendix, we expect to achieve this condition up to refining the time grid sufficiently. For the sake of simplicity, we introduce the following assumption.

$$\overline{E}_{11} \text{ is pointwise invertible on } \mathcal{X} \times \mathcal{X}. \tag{A1}$$

Furthermore, since $\overline{z} = (\overline{z}_1, \overline{z}_2)$ is not given as part of a gradient pair anymore, we will choose $\overline{z}_2$ as a consistent discretization of the time-continuous function z_2.

In a more detailed fashion, also highlighting the partitioned state, we rewrite (18) and (20) combined as

$$\begin{bmatrix} \overline{E}_{11}(x^k, x^{k+1}) & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} x_1^{k+1} - x_1^k \\ x_2^{k+1} - x_2^k \end{bmatrix} = h\big(\overline{J}(x^k, x^{k+1}) - \overline{R}(x^k, x^{k+1})\big) \begin{bmatrix} z_1^{k,k+1} \\ \overline{z}_2(x^k, x^{k+1}) \end{bmatrix} + h\overline{B}(x^k, x^{k+1}) u^{k,k+1}, \tag{21a}$$

$$y^{k,k+1} = \overline{B}(x^k, x^{k+1})^\top \begin{bmatrix} z_1^{k,k+1} \\ \overline{z}_2(x^k, x^{k+1}) \end{bmatrix}, \tag{21b}$$

$$\overline{E}_{11}(x^k, x^{k+1})^\top z_1^{k,k+1} = \overline{\nabla}\mathcal{H}_1(x_1^k, x_1^{k+1}), \tag{21c}$$

which can be solved for the unknowns $(x_1^{k+1}, x_2^{k+1}, z_1^{k,k+1}, y^{k,k+1})$ in each time step (assuming that a solution exists). Note that $z_1^{k,k+1}$, which here replaces the uniquely determined function $\overline{z}_1$, is considered as an unknown of the time-discrete system, whereas $\overline{z}_2$ is a consistent discretization of z_2. This scheme extends the discrete gradient method from [41,54] to semi-explicit pHDAE systems with the specific structure of the descriptor matrix E.

Let us illustrate the proposed method by an example and show that it preserves the power balance equation in discrete time.

Example 5. *We consider again the running example system from Example 1. Its discretization (21) is given by*

$$\begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} x_1^{k+1} - x_1^k \\ x_2^{k+1} - x_2^k \end{bmatrix} = h \begin{bmatrix} 0 & 1 \\ -1 & -1 \end{bmatrix} \begin{bmatrix} z_1^{k,k+1} \\ \overline{z}_2(x^k, x^{k+1}) \end{bmatrix}.$$

$$z_1^{k,k+1} = \overline{\nabla}\mathcal{H}_1(x_1^k, x_1^{k+1}) = \frac{1}{2}(x_1^k + x_1^{k+1}).$$

where we chose the Gonzalez discrete gradient for the latter relation, which corresponds to (21c). While $z_1^{k,k+1}$ is an unknown of the system, $\overline{z}_2(x^k, x^{k+1})$ still requires a consistent discretization of $z_2(x) = x_2$. Sensible choices like

$$\overline{z}_2(x^k, x^{k+1}) = x_2^k \qquad \text{or} \qquad \overline{z}_2(x^k, x^{k+1}) = x_2^{k+1} \qquad \text{or} \qquad \overline{z}_2(x^k, x^{k+1}) = \frac{1}{2}(x_2^k + x_2^{k+1})$$

complete the set of equations. ◊

Theorem 3. *Scheme (21) yields an energy-consistent approximation of the time-continuous power balance (7) given by*

$$\mathcal{H}(x^{k+1}) - \mathcal{H}(x^k) = -h \begin{bmatrix} z_1^{k,k+1} \\ \overline{z}_2(x^k, x^{k+1}) \end{bmatrix}^\top \overline{R}(x^k, x^{k+1}) \begin{bmatrix} z_1^{k,k+1} \\ \overline{z}_2(x^k, x^{k+1}) \end{bmatrix} + h(y^{k,k+1})^\top u^{k,k+1} \le h(y^{k,k+1})^\top u^{k,k+1}. \tag{22}$$

Proof. Combining the directionality property of the discrete gradient $\overline{\nabla}\mathcal{H}_1$ with (21) one obtains

$$\begin{aligned} \mathcal{H}(x^{k+1}) - \mathcal{H}(x^k) &= \mathcal{H}_1(x_1^{k+1}) - \mathcal{H}_1(x_1^k) = \overline{\nabla}\mathcal{H}_1(x^k, x^{k+1})^\top (x^{k+1} - x^k) \\ &= (z_1^{k,k+1})^\top \overline{E}_{11}(x^k, x^{k+1})(x_1^{k+1} - x_1^k) = \begin{bmatrix} z_1^{k,k+1} \\ \overline{z}_2(x^k, x^{k+1}) \end{bmatrix}^\top \overline{E}(x^k, x^{k+1})(x^{k+1} - x^k) \\ &= h \begin{bmatrix} z_1^{k,k+1} \\ \overline{z}_2(x^k, x^{k+1}) \end{bmatrix}^\top \big(\overline{J}(x^k, x^{k+1}) - \overline{R}(x^k, x^{k+1})\big) \begin{bmatrix} z_1^{k,k+1} \\ \overline{z}_2(x^k, x^{k+1}) \end{bmatrix} + h \begin{bmatrix} z_1^{k,k+1} \\ \overline{z}_2(x^k, x^{k+1}) \end{bmatrix}^\top \overline{B}(x^k, x^{k+1}) u^{k,k+1} \\ &= -h \begin{bmatrix} z_1^{k,k+1} \\ \overline{z}_2(x^k, x^{k+1}) \end{bmatrix}^\top \overline{R}(x^k, x^{k+1}) \begin{bmatrix} z_1^{k,k+1} \\ \overline{z}_2(x^k, x^{k+1}) \end{bmatrix} + h(y^{k,k+1})^\top u^{k,k+1} \le h(y^{k,k+1})^\top u^{k,k+1}, \end{aligned}$$

which is the desired result. □

The semi-explicit discrete gradient method introduced in this section can of course be applied to constrained input-output pH systems as introduced in Example 2, always achieving the desired exact PBE. While there is in general no guarantee that the algebraic constraints are satisfied exactly by the discrete solution, specific implementation choices may allow to meet additional requirements stemming from the particular application problem. This is shown for the example of nonlinear multibody systems in Section 6.2.

4.2.2. Convergence analysis for semi-explicit pHDAEs

To further motivate the proposed method, let us show that, under some additional assumptions on the structure of the system, second order convergence can be achieved. Following a similar idea as for the Dirac-dissipative representation, let us introduce the costate variable $f_1 \in \mathbb{R}^{n_1}$ and the corresponding gradient pair equation $E_{11}(x)^\top f_1 = \nabla\mathcal{H}_1(x_1)$. We can then rewrite (15) as a semi-explicit DAE of the form

$$\dot{x}_1 = F(x_1, u, f_1, x_2), \tag{23a}$$

$$0 = G_1(x_1, u, f_1, x_2), \tag{23b}$$

$$0 = G_2(x_1, f_1, x_2), \tag{23c}$$

$$0 = G_3(x_1, f_1, x_2, y), \tag{23d}$$

where

$$F(x_1, u, f_1, x_2) := E_{11}(x)^{-1}\Big(\big(J_{11}(x_1, x_2) - R_{11}(x_1, x_2)\big) f_1 + \big(J_{12}(x_1, x_2) - R_{12}(x_1, x_2)\big) z_2(x_1, x_2) + B_1(x_1, x_2) u\Big),$$

$$
\begin{aligned}
G_1(x_1,u,f_1,x_2) &:= \big(J_{21}(x_1,x_2)-R_{21}(x_1,x_2)\big)f_1+\big(J_{22}(x_1,x_2)-R_{22}(x_1,x_2)\big)z_2(x_1,x_2)+B_2(x_1,x_2)u,\\
G_2(x_1,f_1,x_2) &:= E_{11}(x_1,x_2)^\top f_1-\nabla\mathcal{H}_1(x_1),\\
G_3(x_1,f_1,x_2,y) &:= y-B_1(x_1,x_2)^\top f_1-B_2(x_1,x_2)^\top z_2(x_1,x_2).
\end{aligned}
$$

Suppose now that this augmented DAE has differentiation index 1, i.e., that G_1 is continuously differentiable and its partial Jacobian $\mathrm{D}_{x_2}G_1$ is pointwise invertible. Then there exists $\mathcal{R}\in C^1(\mathbb{R}^{n_1},\mathbb{R}^{n_2})$ such that every solution of the augmented DAE satisfies $x_2=\mathcal{R}(x_1)$, due to the implicit function theorem. In particular, every solution also satisfies

$$
\dot{x}_1=\widetilde{F}\big(x_1,\nabla\mathcal{H}_1(x_1),u\big) := F\Big(x_1,u,E_{11}\big(x_1,\mathcal{R}(x_1)\big)^{-\top}\nabla\mathcal{H}_1(x_1),\mathcal{R}(x_1)\Big), \tag{24}
$$

which is an ODE in the variable x_1.

Let us now consider the discrete system (21) obtained using a discrete gradient $\overline{\nabla}\mathcal{H}_1$ and the consistent discretizations stemming from midpoint evaluations, which we write as

$$
\begin{aligned}
x_1^{k+1}-x_1^k &= hF\big(x_1^{k+1/2},u^{k,k+1},z_1^{k,k+1},x_2^{k+1/2}\big),\\
0 &= \begin{bmatrix} G_1\big(x_1^{k+1/2},u^{k,k+1},z_1^{k,k+1},x_2^{k+1/2}\big)\\ G_2\big(x_1^{k+1/2},z_1^{k,k+1},x_2^{k+1/2}\big)\\ G_3\big(x_1^{k+1/2},z_1^{k,k+1},x_2^{k+1/2},y^{k,k+1}\big)\end{bmatrix},
\end{aligned}
$$

where $x_1^{k+1/2}=\frac{x_1^k+x_1^{k+1}}{2}$ and $x_2^{k+1/2}=\frac{x_2^k+x_2^{k+1}}{2}$. In particular, the discrete solutions also satisfy $x_2^{k+1/2}=\mathcal{R}(x_1^{k+1/2})$ for all $k\geq 0$, for the same map $\mathcal{R}$, and therefore

$$
x_1^{k+1}-x_1^k=hF\Big(x_1^{k+1/2},u^{k,k+1},E_{11}\big(x_1^{k+1/2},\mathcal{R}(x_1^{k+1/2})\big)^{-\top}\overline{\nabla}\mathcal{H}_1(x_1^k,x_1^{k+1}),\mathcal{R}(x_1^{k+1/2})\Big)=h\widetilde{F}\big(x_1^{k+1/2},\overline{\nabla}\mathcal{H}_1(x^k,x^{k+1}),u^{k,k+1}\big).
$$

In particular, applying a discrete gradient to a semi-explicit pHDAE using midpoint evaluations yields the same discrete sequence for x_1 as if we applied the same discrete gradient and midpoint evaluations to the ODE (24). Thus, the convergence error for the differential state variable x_1 will also be the same; in the case of the Gonzalez discrete gradient, this ensures second convergence order for x_1 [34,50]. Then, proceeding analogously as in the second part of the proof of [46, Theorem 5.16], one can deduce that x_2 also converges with order 2. We summarize this discussion in the following statement.

Proposition 1. *Consider a semi-explicit pHDAE of the form (15), to which the discretization scheme (21) obtained using the Gonzalez discrete gradient and midpoint evaluations is applied. If the augmented DAE (23) has differentiation index 1, then the method has convergence order 2.*

More in general, the convergence of the method both depends on the differentiation index of the DAE and on the choice of discrete gradient and consistent discretizations. In the numerical example that we present in Section 6, which is a semi-explicit pHDAE with differentiation index 2, this same method appears to have convergence order 2 for the differential variables, but only convergence order 1 for the algebraic variable. We postpone further analysis to future works.

4.3. Discrete gradient methods applied to the Dirac-dissipative representation

We will now discuss an alternative structure-preserving discretization method, which requires neither a semi-explicit form nor a discrete gradient pair, based on the Dirac-dissipative representation, that can also be linked to previous works for ODE systems [41,54,55]. Given a DDR-pHDAE (11), the DDR-method governs time-stepping via

$$
\begin{bmatrix}\overline{\nabla}\mathcal{H}(x^k,x^{k+1})\\ 0\\ y^{k,k+1}\end{bmatrix}+\begin{bmatrix}0 & -\overline{E}(x^k,x^{k+1})^\top & 0\\ \overline{E}(x^k,x^{k+1}) & \overline{J}(x^k,x^{k+1})-\overline{R}(x^k,x^{k+1}) & \overline{B}(x^k,x^{k+1})\\ 0 & -\overline{B}(x^k,x^{k+1})^\top & 0\end{bmatrix}\begin{bmatrix}-\frac{1}{h}(x^{k+1}-x^k)\\ f^{k,k+1}\\ u^{k,k+1}\end{bmatrix}=0. \tag{25}
$$

or written out

$$
\begin{aligned}
\overline{E}(x^k,x^{k+1})(x^{k+1}-x^k) &= h\big(\overline{J}(x^k,x^{k+1})-\overline{R}(x^k,x^{k+1})\big)f^{k,k+1}+h\overline{B}(x^k,x^{k+1})u^{k,k+1},\\
y^{k,k+1} &= \overline{B}(x^k,x^{k+1})^\top f^{k,k+1},
\end{aligned} \tag{26a}
$$

as well as

$$
\overline{E}(x^k,x^{k+1})^\top f^{k,k+1}=\overline{\nabla}\mathcal{H}(x^k,x^{k+1}). \tag{26b}
$$

Therein, $f^{k,k+1}$ are discrete-time approximations of the costate quantities. Additionally, we have borrowed definitions from Section 4.1 concerning the discrete state and matrices.

It is in general unclear whether these equations can be solved simultaneously for the unknowns $(x^{k+1},f^{k,k+1},y^{k,k+1})$ in each time step. While for pointwise invertible $\overline{E}$ one can at least recover $f^{k,k+1}$ as a function of x^{k+1}, and rewrite the discrete system only in terms of x^k and x^{k+1}, for an arbitrary, non-invertible $\overline{E}$ further analysis is required. In particular, (26a) could be underdetermined even if the original DAE was regular, thus it might be necessary to introduce additional constraints. We show this with an example.

Example 6. *Consider the regular linear semi-explicit pHDAE from Example 1 with Hamiltonian* $\mathcal{H}(x) = \frac{1}{2}x_1^2$*, where we can identify*

$$E = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}, \quad J = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}, \quad R = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}, \quad B = \begin{bmatrix} 0 \\ 0 \end{bmatrix}, \quad \nabla\mathcal{H}(x) = \begin{bmatrix} x_1 \\ 0 \end{bmatrix}.$$

The system's DDR (11) reads

$$\begin{bmatrix} x_1 \\ 0 \\ 0 \\ 0 \end{bmatrix} + \begin{bmatrix} 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 \\ 0 & 0 & -1 & -1 \end{bmatrix} \begin{bmatrix} -\dot{x}_1 \\ -\dot{x}_2 \\ f_1 \\ f_2 \end{bmatrix} = 0 \tag{27}$$

with $f = z(x)$*. Discretizing (27) with the Gonzalez discrete gradient and discarding the trivial parts of the equation yields*

$$f_1^{k,k+1} = -f_2^{k,k+1} = \frac{x_1^k + x_1^{k+1}}{2}, \qquad x_1^{k+1} = x_1^k - h\frac{x_1^k + x_1^{k+1}}{2}, \tag{28}$$

which is equivalent to reducing (16) to $\dot{x}_1 = -x_1$ *and solving this subsystem with the implicit midpoint method. However,* x_2 *remains undetermined, since the DDR-method discarded the connection between* f_2 *and* x_2*.*

One possible solution is to use our original knowledge from (16) and define $x_2^{k+1} = -x_1^{k+1}$*, conforming with the algebraic condition* $x_1 + x_2 = 0$*. Another possibility would be to observe that* $(f_1, f_2) = z(x) = (x_1, x_2)$ *and define* $x_2^{k+1} = f_2^{k,k+1} = -\frac{1}{2}(x_1^k + x_1^{k+1})$*. Note that both these ideas are based on a priori knowledge of the equation structure.*

A more robust and generalizable approach would be to select a consistent discretization $\overline{z}$ *for* z*. Since imposing* $f^{k,k+1} = \overline{z}(x^k, x^{k+1})$ *might make the system overdetermined, we choose* $(x^{k+1}, f^{k,k+1})$ *instead so that it satisfies (28) while minimizing* $\|f^{k,k+1} - \overline{z}(x^k, x^{k+1})\|$*. We investigate three different choices for* $\overline{z}$*:*

1. *If* $\overline{z}(x^k, x^{k+1}) = x^{k+1}$*, then we obtain again* $x_2^{k+1} = f_2^{k,k+1} = -\frac{1}{2}(x_1^k + x_1^{k+1})$ *for all* $k \geq 0$*.*
2. *If* $\overline{z}(x^k, x^{k+1}) = x^k$*, then* x_2^{k+1} *does not appear in* $\|f^{k,k+1} - \overline{z}(x^k, x^{k+1})\|$*. However, since* x_2^k *appears, we obtain* $x_2^k = f_2^{k,k+1} = -\frac{1}{2}(x_1^k + x_1^{k+1})$ *for* $1 \leq k \leq N-1$ *(and additionally* $k = 0$ *if we allow to redefine* x_2^0*). Note that in this case* x_2^k *is to be computed after* x_1^{k+1}*, since the iteration defining* x_1^{k+1} *is independent of* x_2^k*. However, the final state* x_2^N *remains undefined. In fact, this definition suggests that* x_2^k *actually approximates* $x_2(t^k + \frac{h}{2})$ *instead of* $x_2(t^k)$*, thus justifying redefining* x_2^0 *and stopping at* x_2^{N-1}*.*
3. *If* $\overline{z}(x^k, x^{k+1}) = \frac{1}{2}(x^k + x^{k+1})$*, then we obtain* $x_2^{k+1} = -x_1^k - x_1^{k+1} - x_2^k$*. If the initial condition* x^0 *satisfies* $x_2^0 = -x_1^0$*, then* $x_2^{k+1} = -x_1^{k+1}$ *holds inductively for all* $k \geq 0$*.*

◊

Let us emphasize that the choice of additional constraints does not affect the power balance equation, which remains satisfied by (26a) and (26b). We also refer to [48, Ex. 7.4.1] where analogous deductions are made in the context of Galerkin projection schemes.

In the case where E is singular, the question arises whether there exists a discrete gradient of $\mathcal{H}$, which ensures that $\overline{\nabla}\mathcal{H}(x, x')$ is in the column space of $\overline{E}(x, x')^\top$, i.e.,

$$\overline{\nabla}\mathcal{H}(x, x') \in \operatorname{colsp}(\overline{E}(x, x')^\top), \tag{29}$$

for all $x, x' \in \mathbb{R}^n$. This ensures that (26b) can be solved for $f^{k,k+1}$, although not necessarily uniquely. Further details and a corresponding counterexample can be found in Appendix C. Let us now focus on the connections between the discrete methods introduced in this section.

4.4. Relations between the presented methods in the semi-explicit setting

In this subsection, it is demonstrated that the semi-explicit discrete gradient method from Section 4.2 is equivalent to special cases of the discrete gradient pair approach from Section 4.1 and of the DDR approach from Section 4.3.

First, we observe that scheme (21) for semi-explicit pHDAEs of the form (15) corresponds to an underlying discrete gradient pair, see Definition 7. This is stated in the following theorem and corollary.

