ON PROPERTIES OF ADJOINT SYSTEMS FOR EVOLUTIONARY PDES

BRIAN K. TRAN[†], BEN S. SOUTHWORTH[†], AND MELVIN LEOK[‡]

Abstract. We investigate the geometric structure of adjoint systems associated with evolutionary partial differential equations at the fully continuous, semi-discrete, and fully discrete levels and the relations between these levels. We show that the adjoint system associated with an evolutionary partial differential equation has an infinite-dimensional Hamiltonian structure, which is useful for connecting the fully continuous, semi-discrete, and fully discrete levels. We subsequently address the question of discretize-then-optimize versus optimize-then-discrete for both semi-discretization and time integration, by characterizing the commutativity of discretize-then-optimize methods versus optimize-then-discretize methods uniquely in terms of an adjoint-variational quadratic conservation law. For Galerkin semi-discretizations and one-step time integration methods in particular, we explicitly construct these commuting methods by using structure-preserving discretization techniques.

Contents

[†]Los Alamos National Laboratory, Theoretical Division, Los Alamos, New Mexico 87545
[‡]UC San Diego, Department of Mathematics, La Jolla, CA 92093
E-mail addresses: btran@lanl.gov, southworth@lanl.gov, mleok@ucsd.edu.

1. Introduction

In this paper, we investigate adjoint systems associated with evolution equations on infinite-dimensional Banach spaces, at the fully continuous, semi-discrete, and fully discrete levels, with the aim of addressing theoretical and practical questions in the optimization and optimal control of evolutionary partial differential equations (PDEs).

The solution of many nonlinear optimization and optimal control problems involves successive linearization, and as such variational equations and their adjoints play a critical role in a variety of applications. Adjoint equations are of particular interest when the parameter space is significantly higher dimension than that of the output or objective. In particular, the simulation of adjoint equations arise in sensitivity analysis [6; 7], adaptive mesh refinement [28], uncertainty quantification [51], automatic differentiation [18], superconvergent functional recovery [38], optimal control [41], optimal design [16], optimal estimation [34], and deep learning viewed as an optimal control problem [3].

The study of geometric aspects of adjoint systems arose from the observation that the combination of any system of differential equations and its adjoint equations are described by a formal Lagrangian [24; 25]. This naturally leads to the question of when the formation of adjoints and discretization commutes [47], and prior work on this include the Ross–Fahroo lemma [42], and the observation by Sanz-Serna [46] that the adjoints and discretization commute if and only if the discretization is symplectic, in the specific setting of Runge–Kutta methods. Recently, in [49], we investigate the symplectic and presymplectic structures for adjoint systems associated with ordinary differential equations (ODEs) and differential-algebraic equations (DAEs), respectively, and show that the processes of adjoining, discretization, and reduction (for index 1 DAE) commute with appropriate choices of these processes.

In this paper, we extend these previous studies of discretizing adjoint systems by considering evolutionary PDEs and their associated adjoint systems, at the fully continuous, semi-discrete (i.e. discretized in space), and fully discrete levels