Theorem 4. *Let* (E, z) *be a semi-explicit gradient pair for* $\mathcal{H}$ *in the sense of Definition 9 and let* $z = (z_1, z_2)$ *be split correspondingly. Furthermore, let* $\overline{E}_{11} \in C(\mathcal{X} \times \mathcal{X}, \mathbb{R}^{n_1, n_1})$ *and* $\overline{z}_2 \in C(\mathcal{X} \times \mathcal{X}, \mathbb{R}^{n_2})$ *be consistent discretizations of* E_{11} *and* z_2*, respectively, suppose that* $\overline{E}_{11}$ *satisfies the Assumption A1, and let* $\overline{\nabla}\mathcal{H}_1$ *be a discrete gradient for* $\mathcal{H}_1 \in C^1(\mathcal{X}_1, \mathbb{R})$*. Then* $(\overline{E}, \overline{z})$ *with*

$$\overline{E} = \begin{bmatrix} \overline{E}_{11} & 0 \\ 0 & 0 \end{bmatrix}, \qquad \overline{z} = \begin{bmatrix} \overline{E}_{11}^{-\top}(\overline{\nabla}\mathcal{H}_1 \circ \pi_1) \\ \overline{z}_2 \end{bmatrix} \tag{30}$$

is a discrete gradient pair for $(\mathcal{H}, E, z)$*.*

Proof. Property (i) in Definition 7 is part of our hypotheses. We proceed to show that the properties (i) and (iii) are also valid. In fact, it holds that

$$\overline{z}(x, x) = \begin{bmatrix} \overline{E}_{11}(x, x)^{-\top}\overline{\nabla}\mathcal{H}_1(x_1, x_1) \\ \overline{z}_2(x, x) \end{bmatrix} = \begin{bmatrix} E_{11}(x)^{-\top}\nabla\mathcal{H}_1(x_1) \\ z_2(x) \end{bmatrix} = \begin{bmatrix} z_1(x) \\ z_2(x) \end{bmatrix} = z(x)$$

and

$$\overline{z}(x,x')^\top \overline{E}(x,x')(x'-x) = \overline{z}_1(x,x')^\top \overline{E}_{11}(x,x')(x_1'-x_1) = \overline{\nabla}\mathcal{H}_1(x_1,x_1')^\top(x_1'-x_1) = \mathcal{H}_1(x_1') - \mathcal{H}_1(x_1) = \mathcal{H}(x') - \mathcal{H}(x),$$

for all $x = (x_1, x_2), x' = (x_1', x_2') \in \mathcal{X}$. □

Corollary 1. *Consider a semi-explicit pHDAE of the form (15), let $\overline{\nabla}\mathcal{H}_1$, $\overline{E}_{11}$, $\overline{z}_2$, $\overline{E}$, and $\overline{z}$ be defined as in Theorem 4, and let us fix consistent discretizations for J, R, and B. Then the semi-explicit discrete gradient method applied with $\overline{\nabla}\mathcal{H}_1$ governed by (21) and the discrete gradient pair method (18) applied with $(\overline{E}, \overline{z})$ yield the same solution.*

Proof. The claim immediately follows by construction, since

$$\overline{z}(x^k, x^{k+1}) = \begin{bmatrix} \overline{E}_{11}(x^k, x^{k+1})^{-\top} \overline{\nabla}\mathcal{H}_1(x_1^k, x_1^{k+1}) \\ \overline{z}_2(x^k, x^{k+1}) \end{bmatrix} = \begin{bmatrix} z_1^{k,k+1} \\ \overline{z}_2(x^k, x^{k+1}) \end{bmatrix}.$$

holds true. □

We will now see that the discrete gradient method applied to semi-explicit pHDAEs can be equivalently reinterpreted as a specific DDR-method.

Theorem 5. *Under the same assumptions as in Theorem 4, the semi-explicit discrete gradient method (21) yields the same one-step method as the DDR-method (25) with the completing constraint $f_2^{k,k+1} = \overline{z}_2(x^k, x^{k+1})$.*

Proof. Due to the structure of the system, the DDR-method applied to (15) yields the one-step method

$$\begin{bmatrix} \overline{\nabla}\mathcal{H}_1(x_1^k, x_1^{k+1}) \\ 0 \\ 0 \\ 0 \\ y^{k,k+1} \end{bmatrix} + \begin{bmatrix} 0 & 0 & -\overline{E}_{11}^\top & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ \overline{E}_{11} & 0 & \overline{J}_{11} - \overline{R}_{11} & \overline{J}_{12} - \overline{R}_{12} & \overline{B}_1 \\ 0 & 0 & \overline{J}_{21} - \overline{R}_{21} & \overline{J}_{22} - \overline{R}_{22} & \overline{B}_2 \\ 0 & 0 & -\overline{B}_1^\top & -\overline{B}_2^\top & 0 \end{bmatrix} \begin{bmatrix} -\frac{1}{h}(x_1^{k+1} - x_1^k) \\ -\frac{1}{h}(x_2^{k+1} - x_2^k) \\ f_1^{k,k+1} \\ f_2^{k,k+1} \\ u^{k,k+1} \end{bmatrix} = 0, \tag{31}$$

where the arguments (x^k, x^{k+1}) have been omitted for simplicity. In particular, the first equation of (31) yields

$$\overline{E}_{11}(x^k, x^{k+1})^\top f_1^{k,k+1} = \overline{\nabla}\mathcal{H}_1(x^k, x^{k+1}),$$

thus it is equivalent to the Eq. (21c), up to replacing $f_1^{k,k+1}$ with $z_1^{k,k+1}$. Then, since the second equation of (31) is trivial, we can remove it. Finally, by replacing $f_2^{k,k+1}$ with $\overline{z}_2(x^k, x^{k+1})$ due to the stated constraint, we get exactly (21). □

In summary, Corollary 1 and Theorem 5 demonstrate that the concrete time discretization scheme for semi-explicit pHDAEs provided in Section 4.2 may be regarded as a special case of the discrete gradient pair approach from Section 4.1 and of the DDR method discussed in Section 4.3.

5. Relating general pHDAEs to semi-explicit pHDAEs using system transformations

The goal of this section is to investigate when it is possible to reformulate general pHDAEs as semi-explicit pHDAEs, by employing system transformations. To this end, we first analyze in Section 5.1 the behavior of the proposed schemes under system transformations. In Section 5.2 we then shed more light on the existence of semi-explicit representations of pHDAEs.

5.1. Behavior of gradient pairs under system transformations

We are now interested in studying how the methods introduced in Section 4 behave under structure-preserving system transformations. Our motivation is to construct discrete gradient pairs for general gradient pairs. One possibility would be to transform the general system into an equivalent semi-explicit one, apply Theorem 4, and then apply the inverse transformation. However, this requires to understand more accurately the behavior of discrete gradient pairs under invertible transformations.

We start by formalizing what is meant by *structure-preserving system transformation*. In fact, given a pHDAE of the form (6), a diffeomorphism $\varphi \in C^1(\widetilde{\mathcal{X}}, \mathcal{X})$, and a pointwise invertible matrix function $U \in C(\widetilde{\mathcal{X}}, \mathbb{R}^{n,n})$, we call the pair (φ, U) an *(invertible) system transformation*. This is motivated by the fact that we can obtain an equivalent system by applying the change of variables $x = \varphi(\tilde{x})$ and left-multiplication of the first equation of (6) by $U(\tilde{x})^\top$. In fact, this transformation yields the new system

$$\begin{aligned} \widetilde{E}(\tilde{x})\dot{\tilde{x}} &= \big(\widetilde{J}(\tilde{x}) - \widetilde{R}(\tilde{x})\big)\tilde{z}(\tilde{x}) + \widetilde{B}(\tilde{x})u, \\ y &= \widetilde{B}(\tilde{x})\tilde{z}(\tilde{x}), \end{aligned} \tag{32}$$

where $\widetilde{E} = U^\top(E\circ\varphi)\mathrm{D}\varphi$, $\widetilde{J} = U^\top(J\circ\varphi)U$, $\widetilde{R} = U^\top(R\circ\varphi)U$, $\tilde{z} = U^{-1}(z\circ\varphi)$, and $\widetilde{B} = U^\top(B\circ\varphi)$. Remarkably, $(\widetilde{E}, \tilde{z})$ is a gradient pair for $\widetilde{\mathcal{H}} = \mathcal{H}\circ\varphi$, and the system (32) is a pHDAE with Hamiltonian $\widetilde{\mathcal{H}}$, see [4, Thm. 1] for more details. Furthermore, we observe that, if (φ, U) is an invertible system transformation, then (φ^{-1}, U^{-1}) is also an invertible system transformation. In particular, applying (φ^{-1}, U^{-1}) to the transformed system (32) we obtain again the original system (6). This motivates calling (φ^{-1}, U^{-1}) the *inverse* of the system transformation (φ, U). We will discuss the composition and inversion of system transformations further in Appendix D.1.

Remark 8. Note that, if the original system is an ODE and we want to ensure that (32) is also an ODE, we need to choose $U = (\mathrm{D}\varphi)^{-\top}$, while in the more general case of DAEs this requirement is unnecessary and the choice of U is free.

Since $(\widetilde{E}, \tilde{z})$ only depends on the gradient pair (E, z) and on the system transformation (φ, U), we deduce that system transformations can be applied directly to (discrete) gradient pairs. This leads to the following result.

Theorem 6. *Let (E, z) be a gradient pair for $\mathcal{H}$, let (φ, U) be a system transformation. Then*

$$(\widetilde{E}, \tilde{z}) = \big(U^\top (E \circ \varphi) \mathrm{D}\varphi, U^{-1}(z \circ \varphi)\big) \tag{33}$$

is a gradient pair for $\widetilde{\mathcal{H}} = \mathcal{H} \circ \varphi$, which we call the gradient pair transformed from (E, z) via (φ, U). Furthermore, let $(\overline{E}, \overline{z})$ be a discrete gradient pair for $(\mathcal{H}, E, z)$, let $\overline{\mathrm{D}}\varphi$ be a discrete Jacobian for φ, and let $\overline{U} \in C(\widetilde{\mathcal{X}} \times \widetilde{\mathcal{X}}, \mathbb{R}^{n,n})$ be a pointwise invertible consistent discretization for U. Then $(\widehat{E}, \hat{z})$ with

$$\widehat{E} = \overline{U}^\top (\overline{E} \circ \varphi) \overline{\mathrm{D}}\varphi, \qquad \hat{z} = \overline{U}^{-1} (\overline{z} \circ \varphi) \tag{34}$$

is a discrete gradient pair for $(\widetilde{\mathcal{H}}, \widetilde{E}, \tilde{z})$.

Proof. Analogously to what was proven in [4] in the case of pHDAEs, we have

$$\widetilde{E}^\top \tilde{z} = (\mathrm{D}\varphi)^\top (E \circ \varphi)^\top U U^{-1} (z \circ \varphi) = (\mathrm{D}\varphi)^\top (E^\top z \circ \varphi) = (\mathrm{D}\varphi)^\top (\nabla \mathcal{H} \circ \varphi) = \nabla \widetilde{\mathcal{H}},$$

thus $(\widetilde{E}, \tilde{z})$ is a gradient pair for $\widetilde{\mathcal{H}}$. Concerning the second statement, for every $\tilde{x}, \tilde{x}' \in \widetilde{\mathcal{X}}$ we have

$$\begin{aligned}
\hat{z}(\tilde{x}, \tilde{x}')^\top \widehat{E}(\tilde{x}, \tilde{x}')(\tilde{x}' - \tilde{x}) &= \overline{z}\big(\varphi(\tilde{x}), \varphi(\tilde{x}')\big)^\top \overline{E}\big(\varphi(\tilde{x}), \varphi(\tilde{x}')\big) \overline{\mathrm{D}}\varphi(\tilde{x}, \tilde{x}')(\tilde{x}' - \tilde{x}) \\
&= \overline{z}\big(\varphi(\tilde{x}), \varphi(\tilde{x}')\big)^\top \overline{E}\big(\varphi(\tilde{x}), \varphi(\tilde{x}')\big)\big(\varphi(\tilde{x}') - \varphi(\tilde{x})\big) \\
&= \mathcal{H}\big(\varphi(\tilde{x}')\big) - \mathcal{H}\big(\varphi(\tilde{x})\big) = \widetilde{\mathcal{H}}(\tilde{x}') - \widetilde{\mathcal{H}}(\tilde{x}).
\end{aligned}$$

It is furthermore clear that $\widehat{E}(\tilde{x}, \tilde{x}) = \widetilde{E}(\tilde{x})$ and $\hat{z}(\tilde{x}, \tilde{x}) = \tilde{z}(\tilde{x})$ hold for all $\tilde{x} \in \widetilde{\mathcal{X}}$. □

Remark 9. Note that, for $(E, z) = (I_n, \nabla \mathcal{H})$, $(\overline{E}, \overline{z}) = (I_n, \overline{\nabla} \mathcal{H})$ with $\overline{\nabla} \mathcal{H}$ being a discrete gradient of $\mathcal{H}$, and $U = \overline{U} = I_n$, Theorem 6 yields that $(\overline{\mathrm{D}}\varphi, \overline{\nabla} \mathcal{H} \circ \varphi)$ is a discrete gradient pair for $(\widetilde{\mathcal{H}}, I_n, \nabla \widetilde{\mathcal{H}})$, and therefore

$$\overline{\nabla} \widetilde{\mathcal{H}} = (\overline{\mathrm{D}}\varphi)^\top (\overline{\nabla} \mathcal{H} \circ \varphi) \tag{35}$$

is a discrete gradient for $\widetilde{\mathcal{H}}$. This is the well-known chain rule for discrete derivatives, see [50, Prop. 3.4].

Remark 10. One might wonder whether applying the same numerical methods under different coordinate systems would yield different results. To answer this question, we first need to make it more precise. One possibility would be to consider a discrete gradient pair on the original system and the one obtained via a system transformation as in Theorem 6; in this case, the discrete solutions are the same up to applying the same coordinate change. This could still bring some numerical advantages, e.g. by applying preconditioning. Another option would be to use the same discrete gradient construction, e.g. the Gonzalez midpoint discrete gradient, for both the original system and the transformed one; in this other case, the obtained discrete solutions can be in fact different. The interested reader can find more details in Section D.

We also deduce from Theorem 6 the following result, which fulfills our motivation mentioned at the beginning of this subsection.

Corollary 2. *Let (E, z) be a gradient pair for $\mathcal{H}$, and suppose that there exists an invertible system transformation (φ, U) that maps it into a semi-explicit gradient pair. Then $(\mathcal{H}, E, z)$ admits a discrete gradient pair.*

Proof. In this proof we employ the fact that discrete gradients and discrete Jacobians exist regardless of the structure of the state space, as discussed in Remark 5. Let $\widetilde{\mathcal{H}} = \mathcal{H} \circ \varphi \in C^1(\widetilde{\mathcal{X}}, \mathbb{R})$ be the transformed Hamiltonian, $\widetilde{\mathcal{H}}_1$ be defined according to Lemma 2, and $\overline{\nabla} \widetilde{\mathcal{H}}_1$ be any discrete gradient for $\widetilde{\mathcal{H}}_1$. We apply Theorem 4 to construct a discrete gradient pair $(\widehat{E}, \hat{z})$ for $(\widetilde{\mathcal{H}}, \widetilde{E}, \tilde{z})$. Then, we construct a discrete gradient pair $(\overline{E}, \overline{z})$ for $(\mathcal{H}, E, z)$ by applying Theorem 6 to the discrete gradient pair $(\widehat{E}, \hat{z})$ via the inverse system transformation (φ^{-1}, U^{-1}). For that, any consistent discretization of U^{-1} (e.g. the midpoint discretization) and any discrete Jacobian for φ^{-1} can be employed. □

Theorem 6 and Corollary 2 provide us with a basis for determining a discrete gradient pair for any gradient pair which may be transformed to a semi-explicit one. It remains to find conditions under which a gradient pair allows for a semi-explicit representation, which is the content of the next subsection.

5.2. On the existence of a semi-explicit representation

Corollary 2 requires the existence of an invertible system transformation (φ, U) which brings the system to semi-explicit form. In the special case where E is constant, such a transformation can be obtained based on a singular value decomposition (SVD) of E, as detailed in the following proposition.

Proposition 2. *Let (E, z) be a gradient pair for $\mathcal{H} \in C^1(\mathcal{X}, \mathbb{R})$, assume that $E \in \mathbb{R}^{n,n}$ is constant, and let $E = U \Sigma V^\top$ be an SVD of E. Furthermore, let $U = [U_1, U_2]$, $V = [V_1, V_2]$, and $\Sigma = \mathrm{diag}(\Sigma_1, 0)$ with $U_1, W_1 \in \mathbb{R}^{n,r}$, $\Sigma_1 \in \mathbb{R}^{r,r}$, and $r = \mathrm{rank}(E)$. Then the following statements hold:*

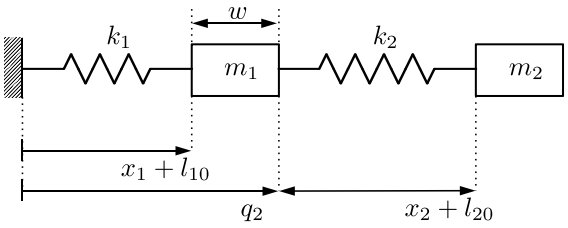

Fig. 1. Mass-spring system.

1. (φ, U) *with* $\varphi(x) = Vx$ *is an invertible system transformation that maps* (E, z) *into a semi-explicit gradient pair.*
2. *The function* $\widetilde{\mathcal{H}}_1 : \widetilde{\mathcal{X}}_1 \to \mathbb{R}$ *associated with* $\widetilde{\mathcal{H}} = \mathcal{H} \circ \varphi$ *via Lemma 2 satisfies* $\widetilde{\mathcal{H}}_1(\tilde{x}_1) = \mathcal{H}(V_1 \tilde{x}_1)$.
3. *If* $\overline{\nabla}\widetilde{\mathcal{H}}_1$ *is a discrete gradient for* $\widetilde{\mathcal{H}}_1$ *and* $\hat{z}_2$ *is a consistent approximation for* $U_2^\top(z \circ \varphi)$, *then* $(E, \overline{z}_2)$ *with* $\overline{z}_2 = U_1 \Sigma_1^{-1} \overline{\nabla}\widetilde{\mathcal{H}}_1 + U_2 \hat{z}$ *is a discrete gradient pair for* $(\mathcal{H}, E, z)$.

Proof. Straightforward calculations yield that the result follows from Theorem 4 and Theorem 6. □

Proposition 2 can find its use in several application instances. We demonstrate this in the following example.

Example 7 (Multibody system with singular mass matrix)**.** *Using Proposition 2, one can design a discrete gradient pair with corresponding integration method for a multibody system example fitting into the aforementioned Example 3. The specific problem as depicted in Fig. 1 (see [56, Sec. 5, Ex. 3] and [57]) has two degrees of freedom but is modeled by means of three redundant coordinates* $q = (x_1, q_2, x_2)$. *This leads to a singular mass matrix with masses* m_1 *and* m_2 *given by*

$$M = \begin{bmatrix} m_1 & 0 & 0 \\ 0 & m_2 & m_2 \\ 0 & m_2 & m_2 \end{bmatrix}, \tag{36}$$

which is contained in the pHDAE's descriptor matrix $E = \operatorname{diag}(I_{3,3}, M, 0)$. *Performing the steps as shown above yields the desired discrete gradient pair. Further details are contained in Appendix E.* ◊

In the general case of a state-dependent E, one might wonder whether it is possible to transform any pHDAE (6) into an equivalent one in the semi-explicit form (15). We start by deducing the following necessary condition:

Theorem 7. *Let* (E, z) *be a gradient pair for* $\mathcal{H}$, *and suppose that there exists an invertible system transformation* (φ, U) *that maps it into a semi-explicit gradient pair. Then* E *has constant rank.*

Proof. Since φ is a diffeomorphism, $\mathrm{D}\varphi$ is pointwise invertible, thus we deduce that

$$\operatorname{rank}\big(E(x)\big) = \operatorname{rank}\big(U(\tilde{x})^\top E(x) \mathrm{D}\varphi(\tilde{x})\big) = \operatorname{rank}\big(\widetilde{E}(\tilde{x})\big) = n_1$$

for all $x \in \mathcal{X}$, where $\tilde{x} = \varphi^{-1}(x)$. □

We investigate now whether this condition is also sufficient. A simple extension of [25, Thm. 3.9] (see Theorem 11 in the appendix) shows that E being continuous and constant rank is sufficient to find pointwise unitary $U, V \in C(\mathcal{X}, \mathbb{R}^{n,n})$ satisfying

$$U^\top E V = \begin{bmatrix} E_{11} & 0 \\ 0 & 0 \end{bmatrix}$$

for some pointwise invertible matrix function E_{11}, at least locally. Unfortunately, since such V is not necessarily the Jacobian of a diffeomorphism φ, we cannot exploit this result directly. However, we are still able to provide a crucial local canonical form for a gradient pair (E, z), as long as E is analytic and has constant rank.

Theorem 8. *Let* (E, z) *be a gradient pair for* $\mathcal{H} \in C^1(\mathcal{X}, \mathbb{R})$, *and suppose that* $E \in C(\mathcal{X}, \mathbb{R}^{n,n})$ *is analytic and has constant rank. Then* (E, z) *is locally equivalent to a gradient pair* $(\widetilde{E}, \tilde{z})$ *for* $\widetilde{\mathcal{H}} \in C^1(\widetilde{\mathcal{X}}, \mathbb{R})$, *such that* $\widetilde{\mathcal{H}}$ *admits an associated function* $\widetilde{\mathcal{H}}_1 \in C^1(\pi_1(\widetilde{\mathcal{X}}), \mathbb{R})$ *in the sense of Lemma 1, and*

$$\widetilde{E} = \begin{bmatrix} I_p & 0 & 0 \\ 0 & 0 & 0 \\ 0 & E_{32} & I_{r-p} \end{bmatrix}, \qquad \tilde{z} = \begin{bmatrix} \nabla \widetilde{\mathcal{H}}_1 \circ \pi_1 \\ z_2 \\ 0 \end{bmatrix}, \tag{37}$$

where $\pi_1 : \mathbb{R}^n \to \mathbb{R}^p$ *denotes the projection onto the first* p *coordinates.*

Proof. See Appendix F. □

The canonical form in Theorem 8 allows us then to find a canonical form for pHDAEs, which allows to split them into a structured semi-explicit DAE and an additional unstructured DAE.

Corollary 3. *Consider a pHDAE of the form (6), and suppose that the descriptor matrix E is analytic and has constant rank. Then the system is locally equivalent to the combination of a parametrized semi-explicit pHDAE of the form*

$$\begin{aligned}\begin{bmatrix} I_{n_1} & 0 \\ 0 & 0 \end{bmatrix}\begin{bmatrix} \dot{x}_1 \\ \dot{x}_2 \end{bmatrix} &= \big(J(x,\theta) - R(x,\theta)\big)\begin{bmatrix} \nabla \mathcal{H}_1(x_1) \\ z_2(x,\theta) \end{bmatrix} + \begin{bmatrix} B_1(x,\theta) \\ B_2(x,\theta) \end{bmatrix} u, \\ y &= \begin{bmatrix} B_1(x,\theta)^\top & B_2(x,\theta)^\top \end{bmatrix}\begin{bmatrix} \nabla \mathcal{H}_1(x_1) \\ z_2(x,\theta) \end{bmatrix}\end{aligned} \tag{38a}$$

with Hamiltonian $\mathcal{H}_1$ depending only on x_1, and an unstructured DAE for the parameter θ given by

$$\dot{\theta} + E_{32}(x,\theta)\dot{x}_2 = A_{31}(x,\theta)\nabla \mathcal{H}_1(x_1) + A_{32}(x,\theta) z_2(x,\theta) + B_3(x,\theta) u, \tag{38b}$$

with state $x = (x_1, x_2)$, up to invertible system transformations.

Proof. Because of Theorem 8 we can assume, up to restricting the state space to an appropriate open neighborhood and applying a certain invertible system transformation, that $\mathcal{H}$ admits an associated function $\mathcal{H}_1 \in C^1(\pi_1(\mathcal{X}), \mathbb{R})$ in the sense of Lemma 1 and

$$E = \begin{bmatrix} I_p & 0 & 0 \\ 0 & 0 & 0 \\ 0 & E_{32} & I_{r-p} \end{bmatrix}, \qquad z = \begin{bmatrix} \nabla \mathcal{H}_1 \circ \pi_1 \\ z_2 \\ 0 \end{bmatrix}.$$

The pHDAE then can be written as

$$\begin{aligned}\begin{bmatrix} \dot{x}_1 \\ 0 \\ E_{32}(x)\dot{x}_2 + \dot{x}_3 \end{bmatrix} &= \begin{bmatrix} J_{11}(x) - R_{11}(x) & J_{12}(x) - R_{12}(x) & J_{13}(x) - R_{13}(x) \\ J_{21}(x) - R_{21}(x) & J_{22}(x) - R_{22}(x) & J_{23}(x) - R_{23}(x) \\ J_{31}(x) - R_{31}(x) & J_{32}(x) - R_{32}(x) & J_{33}(x) - R_{33}(x) \end{bmatrix}\begin{bmatrix} \nabla \mathcal{H}_1(x_1) \\ z_2(x) \\ 0 \end{bmatrix} + \begin{bmatrix} B_1(x) \\ B_2(x) \\ B_3(x) \end{bmatrix} u, \\ y &= \begin{bmatrix} B_1(x)^\top & B_2(x)^\top & B_3(x)^\top \end{bmatrix}\begin{bmatrix} \nabla \mathcal{H}_1(x_1) \\ z_2(x) \\ 0 \end{bmatrix}.\end{aligned}$$

Note that, since $z_3 = 0$, the third block column of $J - R$ can be arbitrarily modified without affecting the solutions of the system. Therefore, $A_{31} = J_{31} - R_{31}$ and $A_{32} = J_{32} - R_{32}$ are actually unstructured, and the system can be equivalently interpreted as (38), up to relabeling $x := (x_1, x_2)$ and $\theta := x_3$.

We finally note that, up to restricting $\mathcal{X}$ further, we can assume that it is an open convex of the form $\mathcal{X}_1 \times \mathcal{X}_2 \times \mathcal{X}_3$ with $\mathcal{X}_1 \subseteq \mathbb{R}^{n_1}$, $\mathcal{X}_2 \subseteq \mathbb{R}^{n_2}$, and $\mathcal{X}_3 \subseteq \mathbb{R}^{n_3}$. □

Remark 11. In the proof of Corollary 3 we reinterpreted part of the state as a time-varying parameter. While this choice might seem arbitrary, it allows us to highlight and exploit the underlying semi-explicit pHDAE structure. In fact, while the full system (38) is not a semi-explicit pHDAE, the fact that the subsystem (38a) is a parametrized semi-explicit pHDAE allows to apply a structure-preserving time-discretization scheme by approximating $\nabla \mathcal{H}_1(x_1)$ by a corresponding discrete gradient. Additionally, one is free to choose an approximation of the unstructured part (38b), which however does not spoil the discrete time power balance equation. It should be emphasized that the derivation of the system (38) requires a suitable system transformation, which may be difficult to obtain in practice.

While we leave further in-depth analyses for future research, we subsequently highlight the applicability of our proposed approach to a mechanical problem class.

6. Application to multibody system dynamics

Let us consider the example of nonlinear and constrained multibody systems (see Example 3). We discuss the modeling as a semi-explicit pHDAE in Section 6.1, showcase the application of a discrete gradient method in Section 6.2 and present a numerical experiment in Section 6.3.

6.1. Modeling multibody systems as semi-explicit pHDAEs

The class of nonlinear multibody systems with redundant coordinates $q \in C(\mathbb{T}, \mathcal{Q})$ fits well into the semi-explicit framework (15). More details on the derivations of the following equations may be found for example in the textbook [58, Ch. 1]. The configuration space $\mathcal{Q}$ is typically a differential manifold, but it can also be regarded as an open subset of $\mathbb{R}^d$ up to switching to local coordinates, where the dimension d of $\mathcal{Q}$ determines the number of coordinates. Correspondingly, admissible velocities $v = \dot{q}$ are elements of the tangent space $T_q\mathcal{Q}$ defined through the presence of holonomic constraints $g \in C^1(\mathcal{Q}, \mathbb{R}^m)$, and can be reinterpreted in local coordinates as vectors in $\mathbb{R}^d$. Since

$$g\big(q(t)\big) = 0 \tag{39}$$

gives rise to the kinematic (i.e. velocity level) constraints (sometimes in the MBS community referred to as *hidden constraints*), admissible velocities need to satisfy

$$\mathrm{D}g\big(q(t)\big)v(t) = 0. \tag{40}$$

These constraints are enforced by means of Lagrange multipliers $\lambda \in C(\mathbb{T}, \mathbb{R}^m)$, which now represent the purely algebraic states, i.e., $x_2 = \lambda$. Correspondingly, with $x_1 = (q, v)$ one defines the non-quadratic Hamiltonian as

$$\mathcal{H}(x) = \mathcal{H}_1(x_1) = \frac{1}{2} v^\top M v + V(q), \tag{41}$$

where the first term represents the kinetic energy with the symmetric and positive-definite mass matrix $M \in \mathbb{R}^{d,d}$ and $V \in C(\mathcal{Q}, \mathbb{R})$ denotes an arbitrary potential energy. The emanating potential forces are derived by taking the partial derivative with respect to the coordinates, i.e., $F_\mathrm{p} = \nabla V(q)$. Additionally, we consider velocity-dependent viscous dissipation governed by the Rayleigh dissipation function $G(q, v) = \frac{1}{2} v^\top R_\mathrm{R}(q) v$, where $R_\mathrm{R}(q) \in C(\mathcal{Q}, \mathbb{R}^{d,d})$ is a symmetric and positive semi-definit dissipation matrix. The non-potential forces appearing in the balance of linear momentum are obtained through differentiation, i.e., $F_\mathrm{np}(q, v) = -\nabla_v G(q, v) = -R_\mathrm{R}(q) v$. This eventually yields the equations of motion as index-2 DAEs given by

$$\dot{q} = v, \tag{42a}$$

$$M \dot{v} = -\nabla V(q) - R_\mathrm{R}(q) v - \mathrm{D}g(q)^\top \lambda + u, \tag{42b}$$

$$0 = \mathrm{D}g(q) v, \tag{42c}$$

where u represents external input loads. These equations can be brought into the semi-explicit pHDAE representation (15) by rewriting them as

$$\begin{bmatrix} I & 0 & 0 \\ 0 & M & 0 \\ 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} \dot{q} \\ \dot{v} \\ \dot{\lambda} \end{bmatrix} = \left(\begin{bmatrix} 0 & I & 0 \\ -I & -R_\mathrm{R}(q) & -\mathrm{D}g(q)^\top \\ 0 & \mathrm{D}g(q) & 0 \end{bmatrix} \right) \begin{bmatrix} \nabla V(q) \\ v \\ \lambda \end{bmatrix} + \begin{bmatrix} 0 \\ I \\ 0 \end{bmatrix} u, \tag{43a}$$

$$y = \begin{bmatrix} 0 & I & 0 \end{bmatrix} \begin{bmatrix} \nabla V(q) \\ v \\ \lambda \end{bmatrix}. \tag{43b}$$

The verification that $E^\top z(x) = \nabla \mathcal{H}(x)$ holds true is straightforward. Moreover, the system output collocated with the input forces coincides with the velocity, i.e., $y = v$.

Note that the pH formulation of the multibody system dynamics is characterized by explicitely accounting for the hidden velocity constraints (40) instead of the constraints on position level (39). Care has to be taken when it comes to the numerical discretization in order to avoid the violation of the constraints on position level during simulations (*drift-off*).

6.2. Structure-preserving time integration of multibody systems

For the time discretization of (43a), we propose the application of the semi-explicit discrete gradient method (21) with additional specifications, leading to the discrete time mapping

$$\begin{bmatrix} I & 0 & 0 \\ 0 & M & 0 \\ 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} q^{k+1} - q^k \\ v^{k+1} - v^k \\ \lambda^{k+1} - \lambda^k \end{bmatrix} = h \begin{bmatrix} 0 & I & 0 \\ -I & -R_\mathrm{R}(q^{k+1/2}) & -\overline{\mathrm{D}} g(q^k, q^{k+1})^\top \\ 0 & \overline{\mathrm{D}} g(q^k, q^{k+1}) & 0 \end{bmatrix} \begin{bmatrix} z_{1,q}^{k,k+1} \\ z_{1,v}^{k,k+1} \\ \lambda^{k,k+1} \end{bmatrix} + h \begin{bmatrix} 0 \\ I \\ 0 \end{bmatrix} u^{k,k+1}, \tag{44a}$$

$$\begin{bmatrix} z_{1,q}^{k,k+1} \\ z_{1,v}^{k,k+1} \end{bmatrix} = \begin{bmatrix} I & 0 \\ 0 & M \end{bmatrix}^{-\top} \overline{\nabla} \mathcal{H}_1(x_1^k, x_1^{k+1}), \tag{44b}$$

$$y^{k,k+1} = z_{1,v}^{k,k+1}, \tag{44c}$$

where $q^{k+1/2} = \frac{1}{2}(q^k + q^{k+1})$ is the midpoint, and $\overline{\mathrm{D}} g$ is a discrete Jacobian for g. Here we discretized the Rayleigh dissipation term using the implicit midpoint rule, but we emphasize that any other consistent approximation which preserves the positive semi-definiteness of R_R would be suitable as well. For the multipliers we make the choice $\lambda^{k,k+1} := \lambda^{k+1}$ such that no appropriate initialization for λ^0 is required.

As already mentioned, one might wonder about the drift-off effect. Since we approximate $\mathrm{D}g$ with a discrete Jacobian, combining the first and third row of (44a) yields

$$g(q^{k+1}) - g(q^k) = \overline{\mathrm{D}} g(q^k, q^{k+1})(q^{k+1} - q^k) = h \overline{\mathrm{D}} g(q^k, q^{k+1}) z_{1,v}^{k,k+1} = 0, \tag{45}$$

and therefore the drift-off vanishes, as long as the initial condition satisfies $g(q^0) = 0$. Thus, this scheme not only yields energy consistency in terms of Theorem 3, but also prevents the drift-off effect.

Remark 12. The choice of using a discrete Jacobian to approximate $\mathrm{D}g$ in general only guarantees that the velocity constraint (40) itself is satisfied approximately. For an energy-consistent multibody system integrator, which captures constraints both on position and on velocity level exactly, the interested reader is referred to [15, Sec. 5].

Remark 13. For lossless systems, one might be additionally interested in preserving momentum maps, like the angular momentum. This can be achieved by using *G-equivariant* discrete gradients, see [51, Ch. 3.7].

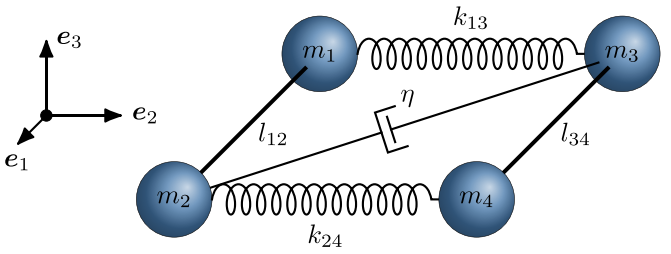

Fig. 2. Four-particle system.

Remark 14. Alternatively to applying the semi-explicit discrete gradient method (21), one could also apply the DDR-method (25) with a discrete gradient $\overline{\nabla}\mathcal{H}$, yielding the discrete time mapping

$$\begin{bmatrix} \overline{\nabla}_q \mathcal{H}(x^k, x^{k+1}) \\ \overline{\nabla}_v \mathcal{H}(x^k, x^{k+1}) \\ \overline{\nabla}_\lambda \mathcal{H}(x^k, x^{k+1}) \\ 0 \\ 0 \\ 0 \\ y^{k,k+1} \end{bmatrix} + \begin{bmatrix} 0 & 0 & 0 & -I & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -M & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ I & 0 & 0 & 0 & I & 0 & 0 \\ 0 & M & 0 & -I & -R_{\mathrm{R}}(q^{k+1/2}) & -\overline{\nabla} g(q^k, q^{k+1})^\top & I \\ 0 & 0 & 0 & 0 & \overline{\nabla} g(q^k, q^{k+1}) & 0 & 0 \\ 0 & 0 & 0 & 0 & -I & 0 & 0 \end{bmatrix} \begin{bmatrix} -\frac{1}{h}(q^{k+1} - q^k) \\ -\frac{1}{h}(v^{k+1} - v^k) \\ -\frac{1}{h}(\lambda^{k+1} - \lambda^k) \\ f_{1,q}^{k,k+1} \\ f_{1,v}^{k,k+1} \\ f_{1,\lambda}^{k,k+1} \\ u^{k,k+1} \end{bmatrix} = 0, \tag{46}$$

where we split $\overline{\nabla}\mathcal{H}$ into its entries $\overline{\nabla}\mathcal{H}_q, \overline{\nabla}\mathcal{H}_v, \overline{\nabla}\mathcal{H}_\lambda$, consistently with the notation introduced in Section 2.3. Note that this is completely equivalent to applying (44), up to constructing the discrete gradient $\overline{\nabla}\mathcal{H}$ based on the discrete gradient $\overline{\nabla}\mathcal{H}_1$ of the Hamiltonian $\mathcal{H}_1$, i.e.,

$$\overline{\nabla}\mathcal{H}(x, x') = \begin{bmatrix} \overline{\nabla}\mathcal{H}_1(q, v, q', v') \\ 0 \end{bmatrix},$$

and adding the constraint $f_{1,q}^{k,k+1} = \lambda^{k+1}$, see also Lemma 1 and Theorem 5.

6.3. Numerical experiment

Let us now focus on a specific problem from the literature to highlight the applicability of our approach and discuss its performance.

6.3.1. Problem description

The four-particle system depicted in Fig. 2 has been adapted from the literature [11,15] and extended to include dissipation. The configuration of the system is characterized by the coordinate vector $q = (q_1, q_2, q_3, q_4) \in \mathbb{R}^{12}$ comprising the Cartesian coordinates of four masses m_i, $i = 1, \dots, 4$ in three dimensions. Two nonlinear springs give rise to the potential function

$$V(q) = \frac{1}{2} k_{13} \left(\|q_3 - q_1\|^2 - 1 \right)^2 + \frac{1}{2} k_{24} \left(\|q_4 - q_2\|^2 - 1 \right)^2, \tag{47}$$

with the spring stiffness parameters k_{13} and k_{24}. The mass matrix is block diagonal, i.e. $M = \mathrm{diag}\{m_1 I, m_2 I, m_3 I, m_4 I\}$. Additionally, we consider configuration-dependent viscous dissipation in terms of the Rayleigh dissipation function

$$G(q, v) = \frac{1}{2} \eta(q) v_{\mathrm{rel}}^2, \qquad v_{\mathrm{rel}} = \|v_3 - v_2\|, \tag{48}$$

where $\eta(q) = \eta_0(1 + \alpha q_{\mathrm{rel}}^2) \geq 0$ is the dynamic viscosity parameter and $q_{\mathrm{rel}} = \|q_3 - q_2\|$. We have also introduced $\eta_0 > 0$ and $\alpha > 0$ as constant parameters. This leads to the dissipation matrix

$$R_{\mathrm{R}}(q) = \eta(q) \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & I & -I & 0 \\ 0 & -I & I & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}. \tag{49}$$

There are two rigid bars connecting two masses, respectively, leading to the constraints on position level given by

$$g_1(q) = \frac{1}{2} \left(\|q_2 - q_1\|^2 - 1 \right) = 0, \qquad g_2(q) = \frac{1}{2} \left(\|q_4 - q_3\|^2 - 1 \right) = 0. \tag{50}$$

In the numerical simulations the initial conditions

$$\begin{aligned} q_1^0 &= \left[0, 0, 0\right]^\top, \; q_2^0 = \left[1, 0, 0\right]^\top, \; q_3^0 = \left[0, 1, 0\right]^\top, \; q_4^0 = \left[1, 1, 0\right]^\top, \\ v_1^0 &= \left[0, 0, 0\right]^\top, \; v_2^0 = \left[0, 0, 0\right]^\top, \; v_3^0 = \left[0, 0, 0\right]^\top, \; v_4^0 = \left[0, 0, \tfrac{20}{17}\right]^\top, \end{aligned} \tag{51}$$

have been chosen consistently with the constraints (50) and their velocity level counterparts induced by (40).

Table 1
Simulation parameters for four-particle system.

h	t_{end}	ϵ_{Newton}	$\{k_{13}, k_{24}\}$	m_i	η_0	α
0.01	10	10^{-10}	$\{50, 500\}$	$\{1, 3, 2.3, 1.7\}$	1	0.5

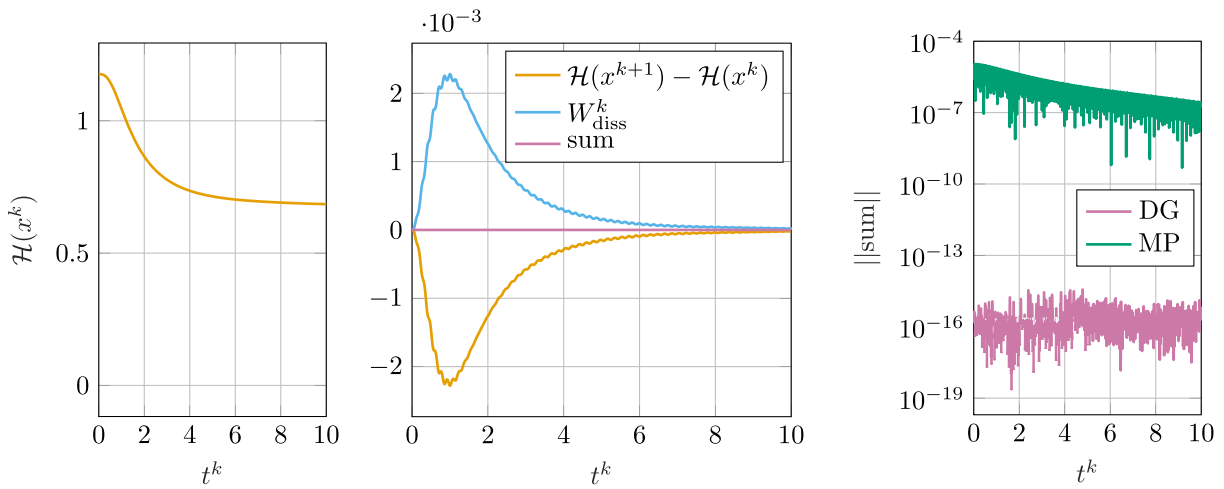

Fig. 3. Hamiltonian evolution (left), increments (center) and comparison with midpoint approach (right). "DG" denotes our approach and "MP" is the midpoint scheme.

6.3.2. Methods

The simulations have been conducted using our discrete gradient scheme for semi-explicit systems (21), or the equivalent DDR-method, implemented as suggested in (44). Results obtained with this scheme are labeled "DG" . The equations have been solved in each time step using Newton's method with a tolerance of ϵ_{Newton}. For the discrete gradients and Jacobians, we use the Gonzalez discrete gradient (12). Since the constraints (50) are quadratic, the application of the Gonzalez discrete Jacobian boils down to a midpoint evaluation. In this example we assume zero inputs.

The generated data along with the source code for the simulations are openly available for verification purposes in the repository https://github.com/plkinon/phdae_discrete_gradients and are archived at [59].

6.3.3. Results & discussion

We simulate the four-particle system using the parameters comprised in Table 6.3.3. On the left part of Fig. 3 one can observe the discrete evolution of the Hamiltonian in time. The exact representation of the power balance in discrete time (see (44) and Theorem 3) is demonstrated in the central part of Fig. 3, since the Hamiltonian increments are always less or equal to zero and the dissipated work in each time step

$$W^{k,k+1}_{\text{diss}} := h \begin{bmatrix} z^{k,k+1}_1 \\ \overline{z}_2(x^k, x^{k+1}) \end{bmatrix}^\top \overline{R}(x^k, x^{k+1}) \begin{bmatrix} z^{k,k+1}_1 \\ \overline{z}_2(x^k, x^{k+1}) \end{bmatrix} = h z^{k,k+1\top}_{1,v} R_{\text{R}}(q^{k+1/2}) z^{k,k+1}_{1,v} \geq 0 \tag{52}$$

is equally large. The sum of the two terms is numerically zero. For comparison, a pure midpoint-based scheme (labeled "MP") does not achieve energy-consistency, as depicted on the right part of Fig. 3.

On the left side of Fig. 4 one can observe that the scheme under investigation does not suffer from drift-off, i.e., it accurately captures the constraints on position level (50), as expected from (45). On the right side of the same figure, the kinematic constraint is shown to have order of magnitude of 10^{-4} for each discrete point in time, due to the intermediate approximation of (40), as discussed in Remark (12). Next, we switch off viscous dissipation by setting $\eta_0 = 0$ in the dissipation law. The discrete-time energy conservation in the non-dissipative case is verified in Fig. 5.

We have also performed a numerical convergence analysis (see Fig. 6, left side) using the relative error measure

$$e_x = \frac{||x_{\text{ref}} - x||}{||x_{\text{ref}}||},$$

where $x \in \{q^k_4, v^k_4, \lambda^{k,k+1}_1\}$ are the solutions evaluated at $t^k = 0.1$ for different time step sizes and methods. The respective reference solution x_{ref} was obtained using our DG method with $h = 10^{-4}$. The scheme exhibits second order accuracy for the differential unknowns of position and velocity and approximately a first order convergence behavior in the Lagrange multiplier. It should be noted that the order of convergence can be affected by the discretization method used for the equation coefficients. The compared midpoint scheme MP yields similar convergence results.

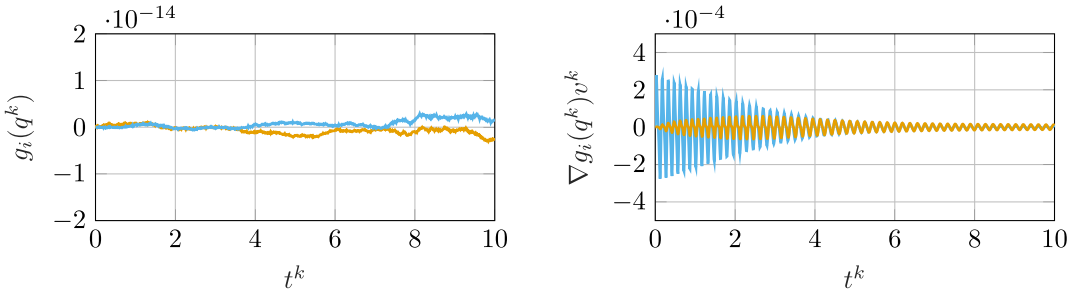

Fig. 4. Constraints on position level (left) and on velocity level (right); $i = 1$, $i = 2$.

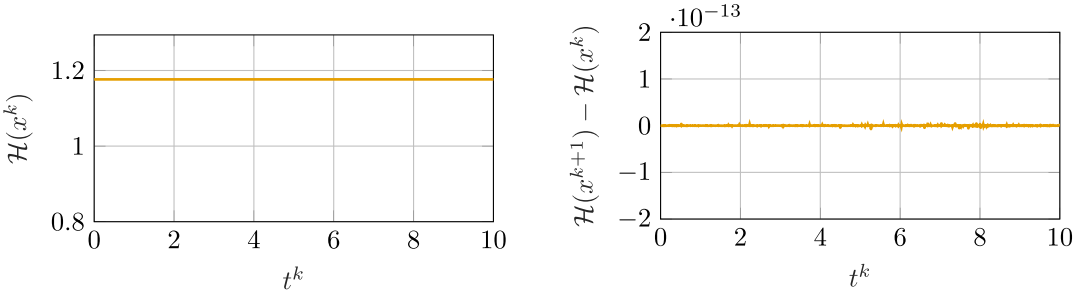

Fig. 5. Hamiltonian evolution (left) and increments (right) without dissipation, i.e., $\eta_0 = 0$.

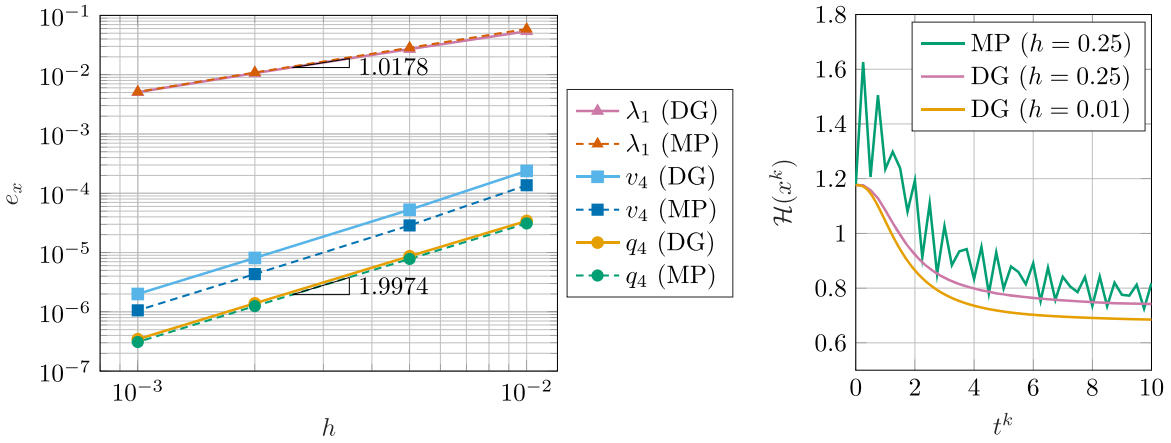

Fig. 6. h-convergence (left) and robustness comparison with larger h (right).

Lastly, we investigated the numerical robustness of the proposed DG scheme compared to the MP scheme when choosing larger time step sizes. Both methods did not converge with time step sizes of 0.4 or larger. However, our DG method provided physically meaningful results up until $h = 0.25$, showing a qualitatively similar behavior as with the previous simulation (see Fig. 6, right side). Contrarily to that, MP exhibits occasional total energy increase, thus violating the dissipativity of the system. This is in accordance with literature showing that discrete gradient methods are relatively robust compared to the midpoint rule in the nonlinear regime, see e.g. [15,60].

7. Conclusion

In this work, we introduced discrete gradient methods for port-Hamiltonian differential-algebraic equations (pHDAEs), addressing the challenges associated with state-dependent and non-invertible descriptor matrices. We developed a promising time integration method for semi-explicit systems, discussed more general pHDAEs, and explored a method based on an alternative representation of pHDAEs. Additionally, we outlined conditions for constructing discrete gradient pairs for general pHDAEs, analyzed state transformations and the equivalence of different methods. In particular we proved that, under appropriate regularity assumptions, every pHDAE can be reinterpreted as the combination of a parametrized semi-explicit pHDAE and an unstructured DAE on the time-varying parameter. Lastly, we applied the proposed framework to the important application case of nonlinear multibody system dynamics, providing convincing simulation results.

Future research could focus on refining the conditions needed to apply discrete gradients to general pHDAEs, improving the numerical efficiency and accuracy. It will be of major interest to apply our framework to large-scale and multiphysics systems, as their modeling is seamlessly possible in the pH framework. Moreover, a rigorous convergence analysis of the time discretization schemes presented in this paper should be pursued in the future.

CRediT authorship contribution statement

Philipp L. Kinon: Writing – review & editing, Writing – original draft, Software, Methodology, Investigation, Formal analysis, Data curation, Conceptualization, Validation, Visualization; **Riccardo Morandin:** Writing – review & editing, Writing – original draft, Methodology, Formal analysis, Conceptualization, Validation; **Philipp Schulze:** Writing – review & editing, Writing – original draft, Methodology, Formal analysis, Conceptualization, Validation.

Data availability

The integration methods as well as the definition of the system have been implemented in the openly available Python package `pydykit`, which can be found at https://github.com/pydykit/pydykit and is archived under [61]. The data generated for this work and the underlying source code for the simulations can be found in the repository https://github.com/plkinon/phdae_discrete_gradients and are archived at [59].

Declaration of competing interest

The authors declare no conflict of interest.

Acknowledgments

R. Morandin is funded by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) – 446856041. P. L. Kinon gratefully acknowledges funding by the Research Travel Grant of the Karlsruhe House of Young Scientists (KHYS). P. Schulze is funded by the Deutsche Forschungsgemeinschaft within the Collaborative Research Centre 1294: Data Assimilation – The Seamless Integration of Data and Models (Project-ID 318763901).

Appendix A. Proof details for Lemma 1

To prove the first claim in Lemma 1, we consider a fixed $\hat{x}_2 \in \mathcal{X}_2$ and define $f_1 : \mathcal{X}_1 \to \mathbb{R},\ x_1 \mapsto f(x_1, \hat{x}_2)$. Since $\mathcal{X}_2$ is convex, we deduce that for every fixed $(x_1, x_2) \in \mathcal{X}$ the map

$$\hat{f} : [0,1] \to \mathbb{R}, \qquad s \mapsto f\big(x_1, sx_2 + (1-s)\hat{x}_2\big)$$

is well-defined, continuously differentiable, and its derivative satisfies

$$\frac{\mathrm{d}\hat{f}}{\mathrm{d}s}(s) = \nabla_{x_2} f\big(x_1, sx_2 + (1-s)\hat{x}_2\big)^\top \big(x_2 - \hat{x}_2\big) = 0$$

for all $s \in [0,1]$, i.e., $\hat{f}$ is constant. Thus,

$$f(x_1, x_2) = \hat{f}(1) = \hat{f}(0) = f\big(x_1, \hat{x}_2\big) = f_1(x_1).$$

We observe that for every $x_1 \in \mathcal{X}_1$ and sufficiently small $h \in \mathbb{R}^{n_1}$ it holds that $(x_1 + h, \hat{x}_2) \in \mathcal{X}$, since $(x_1, \hat{x}_2) \in \mathcal{X}$ and $\mathcal{X}$ is an open set. In particular, we can write

$$f_1(x_1 + h) - f_1(x_1) = f\big(x_1 + h, \hat{x}_2\big) - f\big(x_1, \hat{x}_2\big)$$

for every $x_1 \in \mathcal{X}_1$ and every $h \in \mathbb{R}^{n_1}$ of appropriately bounded norm, from which we immediately deduce that f_1 is continuously differentiable and $\nabla f_1(x_1) = \nabla_{x_1} f(x_1, x_2)$ for every $(x_1, x_2) \in \mathcal{X}$. The second claim of Lemma 1 is proven in the main part of the manuscript.

Appendix B. Details on the synchronous machine

Another example for the present framework is the synchronous machine, see Example 4. The pH system, as shown in [53] reads

$$\begin{bmatrix} \dot{\psi}_s \\ \dot{\psi}_r \\ \dot{p} \\ \dot{\theta} \end{bmatrix} = \begin{bmatrix} -R_s & 0 & 0 & 0 \\ 0 & -R_r & 0 & 0 \\ 0 & 0 & -d & -1 \\ 0 & 0 & 1 & 0 \end{bmatrix} \nabla \widetilde{H}(\psi_s, \psi_r, p, \theta) + \begin{bmatrix} I_3 & 0 & 0 \\ 0 & e_1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} V_s \\ V_f \\ \tau \end{bmatrix}, \tag{B.1a}$$

$$\begin{bmatrix} I_s \\ I_f \\ \omega \end{bmatrix} = \begin{bmatrix} I_3 & 0 & 0 & 0 \\ 0 & e_1^\top & 0 & 0 \\ 0 & 0 & 1 & 0 \end{bmatrix} \nabla \widetilde{H}(\psi_s, \psi_r, p, \theta), \tag{B.1b}$$

with Hamiltonian

$$\widetilde{\mathcal{H}}(\psi_s,\psi_r,p,\theta)=\frac{1}{2}\begin{bmatrix}\psi_s\\ \psi_r\end{bmatrix}^\top L(\theta)^{-1}\begin{bmatrix}\psi_s\\ \psi_r\end{bmatrix}+\frac{1}{2J_r}p^2,$$

from which

$$\nabla\widetilde{\mathcal{H}}(\psi_s,\psi_r,p,\theta)=\begin{bmatrix} L(\theta)^{-1}\begin{bmatrix}\psi_s\\ \psi_r\end{bmatrix}\\ J_r^{-1}p\\ -\frac{1}{2}\begin{bmatrix}\psi_s\\ \psi_r\end{bmatrix}^\top L(\theta)^{-1}L'(\theta)L(\theta)^{-1}\begin{bmatrix}\psi_s\\ \psi_r\end{bmatrix}\end{bmatrix}.$$

Therein, $\psi_s,\psi_r\in\mathbb{R}^3$ represent the stator and rotor fluxes, respectively. For the further variable declarations, please refer to Example 4 in the bulk part of this work. Suppose we now want to rewrite (B.1a), (B.1b) replacing the magnetic fluxes with the corresponding currents, through the constitutive relation

$$\begin{bmatrix}\psi_s\\ \psi_r\end{bmatrix}=L(\theta)I.$$

This change of variables allows us to rewrite the system equivalently in its pHDAE form given in (17a) and (17b) with the corresponding Hamiltonian (4). These fit into the general pHDAE formulation with

$$x=\begin{bmatrix}I\\ p\\ \theta\end{bmatrix}\in\mathbb{R}^8,\qquad u=\begin{bmatrix}V_s\\ V_f\\ \tau\end{bmatrix}\in\mathbb{R}^5,\qquad y=\begin{bmatrix}I_s\\ I_f\\ \omega\end{bmatrix}\in\mathbb{R}^5,$$

$$E(I,\theta)=\begin{bmatrix}L(\theta)&0&L'(\theta)I\\ 0&1&0\\ 0&0&1\end{bmatrix}\in\mathbb{R}^{8,8},\qquad z(I,p,\theta)=\begin{bmatrix}I\\ J_r^{-1}p\\ -\frac{1}{2}I^\top L'(\theta)I\end{bmatrix}\in\mathbb{R}^8,$$

$$J=\begin{bmatrix}0&0&0\\ 0&0&-1\\ 0&1&0\end{bmatrix}\in\mathbb{R}^{8,8},\qquad R=\begin{bmatrix}R_{s,r}&0&0\\ 0&d&0\\ 0&0&0\end{bmatrix}\in\mathbb{R}^{8,8},\qquad B=\begin{bmatrix}I_3&0&0&0\\ 0&e_1^\top&0&0\\ 0&0&1&0\end{bmatrix}^\top.$$

Eventually, the relation $E(x)^\top z(x)=\nabla\mathcal{H}(x)$ can be checked as

$$\begin{bmatrix}L(\theta)&0&0\\ 0&1&0\\ I^\top L'(\theta)&0&1\end{bmatrix}\begin{bmatrix}I\\ J_r^{-1}p\\ -\frac{1}{2}I^\top L'(\theta)I\end{bmatrix}=\begin{bmatrix}L(\theta)I\\ J_r^{-1}p\\ \frac{1}{2}I^\top L'(\theta)I\end{bmatrix}.$$

Appendix C. Further details on the DDR-method with singular descriptor matrix

Towards the end of Section 4.3 we discussed possible limitations of the DDR-approach, questioning whether one can always find a discrete gradient that ensures the solvability of the system Eq. (26b), even for a singular descriptor matrix E. This of course also depends on the choice of $\overline{E}$, but for simplicity one would hope that for some suitable choice of $\overline{E}$, such as the midpoint approximation

$$\overline{E}(x,x'):=E(\tfrac{x+x'}{2}),\tag{C.1}$$

one can always construct a discrete gradient satisfying (29) for all $x,x'\in\mathbb{R}^n$. The following example demonstrates that this is not in general the case when considering a fixed consistent approximation for E, like the one in (C.1).

Example 8. *Consider a (non-semi-explicit) pHDAE with given*

$$\mathcal{H}(x)=\exp(\tfrac{1}{2}x_1^2)-1+\tfrac{1}{2}x_2^2,\quad \nabla\mathcal{H}(x)=\begin{bmatrix}x_1\exp(\frac{1}{2}x_1^2)\\ x_2\end{bmatrix},$$

$$E(x)=\begin{bmatrix}1\\ 1\end{bmatrix}\nabla\mathcal{H}(x)^\top=\begin{bmatrix}x_1\exp(\frac{1}{2}x_1^2)&x_2\\ x_1\exp(\frac{1}{2}x_1^2)&x_2\end{bmatrix},\quad z(x)=\tfrac{1}{2}\begin{bmatrix}1\\ 1\end{bmatrix}.$$

Here, E and z are constructed such that $E^\top z=\nabla\mathcal{H}$ holds, while the choice of the coefficients J,R,B is free and they can be set e.g. to zero, since they do not explicitly influence (26b). Correspondingly, we know that $\operatorname{colsp}(E^\top)=\operatorname{span}(\nabla\mathcal{H})$ *holds pointwise. For E we consider the midpoint approximation $\overline{E}$ as in (C.1), which results in*

$$\operatorname{colsp}\big(\overline{E}(x,x')^\top\big)=\operatorname{colsp}\big(E(\tfrac{x+x'}{2})^\top\big)=\operatorname{span}\big(\nabla\mathcal{H}(\tfrac{x+x'}{2})\big).$$

A priori, we want to allow the choice of an arbitrary discrete gradient $\overline{\nabla}\mathcal{H}$ of $\mathcal{H}$. By [50, Proposition 3.2], $\overline{\nabla}\mathcal{H}$ may be split up into orthogonal contributions as

$$\overline{\nabla}\mathcal{H}(x,x')=\frac{\mathcal{H}(x')-\mathcal{H}(x)}{\|x'-x\|^2}(x'-x)+w(x,x')\tag{C.2}$$

for $x \neq x'$, where w satisfies $w(x,x') \in \operatorname{span}(x'-x)^\perp$ and

$$\lim_{x' \to x} \left(w(x,x') - \pi_{\operatorname{span}(x'-x)^\perp} \nabla \mathcal{H}(x) \right) = 0,$$

where

$$\pi_{\operatorname{span}(x'-x)^\perp} = \frac{I - (x'-x)(x'-x)^\top}{\|x'-x\|^2}$$

denotes the orthogonal projection onto $\operatorname{span}(x'-x)^\perp$. Straightforward calculations yield that for the special choice

$$x = \begin{bmatrix} a \\ 0 \end{bmatrix}, \quad x' = \begin{bmatrix} 0 \\ b \end{bmatrix}, \quad a, b \in \mathbb{R} \setminus \{0\},$$

where $b := \pm a \sqrt{\exp(\frac{1}{2}(a/2)^2)}$, we have $\mathcal{H}(x') \neq \mathcal{H}(x)$ and $\nabla \mathcal{H}(\frac{x+x'}{2})^\top (x'-x) = 0$, and therefore

$$x' - x \in \operatorname{span}\left(\nabla \mathcal{H}(\tfrac{x+x'}{2}) \right)^\perp = \operatorname{colsp}(\overline{E}(x,x')^\top)^\perp.$$

Due to (C.2), this implies $\overline{\nabla} \mathcal{H}(x,x') \notin \operatorname{colsp}(\overline{E}(x,x')^\top)$, i.e., there exists no vector f satisfying $\overline{E}(x,x')^\top f = \overline{\nabla} \mathcal{H}(x,x')$ for this choice of x, x'. The discrete Eq. (26b) is therefore unsolvable. ◊

Appendix D. Interplay of system transformation and discretization

In this section we investigate the impact of system transformations on a subsequent time discretization by the methods discussed in Section 4. To this end, we first provide some preliminary results on inverses and compositions of system transformations and the corresponding discrete Jacobians in Appendix D.1. Afterwards, we analyze the application of the discretization schemes from Section 4 based on different coordinate systems in Appendix D.2.

D.1. Discrete Jacobians of composite and inverse maps

Suppose that $(\varphi, U) : \widetilde{\mathcal{X}} \to \mathcal{X} \times \mathbb{R}^{n,n}$ and $(\tilde{\varphi}, \widetilde{U}) : \widehat{\mathcal{X}} \to \widetilde{\mathcal{X}} \times \mathbb{R}^{n,n}$ are two system transformations. Then it is natural to define their *composition* as

$$(\varphi, U) \circ (\tilde{\varphi}, \widetilde{U}) = \left(\varphi \circ \tilde{\varphi}, (U \circ \tilde{\varphi}) \widetilde{U} \right) : \widehat{\mathcal{X}} \to \mathcal{X} \times \mathbb{R}^{n,n},$$

since applying $(\varphi, U) \circ (\tilde{\varphi}, \widetilde{U})$ to a system or gradient pair is equivalent to applying (φ, U) and $(\tilde{\varphi}, \widetilde{U})$ consecutively.

Let now $\overline{\mathrm{D}}\varphi$ and $\overline{\mathrm{D}}\tilde{\varphi}$ be discrete Jacobians for φ and $\tilde{\varphi}$, and let $\overline{U}$ and $\widehat{U}$ be consistent approximations of U and $\widetilde{U}$, respectively. Because of (35), $(\overline{\mathrm{D}}\varphi \circ \tilde{\varphi}) \overline{\mathrm{D}} \tilde{\varphi}$ is a discrete Jacobian for $\varphi \circ \tilde{\varphi}$, while $(\overline{U} \circ \tilde{\varphi}) \widehat{U}$ is obviously a consistent approximation of $(U \circ \tilde{\varphi}) \widetilde{U}$. Note that this choice is consistent with Theorem 6.

Consider now an invertible state transformation (φ, U). We define its *inverse* as $(\varphi, U)^{-1} = (\varphi^{-1}, U^{-1} \circ \varphi^{-1})$, since the compositions

$$(\varphi^{-1}, U^{-1} \circ \varphi^{-1}) \circ (\varphi, U) = (\mathrm{Id}_{\widetilde{\mathcal{X}}}, I_n) \quad \text{and} \quad (\varphi, U) \circ (\varphi^{-1}, U^{-1} \circ \varphi^{-1}) = (\mathrm{Id}_{\mathcal{X}}, I_n)$$

leave all systems and gradient pairs they are applied to invariant. Let us now denote $\psi = \varphi^{-1}$ and $V = U^{-1} \circ \varphi^{-1}$. Then, given discrete Jacobians $\overline{\mathrm{D}}\varphi$ and $\overline{\mathrm{D}}\psi$ for φ and its inverse, and pointwise invertible consistent approximations $\overline{U}$ and $\overline{V}$ for U and V, by applying Theorem 6 to a discrete gradient pair $(\overline{E}, \overline{z})$ for $(\mathcal{H}, E, z)$ with the system transformation (φ, U) and its inverse (ψ, V) consecutively, we obtain the discrete gradient pair

$$(\widehat{E}, \hat{z}) = \left(\overline{V}^\top (\overline{U} \circ \psi)^\top \overline{E} \, (\overline{\mathrm{D}}\varphi \circ \psi) \overline{\mathrm{D}}\psi \, , \; \overline{V}^{-1} (\overline{U}^{-1} \circ \psi) \overline{z} \right),$$

for the same $(\mathcal{H}, E, z)$ and the same state space. Since the composition of (φ, U) and (ψ, V) leaves the gradient pair unaltered, it is sensible to choose $\overline{\mathrm{D}}\psi$ and $\overline{V}$ in such a way that $(\widehat{E}, \hat{z}) = (\overline{E}, \overline{z})$. If we want this choice to be independent of (E, z), this is equivalent to the conditions $\overline{V} = \overline{U}^{-1} \circ \psi$ and $(\overline{\mathrm{D}}\varphi \circ \psi) \overline{\mathrm{D}}\psi = I_n$. While the former condition can always be imposed and ensures that $\overline{V}$ is a consistent approximation of V, the latter condition requires $\overline{\mathrm{D}}\varphi$ to be pointwise invertible, and in that case is equivalent to $\overline{\mathrm{D}}\psi = (\overline{\mathrm{D}}\varphi \circ \psi)^{-1}$. This leads to the following canonical construction for the inverse discrete Jacobian.

Lemma 3. *Let $\varphi \in C^1(\widetilde{\mathcal{X}}, \mathcal{X})$ be a diffeomorphism between two open spaces $\mathcal{X}, \widetilde{\mathcal{X}} \subseteq \mathbb{R}^n$, and let $\overline{\mathrm{D}}\varphi$ be a pointwise invertible discrete Jacobian for φ. Then a discrete Jacobian for φ^{-1}, which we call the inverse discrete Jacobian of φ based on $\overline{\mathrm{D}}\varphi$, is $\overline{\mathrm{D}}(\varphi^{-1}) = \left(\overline{\mathrm{D}}\varphi \circ \varphi^{-1} \right)^{-1}$.*

Proof. For $x, x' \in \mathcal{X}$ and $\tilde{x} = \varphi^{-1}(x)$, $\tilde{x}' = \varphi^{-1}(x')$ we have

$$\overline{\mathrm{D}}(\varphi^{-1})(x,x')(x'-x) = \overline{\mathrm{D}}\varphi(\tilde{x},\tilde{x}')^{-1} \left(\varphi(\tilde{x}') - \varphi(\tilde{x}) \right) = \overline{\mathrm{D}}\varphi(\tilde{x},\tilde{x}')^{-1} \overline{\mathrm{D}}\varphi(\tilde{x},\tilde{x}')(\tilde{x}' - \tilde{x}) = \varphi^{-1}(x') - \varphi^{-1}(x)$$

and $\overline{\mathrm{D}}(\varphi^{-1})(x,x) = \mathrm{D}\varphi(\tilde{x})^{-1} = \mathrm{D}(\varphi^{-1})(x)$. □

Note that the requirement for $\overline{\mathrm{D}}\varphi$ to be pointwise invertible in the construction of the inverse discrete Jacobian is often in practice not restrictive, since the discrete Jacobians of diffeomorphisms are locally pointwise invertible, as discussed in Remark 15. However, it can happen that such discrete Jacobians are not globally pointwise invertible, as the following example highlights.

Example 9. *Let us consider* $\varphi : \mathbb{R}^2 \to \mathbb{R}^2,\ \varphi(x) = \mathrm{Rot}(x^\top x)x$, *where* $\mathrm{Rot} : \mathbb{R} \to \mathbb{R}^{2,2}$ *is the rotation matrix function, i.e.,*

$$\mathrm{Rot}(\theta) = \begin{bmatrix} \cos(\theta) & -\sin(\theta) \\ \sin(\theta) & \cos(\theta) \end{bmatrix}$$

for all $\theta \in \mathbb{R}$. *We note that* φ *is* C^∞ *and that it is a bijective map, since it decomposes into rotations of fixed angle on every circle centered in* $0 \in \mathbb{R}^2$. *Furthermore, since*

$$\frac{\mathrm{dRot}}{\mathrm{d}\theta}(\theta) = \begin{bmatrix} -\sin(\theta) & -\cos(\theta) \\ \cos(\theta) & -\sin(\theta) \end{bmatrix} = \begin{bmatrix} \cos(\theta+\frac{\pi}{2}) & -\sin(\theta+\frac{\pi}{2}) \\ \sin(\theta+\frac{\pi}{2}) & \cos(\theta+\frac{\pi}{2}) \end{bmatrix} = \mathrm{Rot}(\theta+\tfrac{\pi}{2}) = \mathrm{Rot}(\theta)\mathrm{Rot}(\tfrac{\pi}{2}),$$

we deduce that

$$\mathrm{D}\varphi(x) = \mathrm{D}\big(\mathrm{Rot}(x^\top x)x\big) = \mathrm{Rot}(x^\top x) + \frac{\mathrm{dRot}}{\mathrm{d}\theta}(x^\top x)\nabla(x^\top x)x^\top = \mathrm{Rot}(x^\top x)\big(I_2 + 2\mathrm{Rot}(\tfrac{\pi}{2})xx^\top\big).$$

We now show that $\mathrm{D}\varphi$ *is pointwise invertible. Suppose that* $x, w \in \mathbb{R}^2$ *satisfy* $\mathrm{D}\varphi(x)w = 0$: *then* $\big(I + 2\mathrm{Rot}(\frac{\pi}{2})xx^\top\big)w = 0$, *from which* $w = -2x^\top w\,\mathrm{Rot}(\frac{\pi}{2})x$. *In particular,*

$$x^\top w = -2x^\top w\big(x^\top \mathrm{Rot}(\tfrac{\pi}{2})x\big) = 0,$$

and therefore $w = 0$, *allowing us to conclude that* $\mathrm{D}\varphi$ *is pointwise invertible.*

Let now $\overline{\mathrm{D}}\varphi$ *denote the Gonzalez discrete Jacobian of* φ *(see (1)). In particular, for every* $x, x' \in \mathbb{R}^2$ *and* $z \in (x'-x)^\perp$ *we have*

$$\overline{\mathrm{D}}\varphi(x,x')(x'-x) = \varphi(x') - \varphi(x) \quad \text{and} \quad \overline{\mathrm{D}}\varphi(x,x')z = \mathrm{D}\varphi(\tfrac{x+x'}{2})z.$$

For $x = 0$, $x' = (\sqrt{2\pi}, 0)$, $e_1 = (1,0)$, *and* $e_2 = (0,1)$, *we obtain then* $x' = \sqrt{2\pi}e_1$ *and* $x' - x = x' \perp e_2$, *and therefore*

$$\overline{\mathrm{D}}\varphi(0,x')e_1 = \frac{\overline{\mathrm{D}}\varphi(0,x')x'}{\sqrt{2\pi}} = \frac{\varphi(x')-\varphi(x)}{\sqrt{2\pi}} = \frac{\mathrm{Rot}(2\pi)x' - \mathrm{Rot}(0)0}{\sqrt{2\pi}} = \frac{x'}{\sqrt{2\pi}} = e_1$$

and

$$\overline{\mathrm{D}}\varphi(0,x')e_2 = \mathrm{D}\varphi(\tfrac{x+x'}{2})e_2 = \mathrm{Rot}(\tfrac{\pi}{2})\big(e_2 + \tfrac{1}{2}\mathrm{Rot}(\tfrac{\pi}{2})x'(x')^\top e_2\big) = \mathrm{Rot}(\tfrac{\pi}{2})e_2 = -e_1.$$

Thus,

$$\overline{\mathrm{D}}\varphi(x,x') = [e_1, -e_1] = \begin{bmatrix} 1 & -1 \\ 0 & 0 \end{bmatrix},$$

which is singular. ◊

Note that, while in Example 9 the inverse discrete Jacobian of φ based on $\overline{\mathrm{D}}\varphi$ cannot be constructed, the inverse diffeomorphism φ^{-1} still admits discrete Jacobians, e.g. the Gonzalez one. This in particular shows that the Gonzalez discrete Jacobian of the inverse diffeomorphism does not in general coincide with the inverse discrete Jacobian based on the Gonzalez discrete Jacobian.

We also present the following example, that shows that the Gonzalez discrete gradient construction does not in general commute with system transformations.

Example 10. *Consider the function* $f : \mathbb{R}^2 \to \mathbb{R},\ f(x) = \frac{1}{4}\|x^4\|$ *and the change of variables* $\varphi : \mathbb{R}^2 \to \mathbb{R}^2,\ \varphi(x_1,x_2) = (x_1+x_2, x_2)$, *which yield*

$$\nabla f = \|x\|^2 x, \qquad \mathrm{D}\varphi = \begin{bmatrix} 1 & 1 \\ 0 & 1 \end{bmatrix},$$

and let $\overline{\nabla}_G f$ *and* $\overline{\mathrm{D}}_G\varphi$ *denote the corresponding Gonzalez discrete gradient and Gonzalez discrete Jacobian, noting in particular that* $\overline{\mathrm{D}}_G\varphi = \mathrm{D}\varphi$, *since it is a constant matrix. We have now two natural ways to construct a discrete gradient for the composed map* $\tilde{f} = f\circ\varphi$: *either as its Gonzalez discrete gradient* $\overline{\nabla}_G\tilde{f}$, *or by using the chain rule (35), i.e.,* $\overline{\nabla}\tilde{f} = \overline{\mathrm{D}}_G\varphi^\top\overline{\nabla}_G f$. *We have then*

$$\overline{\nabla}_G\tilde{f}(0,2e_1)^\top e_2 = \nabla\tilde{f}(e_1)^\top e_2 = \nabla f\big(\varphi(e_1)\big)^\top \mathrm{D}\varphi\, e_2 = e_1^\top\begin{bmatrix} 1 & 1 \\ 0 & 1 \end{bmatrix}e_2 = 1$$

and

$$\begin{aligned}\overline{\nabla}\tilde{f}(0,2e_1)^\top e_2 &= \overline{\nabla}_G\tilde{f}(0,2e_1)^\top\overline{\mathrm{D}}\varphi\, e_2 = \overline{\nabla}_G f(0,2e_1)^\top(e_1+e_2)\\ &= \tfrac{1}{2}\overline{\nabla}_G f(0,2e_1)^\top 2e_1 + \overline{\nabla}_G f(0,2e_1)^\top e_2 = \tfrac{1}{2}\big(f(2e_1) - f(0)\big) + \nabla f(e_1)^\top e_2 = 2,\end{aligned}$$

thus $\overline{\nabla}\tilde{f}$ *and* $\overline{\nabla}_G\tilde{f}$ *do not coincide.* ◊

D.2. Discrete system invariance under system transformations

We would like to understand whether applying the same proposed numerical methods under different coordinate systems yields different results. We start by studying the discrete gradient pair scheme (18), in the form of the following theorem.

Theorem 9. *Consider a pHDAE of the form (6), let $(\overline{E}, \overline{z})$ be a discrete gradient pair for $(\mathcal{H}, E, z)$, and let $\overline{J}, \overline{R}, \overline{B}$ be consistent approximations for J, R, B, respectively, such that $\overline{J} = -\overline{J}^\top$ and $\overline{R} = \overline{R}^\top \geq 0$ pointwise. Let (φ, U) be an invertible system transformation, let $\overline{\mathrm{D}}\varphi$ be a discrete Jacobian for φ, and let $\overline{U}$ be a pointwise invertible consistent approximation for U. Then the discrete gradient pair scheme (18) applied to the original system, with the discrete gradient pair $(\overline{E}, \overline{z})$ and the consistent approximations $\overline{J}, \overline{R}, \overline{B}$, is equivalent to the same scheme applied to the system transformed via (φ, U), with the discrete gradient pair $(\widehat{E}, \hat{z})$ defined as in (34) and the consistent approximations $\widehat{J} = \overline{U}^\top(\overline{J}\circ\varphi)\overline{U}$, $\widehat{R} = \overline{U}^\top(\overline{R}\circ\varphi)\overline{U}$, and $\widehat{B} = \overline{U}^\top(\overline{B}\circ\varphi)$, up to the change of variables φ.*

Proof. In this proof we will often omit the arguments (x^k, x^{k+1}) and $(\tilde{x}^k, \tilde{x}^{k+1})$, for the sake of readability. It is clear that $\widehat{J}$, $\widehat{R}$, and $\widehat{B}$ are consistent approximations for the coefficients $\widetilde{J} = U^\top(J\circ\varphi)U$, $\widetilde{R} = U^\top(R\circ\varphi)U$, and $\widetilde{B} = U^\top(B\circ\varphi)$ of the transformed system, and that $\widehat{J} = -\widehat{J}^\top$ and $\widehat{R} = \widehat{R}^\top \geq 0$ hold pointwise. Thus, the discrete gradient pair scheme applied on the transformed system is well-defined.

Let now x^0, $(x^{k+1}, u^{k,k+1}, y^{k,k+1})$ for $k = 0, \dots, N-1$ denote a solution of the discrete gradient pair scheme applied to the original system, and let $\tilde{x}^k = \varphi^{-1}(x^k)$ for $k = 0, \dots, N$. Then we have

$$\begin{aligned}\widehat{E}(\tilde{x}^{k+1} - \tilde{x}^k) - h\big((\widehat{J} - \widehat{R})\hat{z} + \widehat{B}u^{k,k+1}\big) &= \overline{U}^\top\overline{E}(\overline{\mathrm{D}}\varphi)(\tilde{x}^{k+1} - \tilde{x}^k) - h\big((\overline{U}^\top\overline{JU} - \overline{U}^\top\overline{RU})\overline{U}^{-1}\overline{z} + \overline{U}^\top\overline{B}u^{k,k+1}\big)\\ &= \overline{U}^\top\Big(\overline{E}(x^{k+1} - x^k) - h\big((\overline{J} - \overline{R})\overline{z} + \overline{B}u^{k,k+1}\big)\Big) = 0,\\ y^{k,k+1} - \widehat{B}^\top\hat{z} = y^{k,k+1} - \overline{B}^\top\overline{U}\,\overline{U}^{-1}\overline{z} &= y^{k,k+1} - \overline{B}^\top\overline{z} = 0.\end{aligned}$$

Thus, $\tilde{x}^0$, $(\tilde{x}^{k+1}, u^{k,k+1}, y^{k,k+1})$ for $k = 0, \dots, N-1$ is a solution of the scheme applied to the transformed system.

Analogously, if $\tilde{x}^0$, $(\tilde{x}^{k+1}, u^{k,k+1}, y^{k,k+1})$ for $k = 0, \dots, N-1$ is a solution of the transformed discrete system, and we define $x^k = \varphi(\tilde{x}^k)$ for $k = 0, \dots, N$, then

$$\begin{aligned}\overline{E}(x^{k+1} - x^k) - h\big((\overline{J} - \overline{R})\overline{z} + \overline{B}u^{k,k+1}\big) &= \overline{U}^{-\top}\Big(\overline{U}^\top\overline{E}(\overline{\mathrm{D}}\varphi)(\tilde{x}^{k+1} - \tilde{x}^k) - h\big((\overline{U}^\top\overline{JU} - \overline{U}^\top\overline{RU})\overline{U}^{-1}\overline{z} + \overline{U}^\top\overline{B}u^{k,k+1}\big)\Big)\\ &= \overline{U}^{-\top}\Big(\widehat{E}(\tilde{x}^{k+1} - \tilde{x}^k) - h\big((\widehat{J} - \widehat{R})\hat{z} + \widehat{B}u^{k,k+1}\big)\Big) = 0,\\ y^{k,k+1} - \overline{B}^\top\overline{z} = y^{k,k+1} - \overline{B}^\top\overline{U}\,\overline{U}^{-1}\overline{z} &= y^{k,k+1} - \widehat{B}^\top\hat{z} = 0,\end{aligned}$$

such that x^0, $(x^{k+1}, u^{k,k+1}, y^{k,k+1})$ for $k = 0, \dots, N-1$ is a solution of the original discrete system. □

Next, we analyze the semi-explicit discrete gradient scheme (21). For that purpose, we first have to investigate which system transformations preserve the semi-explicit structure.

Proposition 3. *Let (E, z) be a semi-explicit gradient pair for $\mathcal{H}$, let (φ, U) be an invertible system transformation from another open state space $\widetilde{\mathcal{X}} = \widetilde{\mathcal{X}}_1 \times \widetilde{\mathcal{X}}_2$, where $\widetilde{\mathcal{X}}_2$ is convex, and let us split $\varphi = (\varphi_1, \varphi_2)$ and $U = \left[\begin{smallmatrix} U_{11} & U_{12} \\ U_{21} & U_{22}\end{smallmatrix}\right]$ accordingly. Then the transformed gradient pair is semi-explicit if and only if $\mathrm{D}_{\tilde{x}_2}\varphi_1 = 0$ and $U_{12} = 0$.*

Proof. Denoting by $(\widetilde{E}, \tilde{z})$ the transformed gradient pair, we have

$$\widetilde{E} = U^\top(E\circ\varphi)\mathrm{D}\varphi = \begin{bmatrix} U_{11} & U_{12} \\ U_{21} & U_{22}\end{bmatrix}^\top\begin{bmatrix} E_{11}\circ\varphi & 0 \\ 0 & 0\end{bmatrix}\begin{bmatrix} \mathrm{D}_{\tilde{x}_1}\varphi_1 & \mathrm{D}_{\tilde{x}_2}\varphi_1 \\ \mathrm{D}_{\tilde{x}_1}\varphi_2 & \mathrm{D}_{\tilde{x}_2}\varphi_2\end{bmatrix} = \begin{bmatrix} U_{11}^\top(E_{11}\circ\varphi)\mathrm{D}_{\tilde{x}_1}\varphi_1 & U_{11}^\top(E_{11}\circ\varphi)\mathrm{D}_{\tilde{x}_2}\varphi_1 \\ U_{12}^\top(E_{11}\circ\varphi)\mathrm{D}_{\tilde{x}_1}\varphi_1 & U_{12}^\top(E_{11}\circ\varphi)\mathrm{D}_{\tilde{x}_2}\varphi_1\end{bmatrix}.$$

Note that, since U and $\mathrm{D}\varphi$ are pointwise invertible, $\operatorname{rank}(\widetilde{E}) = \operatorname{rank}(E)$ pointwise, and therefore $(\widetilde{E}, \tilde{z})$ is a semi-explicit gradient pair if and only if $\widetilde{E}_{ij} = U_{1i}^\top(E_{11}\circ\varphi)\mathrm{D}_{\tilde{x}_j}\varphi_1$ is invertible for $i = j = 1$ and zero otherwise.

Suppose first that $\widetilde{E}$ has the wished structure. Since $\widetilde{E}_{11}$ is invertible, so are U_{11} and $\mathrm{D}_{\tilde{x}_1}\varphi_1$. Then we deduce from $\widetilde{E}_{12}, \widetilde{E}_{21} = 0$ that $U_{12}, \mathrm{D}_{\tilde{x}_2}\varphi_1 = 0$. Suppose now that $U_{12}, \mathrm{D}_{\tilde{x}_2}\varphi_1 = 0$. Then it is clear that $\widetilde{E}_{ij} = 0$ for $(i, j) \neq (1, 1)$. Furthermore, since U and $\mathrm{D}\varphi$ are pointwise invertible and block lower triangular, we deduce that U_{11} and $\mathrm{D}_{\tilde{x}_1}\varphi_1$ are also pointwise invertible, and so is $\widetilde{E}_{11}$. □

We also need the following result, which provides conditions ensuring that the Hamiltonian of the transformed system only depends on the differential state.

Lemma 4. *Let φ be a diffeomorphism as in Lemma 3 satisfying $\mathrm{D}_{\tilde{x}_2}\varphi_1 = 0$. Then, the following assertions hold.*

1. *There is a diffeomorphism $\varphi_{11} \in C^1(\widetilde{\mathcal{X}}_1, \mathcal{X}_1)$ such that $\varphi_{11}\circ\pi_1 = \varphi_1$ and $\mathrm{D}\varphi_{11}\circ\pi_1 = \mathrm{D}_{\tilde{x}_1}\varphi_1$.*
2. *Let $\mathcal{H} \in C^1(\mathcal{X}, \mathbb{R})$ be such that $\nabla_{x_2}\mathcal{H} = 0$, let $\mathcal{H}_1 \in C^1(\mathcal{X}_1, \mathbb{R})$ be the associated function defined as in Lemma 1, let $\overline{\nabla}\mathcal{H}_1$ be a discrete gradient for $\mathcal{H}_1$, and let $\overline{\mathrm{D}}\varphi_{11}$ be a discrete Jacobian for φ_{11}. Then $\widetilde{\mathcal{H}} = \mathcal{H}\circ\varphi$ satisfies the assumptions of Lemma 1 with associated function $\widetilde{\mathcal{H}}_1 \in C^1(\widetilde{\mathcal{X}}_1, \mathbb{R})$, and*

$$\overline{\nabla}\widetilde{\mathcal{H}}_1 = (\overline{\mathrm{D}}\varphi_{11})^\top(\overline{\nabla}\mathcal{H}_1\circ\varphi_{11}) \tag{D.1}$$

is a discrete gradient for $\widetilde{\mathcal{H}}_1$.

Proof. Let us prove the two statements separately:

1. It is clear that $\varphi_{11} \in C^1(\widetilde{\mathcal{X}}_1, \mathcal{X}_1)$ satisfying $\varphi_{11} \circ \pi_1 = \varphi_1$ and $\mathrm{D}\varphi \circ \pi_1 = \mathrm{D}_{\tilde{x}_1}\varphi_1$ exists because of Lemma 1. Let now $\psi = (\psi_1, \psi_2) = \varphi^{-1}$. Since $\mathrm{D}\psi = (\mathrm{D}\varphi \circ \psi)^{-1}$ has the same block lower triangular structure as $\mathrm{D}\varphi$, we construct $\psi_{11} \in C^1(\mathcal{X}_1, \widetilde{\mathcal{X}}_1)$ analogously to φ_{11}, and deduce that $\varphi_{11} \circ \psi_{11}$ and $\psi_{11} \circ \varphi_{11}$ are both the identity. Since $\mathrm{D}\varphi_{11}$ inherits from $\mathrm{D}_{\tilde{x}_1}\varphi_1$ (and therefore from $\mathrm{D}\varphi$) the property of being pointwise invertible, we conclude that φ_{11} is indeed a diffeomorphism.
2. Since
$$\nabla \widetilde{\mathcal{H}} = (\mathrm{D}\varphi)^\top (\nabla \mathcal{H} \circ \varphi) = \begin{bmatrix} \mathrm{D}_{\tilde{x}_1}\varphi_1^\top & \mathrm{D}_{\tilde{x}_1}\varphi_2^\top \\ 0 & \mathrm{D}_{\tilde{x}_2}\varphi_2^\top \end{bmatrix} \begin{bmatrix} \nabla_{x_1}\mathcal{H} \circ \varphi \\ 0 \end{bmatrix} = \begin{bmatrix} \mathrm{D}_{\tilde{x}_1}\varphi_1^\top (\nabla_{x_1}\mathcal{H} \circ \varphi) \\ 0 \end{bmatrix},$$
the assumptions of Lemma 1 are satisfied and $\widetilde{\mathcal{H}}_1$ is well-defined, and clearly satisfies $\widetilde{\mathcal{H}}_1 = \mathcal{H}_1 \circ \varphi_{11}$. The fact that $\overline{\nabla}\widetilde{\mathcal{H}}_1$ is a discrete gradient for $\widetilde{\mathcal{H}}_1$ follows immediately from the chain rule (35).

This proves the Lemma. □

We can now prove the following result, which states that applying the semi-explicit discrete gradient scheme from Section 4.2 to a semi-explicit system and to a corresponding transformed semi-explicit system leads to equivalent time-discrete systems.

Theorem 10. *Consider a semi-explicit pHDAE of the form (15), let $\overline{\nabla}\mathcal{H}_1$ be a discrete gradient for the Hamiltonian $\mathcal{H}_1$, and let $\overline{E}_{11}, \overline{z}_2, \overline{J}, \overline{R}, \overline{B}$ be consistent approximations for E_{11}, z_2, J, R, B, respectively, such that Assumption A1 is satisfied, and $\overline{J} = -\overline{J}^\top$ and $\overline{R} = \overline{R}^\top \succeq 0$ hold pointwise. Let (φ, U) be an invertible system transformation preserving the semi-explicit structure as in Lemma 3, let $\overline{\mathrm{D}}\varphi_{11}$ be a pointwise invertible discrete Jacobian of φ_{11} as specified in Lemma 4, and let $\overline{U} = \left[\begin{smallmatrix} \overline{U}_{11} & 0 \\ \overline{U}_{21} & \overline{U}_{22} \end{smallmatrix}\right]$ be a pointwise invertible consistent approximation for U. Then the semi-explicit discrete gradient scheme (21) applied to the original system, with the discrete gradient $\overline{\nabla}\mathcal{H}_1$ and the consistent approximations $\overline{E}_{11}, \overline{z}_2, \overline{J}, \overline{R}, \overline{B}$, is equivalent to the same scheme applied to the system transformed via (φ, U), with the discrete gradient $\overline{\nabla}\widetilde{\mathcal{H}}_1$ defined as in (D.1) and the consistent approximations $\hat{E}_{11} = \overline{U}_{11}^\top (\overline{E}_{11} \circ \varphi)(\overline{\mathrm{D}}\varphi_{11} \circ \pi_1)$, $\hat{z}_2 = \overline{U}_{22}^{-1}\big((\overline{z}_2 \circ \varphi) - \overline{U}_{21}\hat{E}_{11}^{-\top}(\overline{\nabla}\widetilde{\mathcal{H}}_1 \circ \pi_1)\big)$, $\hat{J} = \overline{U}^\top (\overline{J} \circ \varphi)\overline{U}$, $\hat{R} = \overline{U}^\top (\overline{R} \circ \varphi)\overline{U}$, and $\hat{B} = \overline{U}^\top (\overline{B} \circ \varphi)$, up to the change of variables φ.*

Proof. We first show that the semi-explicit discrete gradient scheme applied to the transformed system is well-defined. To this end, we observe that the transformed system is semi-explicit by assumption, $\overline{\nabla}\widetilde{\mathcal{H}}_1$ is a discrete gradient of $\widetilde{\mathcal{H}}_1$ because of Lemma 4, $\hat{E}_{11}$, $\hat{J}$, $\hat{R}$, and $\hat{B}$ are consistent approximations of $\widetilde{E}_{11} = U_{11}^\top (E_{11} \circ \varphi)\mathrm{D}_{\tilde{x}_1}\varphi_1 = U_{11}^\top (E_{11} \circ \varphi)(\mathrm{D}\varphi_{11} \circ \pi_1)$, $\widetilde{J} = U^\top (J \circ \varphi)U$, $\widetilde{R} = U^\top (R \circ \varphi)U$, and $\widetilde{B} = U^\top (B \circ \varphi)$, respectively, and $\hat{J} = -\hat{J}^\top$ and $\hat{R} = \hat{R}^\top \succeq 0$ hold pointwise. Furthermore, note that $\hat{E}_{11}$ satisfies Assumption A1 and that, since
$$\begin{aligned} \tilde{z}_2 &= [0, I_{n_2}]U^{-1}(z \circ \varphi) = U_{22}^{-1}\big((z_2 \circ \varphi) - U_{21}U_{11}^{-1}(z_1 \circ \varphi)\big) \\ &= U_{22}^{-1}\big((z_2 \circ \varphi) - U_{21}U_{11}^{-1}(E_{11} \circ \varphi)^{-\top}(\nabla_{x_1}\mathcal{H} \circ \varphi)\big) = U_{22}^{-1}\big((z_2 \circ \varphi) - U_{21}\widetilde{E}_{11}^{-\top}(\nabla\widetilde{\mathcal{H}}_1 \circ \pi_1)\big), \end{aligned}$$
$\hat{z}_2$ is a consistent approximation of $\tilde{z}_2$.

Let us now construct a discrete Jacobian $\overline{\mathrm{D}}\varphi$ of φ, in such a way that $\overline{\mathrm{D}}_{\tilde{x}_1}\varphi_1 = \overline{\mathrm{D}}\varphi_{11} \circ \pi_1$. This can be simply done by choosing a discrete Jacobian $\overline{\mathrm{D}}\varphi_2$ of $\varphi_2 = \pi_2 \circ \varphi$ and defining
$$\overline{\mathrm{D}}\varphi = \begin{bmatrix} \overline{\mathrm{D}}\varphi_{11} \circ \pi_1 & 0 \\ \overline{\mathrm{D}}_{\tilde{x}_1}\varphi_2 & \overline{\mathrm{D}}_{\tilde{x}_2}\varphi_2 \end{bmatrix},$$
which, as it can be easily verified, fulfills the discrete Jacobian definition.

To prove the statement of the theorem it is then sufficient to combine Corollary 1 and Theorem 9. In fact, the semi-explicit discrete gradient scheme applied to the original system is equivalent to the discrete gradient pair scheme applied to the same system with the discrete gradient pair $(\overline{E}, \overline{z})$ defined as in (30), i.e.,
$$\overline{E} = \begin{bmatrix} \overline{E}_{11} & 0 \\ 0 & 0 \end{bmatrix}, \qquad \overline{z} = \begin{bmatrix} \overline{E}_{11}^{-\top}(\overline{\nabla}\mathcal{H}_1 \circ \pi_1) \\ \overline{z}_2 \end{bmatrix},$$
where π_1 here is to be intended as the projection of $\mathcal{X}$ onto $\mathcal{X}_1$. This discrete system is then equivalent up to the change of variables φ to the one yielded by the discrete gradient pair scheme applied to the transformed system with the discrete gradient pair $(\hat{E}, \hat{z})$ defined as in Theorem 9, i.e.,
$$\hat{E} = \overline{U}^\top (\overline{E} \circ \varphi)\overline{\mathrm{D}}\varphi = \begin{bmatrix} \overline{U}_{11}^\top (\overline{E}_{11} \circ \varphi)(\overline{\mathrm{D}}\varphi_{11} \circ \pi_1) & 0 \\ 0 & 0 \end{bmatrix} = \begin{bmatrix} \hat{E}_{11} & 0 \\ 0 & 0 \end{bmatrix},$$
$$\hat{z} = \overline{U}^{-1}(\overline{z} \circ \varphi) = \begin{bmatrix} \overline{U}_{11}^{-1}(\overline{E}_{11} \circ \varphi)^{-\top}(\overline{\nabla}\mathcal{H}_1 \circ \pi_1 \circ \varphi) \\ \overline{U}_{22}^{-1}\big((\overline{z}_2 \circ \varphi) - \overline{U}_{21}\overline{U}_{11}^{-1}(\overline{E}_{11} \circ \varphi)^{-\top}(\overline{\nabla}\mathcal{H}_1 \circ \pi_1 \circ \varphi)\big) \end{bmatrix} = \begin{bmatrix} \hat{E}_{11}^{-\top}(\overline{\nabla}\widetilde{\mathcal{H}}_1 \circ \pi_1) \\ \hat{z}_2 \end{bmatrix},$$
and the consistent approximations $\hat{J}, \hat{R}, \hat{B}$. Finally, due to the structure of $(\hat{E}, \hat{z})$, we can apply again Corollary 1 and conclude that the latest discrete system is equivalent to the one obtained by applying the semi-explicit discrete gradient scheme to the transformed system with the discrete gradient $\overline{\nabla}\widetilde{\mathcal{H}}_1$ and the consistent approximations $\hat{E}_{11}$, $\hat{z}_2$, $\hat{J}$, $\hat{R}$, and $\hat{B}$. □

Remark 15. A similar result holds for the DDR-method applied to a given DDR-pHDAE (11). On the one hand, its corresponding DDR-pHDAE transformed via (φ, U) is

$$\begin{bmatrix} (\mathrm{D}\varphi)^\top(\nabla\mathcal{H}\circ\varphi) \\ 0 \\ y \end{bmatrix} + \begin{bmatrix} 0 & -\mathrm{D}\varphi^\top(E\circ\varphi)^\top U & 0 \\ U^\top(E\circ\varphi)\mathrm{D}\varphi & U^\top\big((J-R)\circ\varphi\big)U & U^\top(B\circ\varphi) \\ 0 & (B\circ\varphi)^\top U & 0 \end{bmatrix} \begin{bmatrix} -\dot{\tilde{x}} \\ \tilde{f} \\ u \end{bmatrix} = 0, \tag{D.2}$$

together with $\tilde{f} = U^{-1}(z\circ\varphi)$. On the other hand, by applying the DDR-method (25) for a fixed discrete gradient $\overline{\nabla}\mathcal{H}$ of $\mathcal{H}$ and some given consistent approximations $\overline{E}$, $\overline{J}$, $\overline{R}$, and $\overline{B}$ of E, J, R, and B, respectively, and multiplying the first block row by $(\overline{\mathrm{D}}\varphi)^\top$ and the second block row by $\overline{U}^\top$, where $\overline{\mathrm{D}}\varphi$ is a discrete Jacobian for φ and $\overline{U}$ is a consistent approximation of U, and replacing $x^{k+1} - x^k = \overline{\mathrm{D}}\varphi(\tilde{x}^k, \tilde{x}^{k+1})(\tilde{x}^{k+1} - \tilde{x}^k)$ and $f^{k,k+1} = \overline{U}(\tilde{x}^k, \tilde{x}^{k+1})\tilde{f}^{k,k+1}$ with $\tilde{x}^k = \varphi^{-1}(x^k)$ and $\tilde{x}^{k+1} = \varphi^{-1}(x^{k+1})$, we obtain the one-step method

$$\begin{bmatrix} (\overline{\mathrm{D}}\varphi)^\top(\overline{\nabla}\mathcal{H}\circ\varphi) \\ 0 \\ y^{k,k+1} \end{bmatrix} + \begin{bmatrix} 0 & -\overline{\mathrm{D}}\varphi^\top(\overline{E}\circ\varphi)^\top\overline{U} & 0 \\ \overline{U}^\top(\overline{E}\circ\varphi)\overline{\mathrm{D}}\varphi & \overline{U}^\top\big((\overline{J}-\overline{R})\circ\varphi\big)\overline{U} & \overline{U}^\top(\overline{B}\circ\varphi) \\ 0 & (\overline{B}\circ\varphi)^\top\overline{U} & 0 \end{bmatrix} \begin{bmatrix} -\frac{\tilde{x}^{k+1}-\tilde{x}^k}{h} \\ \tilde{f}^{k,k+1} \\ u^{k,k+1} \end{bmatrix} = 0, \tag{D.3}$$

where the arguments $(\tilde{x}^k, \tilde{x}^{k+1})$ have been omitted to keep the notation short. Note that, since $\overline{\nabla}\widetilde{\mathcal{H}} = (\overline{\mathrm{D}}\varphi)^\top(\overline{\nabla}\mathcal{H}\circ\varphi)$ is a discrete gradient for $\widetilde{\mathcal{H}} = \mathcal{H}\circ\varphi$ because of the chain rule, and $\hat{E} = \overline{U}^\top(\overline{E}\circ\varphi)\overline{\mathrm{D}}\varphi$, $\hat{J} = \overline{U}^\top(\overline{J}\circ\varphi)\overline{U}$, $\hat{R} = \overline{U}^\top(\overline{R}\circ\varphi)\overline{U}$, and $\hat{B} = \overline{U}^\top(\overline{B}\circ\varphi)$ are consistent approximations of the correspondent coefficients of the transformed system (32), the one-step method (D.3) is equivalent to an appropriate DDR-method applied to the transformed system.

This construction immediately shows that every solution of the original discrete DDR system is uniquely mapped into a solution of the transformed discrete DDR system. However, to be able to uniquely associate to every solution of the transformed discrete DDR system one solution of the original discrete DDR system, we need to invert the construction, which requires the discrete Jacobian $\overline{\mathrm{D}}\varphi(x^k, x^{k+1})$ to be invertible.

Similarly to our considerations leading to Assumption A1 we note that, for small enough time steps, this is guaranteed by consistency, since $\overline{\mathrm{D}}\varphi(x^k, x^k) = \mathrm{D}\varphi(x^k)$ is invertible for every $x^k \in \mathcal{X}$. However, there is in general no guarantee that the discrete Jacobian of a diffeomorphism is pointwise invertible, cf. Example 9.

It remains to discuss how the additional constraints used in the DDR-methods change under system transformations. This strongly depends on the specific form of these constraints, which can be quite diverse. For example, if in the original coordinates we have a constraint of the form $F(x^k, x^{k+1}, f^{k,k+1}) = 0$ for some function $F : \mathcal{X}\times\mathcal{X}\times\mathbb{R}^m \to \mathbb{R}^p$, then to obtain an equivalent one-step method the corresponding constraint in the new coordinates would be $\widetilde{F}(\tilde{x}^k, \tilde{x}^{k+1}, \tilde{f}^{k,k+1}) = 0$ with

$$\widetilde{F}(\tilde{x}^k, \tilde{x}^{k+1}, \tilde{f}^{k,k+1}) = F(\varphi(\tilde{x}^k), \varphi(\tilde{x}^{k+1}), \overline{U}(\tilde{x}^k, \tilde{x}^{k+1})\tilde{f}^{k,k+1}).$$

Similarly, if in the original coordinates we require $\|f^{k,k+1} - \overline{z}(x^k, x^{k+1})\|$ to be minimal for some fixed consistent discretization $\overline{z}$ of z, in the new coordinates we would minimize

$$\|f^{k,k+1} - \overline{z}(x^k, x^{k+1})\| = \|\overline{U}(\tilde{x}^k, \tilde{x}^{k+1})(\tilde{f}^{k,k+1} - \hat{z}(\tilde{x}^k, \tilde{x}^{k+1}))\|$$

instead, where $\hat{z} = \overline{U}^{-1}(\overline{z}\circ\varphi)$ is a consistent discretization of $\tilde{z}$.

Appendix E. Details on the mass-spring multibody system example

The multibody system with singular mass matrix from Example 7, with masses m_i and springs with constants k_i and resting lengths l_{i0}, with $i \in \{1, 2\}$, takes up the considerations in Section 6.1. The system can be regarded as a modular multibody system comprising two separate subsystems with two degrees of freedom. However, we decide to use two coordinates for the elongations of the springs (x_1 and x_2) and one coordinate q_2 for the point where the two subsystems are interconnected. Correspondingly, we use

$$q = \begin{bmatrix} x_1 \\ q_2 \\ x_2 \end{bmatrix} \quad \text{and} \quad v = \begin{bmatrix} v_1 \\ v_2 \\ v_3 \end{bmatrix} = \begin{bmatrix} \dot{x}_1 \\ \dot{q}_2 \\ \dot{x}_2 \end{bmatrix}$$

and the interconnection constraint $q_2 = x_1 + l_{10} + w$ arises. The total kinetic energy is given by

$$T(v) = \frac{1}{2}m_1 v_1^2 + \frac{1}{2}m_2(v_2 + v_3)^2 = \frac{1}{2}v^\top M v \tag{E.1}$$

and thus we identify the mass matrix M from (36), which is constant and singular for all configurations.

Following Proposition 2, we perform a singular value decomposition to arrive at a semi-explicit pHDAE formulation. For the present case, we have

$$E = \begin{bmatrix} I_{3\times3} & 0 & 0 \\ 0 & M & 0 \\ 0 & 0 & 0 \end{bmatrix}. \tag{E.2}$$

Here we identify the SVD of E given by $E = U\Sigma V^\top = [U_1, U_2]\mathrm{diag}(\Sigma_1, 0)[V_1, V_2]^\top$, where $\Sigma_1 = \mathrm{diag}(1, 1, 1, m_1, 2m_2)$ and

$$V_1 = W_1 = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & \frac{1}{\sqrt{2}} \\ 0 & 0 & 0 & 0 & \frac{1}{\sqrt{2}} \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}, V_2 = W_2 = \begin{bmatrix} 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ -\frac{1}{\sqrt{2}} & 0 \\ \frac{1}{\sqrt{2}} & 0 \\ 0 & 1 \end{bmatrix}. \tag{E.3}$$

Appendix F. Transformation to semi-explicit form

The following theorem provides an SVD-like decomposition for a matrix function with constant rank. This result is helpful in deriving conditions for the existence of a semi-explicit representation of a pHDAE.

Theorem 11. *Let $E \in C(\mathcal{X}, \mathbb{R}^{m,n})$, with $\mathrm{rank}(E(x)) = r$ for all $x \in \mathcal{X}$. Then for every $x_0 \in \mathcal{X}$ there exists an open neighborhood $\mathcal{X}_0 \subseteq \mathcal{X}$ of x_0 and pointwise unitary functions $U \in C(\mathcal{X}_0, \mathbb{R}^{m,m})$ and $V \in C(\mathcal{X}_0, \mathbb{R}^{n,n})$ such that*

$$U^\top E V = \begin{bmatrix} \Sigma & 0 \\ 0 & 0 \end{bmatrix}, \tag{F.1}$$

with pointwise invertible $\Sigma \in C(\mathcal{X}_0, \mathbb{R}^{r,r})$. Furthermore, if the entries of E are analytic or C^ℓ for some $\ell \in \mathbb{N}_0 \cup \{\infty\}$, then U, V, and Σ can be chosen to have that same regularity.

Proof. Let

$$U_0^\top E(x_0) V_0 = \begin{bmatrix} \Sigma_0 & 0 \\ 0 & 0 \end{bmatrix}$$

denote the singular value decomposition of $E(x_0)$, with $U_0 \in \mathbb{R}^{m,m}$ and $V_0 \in \mathbb{R}^{n,n}$ unitary matrices, and $\Sigma_0 \in \mathbb{R}^{r,r}$ nonsingular, and let us split correspondingly

$$U_0^\top E(x) V_0 = \begin{bmatrix} E_{11}(x) & E_{12}(x) \\ E_{21}(x) & E_{22}(x) \end{bmatrix}$$

for all $x \in \mathcal{X}$. Since $E_{11}(x_0) = \Sigma_0$ is invertible and E is continuous, there is an open neighborhood $\mathcal{X}_0 \subseteq \mathcal{X}$ of x_0 such that $E_{11}(x)$ is invertible for all $x \in \mathcal{X}_0$. We note that E_{ij} has at least the same regularity as E for all i, j, and that, since the determinant of a matrix function clearly has the same regularity as its entries, and the pointwise inverse of E_{11} on $\mathcal{X}_0$ can be expressed in the form

$$E_{11}(x)^{-1} = \frac{\mathrm{adj}(E_{11}(x))}{\det(E_{11}(x))},$$

where $\mathrm{adj}(E_{11}(x))$ denotes the adjugate matrix of $E_{11}(x)$ (whose entries are determinants of submatrices of $E_{11}(x)$), and $\det(E_{11}(x))$ does not vanish on $\mathcal{X}_0$, E_{11} will also have the same regularity as E on $\mathcal{X}_0$.

Let now

$$\widetilde{U}(x)^\top := \begin{bmatrix} I_r & 0 \\ -E_{21}(x)E_{11}(x)^{-1} & I_{m-r} \end{bmatrix} U_0^\top, \qquad \widetilde{V}(x) := V_0 \begin{bmatrix} I_r & -E_{11}(x)^{-1}E_{12}(x) \\ 0 & I_{n-r} \end{bmatrix},$$

so that

$$\widetilde{U}(x)^\top E(x) \widetilde{V}(x) = \begin{bmatrix} E_{11}(x) & 0 \\ 0 & E_{22}(x) - E_{21}(x)E_{11}(x)^{-1}E_{12}(x) \end{bmatrix}$$

for all $x \in \mathcal{X}_0$. Since $E_{11}(x) \in \mathbb{R}^{r,r}$ is invertible for all $x \in \mathcal{X}_0$ and the rank of E is constantly r, we deduce that actually

$$\widetilde{U}(x)^\top E(x) \widetilde{V}(x) = \begin{bmatrix} E_{11}(x) & 0 \\ 0 & 0 \end{bmatrix}$$

for all $x \in \mathcal{X}_0$. We note that $\widetilde{U}$ and $\widetilde{V}$ also have the same regularity as E.

It remains to show that $\widetilde{U}$ and $\widetilde{V}$ can be replaced by pointwise unitary matrix functions with the same regularity. Let $\widetilde{U}(x) = U(x)L_U(x)$ and $\widetilde{V}(x) = V(x)L_V(x)$ be the QL factorizations of $\widetilde{U}$ and $\widetilde{V}$, which can be computed for all $x \in \mathcal{X}_0$ with the Gram-Schmidt orthogonalization process, in particular U and V are pointwise unitary, and L_U and L_V are pointwise lower triangular with positive diagonal entries. Note that, due to the pointwise invertibility of $\widetilde{U}$ and $\widetilde{V}$, the construction of the Gram-Schmidt process ensures that U, V, L_U, L_V have the same regularity as $\widetilde{U}, \widetilde{V}$. Furthermore, since lower triangular matrices form a multiplicative group, we deduce that

$$U(x)^\top E(x) V(x) = L_U(x)^{-\top} \widetilde{U}(x)^\top E(x) \widetilde{V}(x) L_V(x)^{-1} = \begin{bmatrix} \widetilde{L}_{11}(x)^\top & \widetilde{L}_{21}(x)^\top \\ 0 & \widetilde{L}_{22}(x)^\top \end{bmatrix} \begin{bmatrix} E_{11}(x) & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} \widehat{L}_{11}(x) & \widehat{L}_{21}(x) \\ 0 & \widehat{L}_{22}(x) \end{bmatrix}$$

$$= \begin{bmatrix} \widetilde{L}_{11}(x)^\top E_{11}(x) \widehat{L}_{11}(x) & 0 \\ 0 & 0 \end{bmatrix},$$

where $\widetilde{L}(x) = L_U(x)^{-1}$ and $\widehat{L}(x) = L_V(x)^{-1}$ have again the same regularity as L_U and L_V, due to the same observations that we made for E_{11}. We conclude that U and V have all the requested properties. □

While Theorem 11 is quite powerful, unfortunately it cannot be directly applied to obtain system transformations that bring a descriptor matrix E into its semi-explicit form, since the matrix function V is not guaranteed to be the Jacobian of a diffeomorphism. However, this result is the first step in the direction of proving Theorem 8. The second step is to deduce the following corollary.

Corollary 4. *Let $E \in C(\mathcal{X}, \mathbb{R}^{m,n})$ with $\operatorname{rank}(E(x)) = r$ for all $x \in \mathcal{X}$. Then for every $x_0 \in \mathcal{X}$ there exist an open neighborhood $\mathcal{X}_0 \subseteq \mathcal{X}$ of x_0, a pointwise invertible matrix function $U \in C(\mathcal{X}_0, \mathbb{R}^{m,m})$, and a permutation matrix $\Pi \in \mathbb{R}^{n,n}$, such that*

$$U^\top E \Pi = \begin{bmatrix} I_r & E_{12} \\ 0 & 0 \end{bmatrix}, \tag{F.2}$$

with $E_{12} \in C(\mathcal{X}_0, \mathbb{R}^{r,n-r})$. Furthermore, if the entries of E are analytic or C^ℓ for some $\ell \in \mathbb{N}_0 \cup \{\infty\}$, then U and E_{12} can be chosen to have that same regularity.

Proof. Because of Theorem 11, for every $x_0 \in \mathcal{X}$ there exist an open neighborhood $\mathcal{X}_0 \subseteq \mathcal{X}$ of x_0, pointwise unitary $\widetilde{U}, \widetilde{V}$, and a pointwise invertible $\Sigma \in C(\mathcal{X}_0, \mathbb{R}^{r,r})$, such that $\widetilde{U}, \widetilde{V}, \Sigma$ have the same regularity as E, and

$$\widetilde{U}^\top E \widetilde{V} = \begin{bmatrix} \Sigma & 0 \\ 0 & 0 \end{bmatrix}.$$

In particular,

$$\widetilde{U}^\top E = \begin{bmatrix} \Sigma & 0 \\ 0 & 0 \end{bmatrix} \widetilde{V}^\top = \begin{bmatrix} \widetilde{E}_{11} & \widetilde{E}_{12} \\ 0 & 0 \end{bmatrix}.$$

Since $\operatorname{rank}(U^\top E(x_0)) = \operatorname{rank}(E(x_0)) = r$, there is a permutation matrix $\Pi \in \mathbb{R}^{n,n}$ such that

$$\widetilde{U}^\top E \Pi = \begin{bmatrix} \widehat{E}_{11} & \widehat{E}_{12} \\ 0 & 0 \end{bmatrix},$$

with $\widehat{E}_{11}(x_0)$ invertible. Since $\widehat{E}_{11}$ is continuous, up to further restricting the open neighborhood $\mathcal{X}_0$, we obtain that $\widehat{E}_{11}$ is invertible in $\mathcal{X}_0$. Then, by choosing

$$U = \widetilde{U} \begin{bmatrix} \widehat{E}_{11}^{-\top} & 0 \\ 0 & I_{n-r} \end{bmatrix},$$

we obtain that

$$U^\top E \Pi = \begin{bmatrix} \widehat{E}_{11}^{-1} & 0 \\ 0 & I_{n-r} \end{bmatrix} \widetilde{U}^\top E \Pi = \begin{bmatrix} I_r & E_{12} \\ 0 & 0 \end{bmatrix}$$

for $E_{12} = \widehat{E}_{11}^{-1} \widehat{E}_{12}$. Finally, $\widetilde{E}$ and E_{12} have the same regularity as E, by construction. □

One advantage of Lemma 4 over Theorem 11 is that Π can be interpreted as the Jacobian of a diffeomorphism, in fact $\Pi = \mathrm{D}\sigma$ with $\sigma(x) = \Pi x$. We can now proceed with the proof of Theorem 8.

Proof of Theorem 8. Let us fix $x_0 \in \mathcal{X}$, and let us choose $\mathcal{X}_0$, U, Π, E_{12} as in Lemma 4. Then, up to applying the invertible system transformation (σ, U) with $\sigma(x) = \Pi x$ to E, we assume without loss of generality that

$$E = \begin{bmatrix} I_r & E_{12} \\ 0 & 0 \end{bmatrix},$$

where $E_{12} \in C(\mathcal{X}, \mathbb{R}^{r,n-r})$ is a matrix function with analytic entries. Consider now the linear first order PDE system

$$\nabla_{x_2} v(x) = E_{12}(x)^\top \nabla_{x_1} v(x), \tag{F.3}$$

and let $f_1, \dots, f_p \in C^1(\mathcal{X}, \mathbb{R})$ be functionally independent functions that generate the solutions of (F.3), i.e., such that $\nabla f_1, \dots, \nabla f_p$ are (pointwise) linearly independent, and that the solutions of (F.3) are the functions of the form $v(x) = V(f_1(x), \dots, f_p(x))$ for any $V \in C^1(\mathbb{R}^k, \mathbb{R})$. For the existence of such set of solutions for E_{12} with analytic entries, see e.g. [62,63].

Let us now define $\psi_1 = (f_1, \dots, f_p) \in C^1(\mathcal{X}, \mathbb{R}^p)$. In particular, we have that $\mathrm{D}_{x_2}\psi_1 = (\mathrm{D}_{x_1}\psi_1)E_{12}$. Let us now complete $f_1, \dots, f_p$ to a maximal set of functionally independent functions $f_1, \dots, f_n \in C^1(\mathcal{X}, \mathbb{R})$, which can be done locally e.g. by selecting an appropriate subset of $x_1, \dots, x_n$, and let

$$\psi = (f_1, \dots, f_n) = (\psi_1, f_{p+1}, \dots, f_n) \in C^1(\mathcal{X}, \mathbb{R}^n)$$

be the corresponding local diffeomorphism. In particular, up to further restricting the open neighborhood $\mathcal{X}_0$ of x_0, we assume that $\psi : \mathcal{X}_0 \to \psi(\mathcal{X}_0)$ is a diffeomorphism. Let then $\widetilde{\mathcal{X}}_0 = \psi(\mathcal{X}_0)$ and let $\varphi = \psi^{-1} \in C^1(\widetilde{\mathcal{X}}_0, \mathcal{X}_0)$ denote the inverse diffeomorphism.

Note that, since the original Hamiltonian $\mathcal{H}$ is also a solution of (F.3), it must be of the form $\mathcal{H} = \widetilde{\mathcal{H}}_1 \circ \psi_1$ for some $\widetilde{\mathcal{H}}_1 \in C^1(\pi_1(\widetilde{\mathcal{X}}_0), \mathbb{R})$, where $\pi_1 : \mathbb{R}^n \to \mathbb{R}^p$ denotes the projection onto the first p coordinates. Furthermore, it holds that

$$\mathrm{D}\psi \begin{bmatrix} I_r & E_{12} \\ 0 & 0 \end{bmatrix} (\mathrm{D}\varphi \circ \psi) = \begin{bmatrix} \mathrm{D}_{x_1}\psi_1 & (\mathrm{D}_{x_1}\psi_1)E_{12} \\ \star & \star \end{bmatrix} (\mathrm{D}\psi)^{-1} = \begin{bmatrix} \mathrm{D}\psi_1 \\ \star \end{bmatrix} (\mathrm{D}\psi)^{-1} = \begin{bmatrix} I_p & 0 \\ \star & \star \end{bmatrix}.$$

Then, up to applying the invertible system transformation $(\varphi, (\mathrm{D}\psi \circ \varphi))$, we assume without loss of generality that E is of the form

$$E(x) = \begin{bmatrix} I_p & 0 \\ E_{12}(x) & E_{22}(x) \end{bmatrix}.$$

and that $\mathcal{H}$ only depends on the first block component of the state, which allows to introduce $\mathcal{H}_1 \in C^1(\pi_1(\mathcal{X}_0), \mathbb{R})$ as in Lemma 1.

With subsequent left multiplications and right permutations (and therefore system transformations of the form (σ, U) with $\sigma(x) = \Pi x$), we further bring E to the form

$$E(x) = \begin{bmatrix} I_p & 0 & 0 \\ 0 & 0 & 0 \\ 0 & E_{32}(x) & E_{33}(x) \end{bmatrix},$$

where $E_{32} \in C(\mathcal{X}_0, \mathbb{R}^{r-p,n-r})$ and $E_{33} \in C(\mathcal{X}_0, \mathbb{R}^{r-p,r-p})$, with $E_{33}(x_0)$ invertible. In particular, up to restricting $\mathcal{X}_0$ to an open neighborhood of x_0 where E_{33} is pointwise invertible, and applying an appropriate left multiplication with its inverse, we can assume without loss of generality that E is of the form

$$E(x) = \begin{bmatrix} I_p & 0 & 0 \\ 0 & 0 & 0 \\ 0 & E_{32}(x) & I_{r-p} \end{bmatrix}.$$

Let us partition $x = (x_1, x_2, x_3) \in \mathbb{R}^p \times \mathbb{R}^{n-r} \times \mathbb{R}^{r-p}$ and $z = (z_1, z_2, z_3) \in \mathbb{R}^p \times \mathbb{R}^{n-r} \times \mathbb{R}^{r-p}$. The gradient pair property $E^\top z = \nabla \mathcal{H}$ then implies

$$\begin{bmatrix} z_1 \\ E_{32}^\top z_3 \\ z_3 \end{bmatrix} = \begin{bmatrix} I_p & 0 & 0 \\ 0 & 0 & E_{32}^\top \\ 0 & 0 & I_{r-p} \end{bmatrix} \begin{bmatrix} z_1 \\ z_2 \\ z_3 \end{bmatrix} = E^\top z = \nabla \mathcal{H} = \begin{bmatrix} \nabla \mathcal{H}_1 \circ \pi_1 \\ 0 \\ 0 \end{bmatrix},$$

i.e., $z_1 = \nabla \mathcal{H}_1 \circ \pi_1$ and $z_3 = 0$.

References

[1] V. Duindam, A. Macchelli, S. Stramigioli, H. Bruyninckx, Modeling and Control of Complex Physical Systems: The Port-Hamiltonian Approach, Springer Berlin Heidelberg, 2009. https://doi.org/10.1007/978-3-642-03196-0

[2] A. van der Schaft, D. Jeltsema, Port-Hamiltonian systems theory: an introductory overview, Found. Trends Syst. Control 1 (2–3) (2014) 173–378. https://doi.org/10.1561/2600000002

[3] C. Beattie, V. Mehrmann, H. Xu, H. Zwart, Linear port-Hamiltonian descriptor systems, Math. Control Signals Syst. 30 (2018) 1–27. https://doi.org/10.1007/s00498-018-0223-3

[4] V. Mehrmann, R. Morandin, Structure-preserving discretization for port-Hamiltonian descriptor systems, in: 2019 IEEE 58th Conference on Decision and Control (CDC), IEEE, 2019, pp. 6863–6868. https://doi.org/10.1109/CDC40024.2019.9030180

[5] A. van der Schaft, Port-Hamiltonian differential-algebraic systems, in: A. Ilchmann, T. Reis (Eds.), Surveys in Differential-Algebraic Equations I, Springer Berlin Heidelberg, Berlin, Heidelberg, 2013, pp. 173–226. https://doi.org/10.1007/978-3-642-34928-7_5

[6] A. van der Schaft, B. Maschke, Dirac and Lagrange algebraic constraints in nonlinear port-Hamiltonian systems, Vietnam J. Math. 48 (2020) 929–939. https://doi.org/10.1007/s10013-020-00419-x

[7] A. van der Schaft, B. Maschke, Generalized port-Hamiltonian DAE systems, Syst. Control Lett. 121 (2018) 31–37. https://doi.org/10.1016/j.sysconle.2018.09.008

[8] E. Hairer, C. Lubich, G. Wanner, Geometric Numerical Integration, Springer, Berlin, Berlin, 2006. https://doi.org/10.1007/3-540-30666-8

[9] M.W. Hirsch, S. Smale, Differential Equations, Dynamical Systems, and Linear Algebra, Academic Press, New York, NY, USA, New York, NY, USA, 1974.

[10] V.I. Arnold, Mathematical Methods of Classical Mechanics, Springer, New York, 2nd edition edition, New York, 1989. https://doi.org/10.1007/978-1-4757-2063-1

[11] O. Gonzalez, Mechanical systems subject to holonomic constraints: differential–algebraic formulations and conservative integration, Physica D 132 (1–2) (1999) 165–174. https://doi.org/10.1016/S0167-2789(99)00054-8

[12] O. Gonzalez, Exact energy and momentum conserving algorithms for general models in nonlinear elasticity, Comput. Methods Appl. Mech. Eng. 190 (13–14) (2000) 1763–1783. https://doi.org/10.1016/s0045-7825(00)00189-4

[13] J.C. Simo, N. Tarnow, The discrete energy-momentum method. Conserving algorithms for nonlinear elastodynamics, J. Appl. Math. Phys. (ZAMP) 43 (5) (1992) 757–792. https://doi.org/10.1007/bf00913408

[14] P. Betsch (Ed.), Structure-Preserving Integrators in Nonlinear Structural Dynamics and Flexible Multibody Dynamics, 565 of *CISM International Centre for Mechanical Sciences*, Springer International Publishing, Cham, Cham, 2016. https://doi.org/10.1007/978-3-319-31879-0

[15] P.L. Kinon, P. Betsch, S. Schneider, Structure-preserving integrators based on a new variational principle for constrained mechanical systems, Nonlinear Dyn. 111 (2023) 14231–14261. https://doi.org/10.1007/s11071-023-08522-7

[16] J.E. Marsden, M. West, Discrete mechanics and variational integrators, Acta Numer. 10 (2001) 357–514. https://doi.org/10.1017/S096249290100006X

[17] S. Leyendecker, J.E. Marsden, M. Ortiz, et al., Variational integrators for constrained dynamical systems, ZAMM (J. Appl. Math. Mech.) 88 (9) (2008) 677–708. https://doi.org/10.1002/zamm.200700173

[18] B.J. Leimkuhler, R.D. Skeel, Symplectic numerical integrators in constrained Hamiltonian systems, J. Comput. Phys. 112 (1) (1994) 117–125. https://doi.org/10.1006/jcph.1994.1085

[19] M. May, P. Betsch, Galerkin-based time integration approaches to rigid body dynamics in terms of unit quaternions, 2025. PREPRINT available at Research Square. https://doi.org/10.21203/rs.3.rs-6354821/v1

[20] P. Betsch, P. Steinmann, Conservation properties of a time FE method. Part I: time-stepping schemes for N-body problems, Int. J. Numer. Methods Eng. 49 (5) (2000) 599–638. https://doi.org/10.1002/1097-0207(20001020)49:5<599::AID-NME960>3.0.CO;2-9

[21] P. Betsch, P. Steinmann, Conservation properties of a time FE method — part II: Time-stepping schemes for non-linear elastodynamics, Int. J. Numer. Methods Eng. 50 (8) (2001) 1931–1955. https://doi.org/10.1002/nme.103

[22] P. Betsch, P. Steinmann, Conservation properties of a time FE method — part III: Mechanical systems with holonomic constraints, Int. J. Numer. Methods Eng. 53 (10) (2002) 2271–2304. https://doi.org/10.1002/nme.347
[23] H. Egger, O. Habrich, V. Shashkov, On the energy stable approximation of Hamiltonian and gradient systems, Comput. Methods Appl. Math. 21 (2) (2021) 335–349. https://doi.org/10.1515/cmam-2020-0025
[24] A. Jüngel, U. Stefanelli, L. Trussardi, Two structure-preserving time discretizations for gradient flows, Appl. Math. Optim. 80 (2019) 733–764. https://doi.org/10.1007/s00245-019-09605-x
[25] P. Kunkel, V. Mehrmann, Discretization of inherent ODEs and the geometric integration of DAEs with symmetries, BIT Numer. Math. 63 (2023) 29. https://doi.org/10.1007/s10543-023-00966-y
[26] H.C. Öttinger, GENERIC Integrators: structure preserving time integration for thermodynamic systems, J. Non-Equilib. Thermodyn. 43 (2) (2018) 89–100. https://doi.org/10.1515/jnet-2017-0034
[27] A.A. Simoes, D.M. de Diego, B. Maschke, Discrete gradient methods for irreversible port-Hamiltonian systems, 2023. arXiv:2303.08034, https://doi.org/10.48550/arXiv.2303.08034
[28] P. Kotyczka, L. Lefèvre, Discrete-time port-Hamiltonian systems: a definition based on symplectic integration, Syst. Control Lett. 133 (2019) 104530. https://doi.org/10.1016/j.sysconle.2019.104530
[29] J. Giesselmann, A. Karsai, T. Tscherpel, Energy-consistent Petrov-Galerkin time discretization of port-Hamiltonian systems, 2024. arXiv:2404.12480, https://doi.org/10.48550/arXiv.2404.12480
[30] A. Bartel, M. Diab, A. Frommer, M. Günther, Operator splitting for semi-explicit differential-algebraic equations and port-Hamiltonian DAEs, 2023. arXiv:2308.16736, https://doi.org/10.48550/arXiv.2308.16736
[31] A. Bartel, M. Diab, A. Frommer, M. Günther, N. Marheineke, Splitting techniques for DAEs with port-Hamiltonian applications, Appl. Numer. Math. 214 (2025) 28–53. https://doi.org/10.1016/j.apnum.2025.03.004
[32] M. Mönch, N. Marheineke, Commutator-based operator splitting for linear port-Hamiltonian systems, Appl. Numer. Math. 210 (2025) 25–38. https://doi.org/10.1016/j.apnum.2024.12.007
[33] A. Bartel, M. Schaller, Goal-oriented time adaptivity for port-Hamiltonian systems, J. Comput. Appl. Math. 461 (2025) 116450. https://doi.org/10.1016/j.cam.2024.116450
[34] S. Eidnes, Order theory for discrete gradient methods, BIT Numer. Math. 62 (4) (2022) 1207–1255. https://doi.org/10.1007/s10543-022-00909-z
[35] S. Sato, Linear gradient structures and discrete gradient methods for conservative/dissipative differential-algebraic equations, BIT Numer. Math. 59 (4) (2019) 1063–1091. https://doi.org/10.1007/s10543-019-00759-2
[36] S. Aoues, M. di Loreto, D. Eberard, W. Marquis-Favre, Hamiltonian systems discrete-time approximation: losslessness, passivity and composability, Syst. Control Lett. 110 (2017) 9–14. https://doi.org/10.1016/j.sysconle.2017.10.003
[37] A. Falaize, T. Hélie, Passive guaranteed simulation of analog audio circuits: a port-Hamiltonian approach, Appl. Sci. 6 (10) (2016) 273. https://doi.org/10.3390/app6100273
[38] L. Gören-Sümer, Y. Yalçín, Gradient based discrete-time modeling and control of Hamiltonian systems, IFAC Proc. Vol. 41 (2) (2008) 212–217. https://doi.org/10.3182/20080706-5-kr-1001.00036
[39] E. Celledoni, E.H. Høiseth, Energy-preserving and passivity-consistent numerical discretization of port-Hamiltonian systems, 2017. arXiv:1706.08621, https://doi.org/10.48550/arXiv.1706.08621
[40] A. Frommer, M. Günther, B. Liljegren-Sailer, N. Marheineke, Operator splitting for port-Hamiltonian systems, 2023. arXiv:2304.01766, https://doi.org/10.48550/arXiv.2304.01766
[41] P.L. Kinon, T. Thoma, P. Betsch, P. Kotyczka, Discrete nonlinear elastodynamics in a port-Hamiltonian framework, PAMM (Proc. Appl. Math. Mech.) 23 (3) (2023) e202300144. https://doi.org/10.1002/pamm.202300144
[42] A. Moreschini, M. Mattioni, S. Monaco, D. Normand-Cyrot, et al., Discrete port-controlled Hamiltonian dynamics and average passivation, in: Proceedings of the 58th IEEE Conference on Decision and Control, Nice, France, 2019, pp. 1430–1435. https://doi.org/10.1109/CDC40024.2019.9029809
[43] P. Schulze, Structure-preserving time discretization of port-Hamiltonian systems via discrete gradient pairs, 2023. arXiv:2311.00403, https://doi.org/10.48550/arXiv.2311.00403
[44] P.J. Rabier, W.C. Rheinboldt, On impasse points of quasilinear differential-algebraic equations, J. Math. Anal. Appl. 181 (2) (1994) 429–454. https://doi.org/10.1006/jmaa.1994.1033
[45] A. Steinbrecher, Numerical Solution of Quasi-Linear Differential-Algebraic Equations and Industrial Simulation of Multibody Systems, Ph.D. thesis, Technische Universität Berlin, 2006. https://doi.org/10.14279/depositonce-1360
[46] P. Kunkel, V. Mehrmann, Differential-Algebraic Equations: Analysis and Numerical Solution, EMS Textbooks in Mathematics, European Mathematical Society Publ. House, Zürich, Zürich, 2006. https://doi.org/10.4171/017
[47] V. Mehrmann, B. Unger, Control of port-Hamiltonian differential-algebraic systems and applications, Acta Numer. 32 (2023) 395–515. https://doi.org/10.1017/S0962492922000083
[48] R. Morandin, Modeling and Numerical Treatment of Port-Hamiltonian Descriptor Systems, Ph.D. thesis, TU Berlin, 2023. https://doi.org/10.14279/depositonce-19826
[49] A. Moreschini, S. Monaco, D. Normand-Cyrot, Dirac structures for a class of port-Hamiltonian systems in discrete time, IEEE Trans. Automat. Contr. 69 (3) (2024) 1999–2006. https://doi.org/10.1109/TAC.2023.3313327
[50] R.I. McLachlan, G.R.W. Quispel, N. Robidoux, Geometric integration using discrete gradients, Phil. Trans. R. Soc. A 357 (1754) (1999) 1021–1045. https://doi.org/10.1098/rsta.1999.0363
[51] O. Gonzalez, et al., Time integration and discrete Hamiltonian systems, J. Nonlinear Sci. 6 (5) (1996) 449–467. https://doi.org/10.1007/BF02440162
[52] P. Kundur, Power System Stability and Control, The EPRI Power System Engineering Series, McGraw-Hill, New York, New York, 1994.
[53] S. Fiaz, D. Zonetti, R. Ortega, J.M.A. Scherpen, A. van der Schaft, A port-Hamiltonian approach to power network modeling and analysis, Eur. J. Control 19 (6) (2013) 477–485. https://doi.org/10.1016/j.ejcon.2013.09.002
[54] P.L. Kinon, T. Thoma, P. Betsch, P. Kotyczka, Port-Hamiltonian formulation and structure-preserving discretization of hyperelastic strings, in: Proceedings of the 11th ECCOMAS Thematic Conference on Multibody Dynamics, Lisbon, Portugal, 2023, pp. 1–10. https://doi.org/10.48550/arXiv.2304.10957
[55] P.L. Kinon, T. Thoma, P. Betsch, P. Kotyczka, Generalized Maxwell viscoelasticity for geometrically exact strings: nonlinear port-Hamiltonian formulation and structure-preserving discretization, IFAC-PapersOnLine 58 (6) (2024) 101–106. https://doi.org/10.1016/j.ifacol.2024.08.264
[56] F.E. Udwadia, P. Phohomsiri, Explicit equations of motion for constrained mechanical systems with singular mass matrices and applications to multi-body dynamics, Proc. R. Soc. A 462 (2071) (2006) 2097–2117. https://doi.org/10.1098/rspa.2006.1662
[57] P.L. Kinon, P. Betsch, Conserving integration of multibody systems with singular and non-constant mass matrix including quaternion-based rigid body dynamics, Multibody Sys. Dyn. 63 (1) (2024) 303–340. https://doi.org/10.1007/s11044-024-10001-9
[58] D.D. Holm, T. Schmah, C. Stoica, Geometric Mechanics and Symmetry: From Finite to Infinite Dimensions, Oxford University Press, New York, New York, 2009. https://doi.org/10.1093/oso/9780199212903.001.0001
[59] P.L. Kinon, GitHub repository: plkinon/phdae_discrete_gradients: v1.0.0, 2026, https://doi.org/10.5281/zenodo.15007241
[60] O. Gonzalez, J.C. Simo, On the stability of symplectic and energy-momentum algorithms for non-linear Hamiltonian systems with symmetry, Comput. Methods Appl. Mech. Eng. 134 (3–4) (1996) 197–222. https://doi.org/10.1016/0045-7825(96)01009-2
[61] P.L. Kinon, J.K. Bauer, GitHub repository: pydykit/pydykit: v0.0.6, 2025, https://doi.org/10.5281/zenodo.14849865
[62] J. Jonasson, Systems of Linear First Order Partial Differential Equations Admitting a Bilinear Multiplication of Solutions, Ph.D. thesis, Linköping University, Sweden, 2007.
[63] É. Goursat, A Course in Mathematical Analysis. Vol. 2, Pt. 2: Differential Equations, Dover, 1959.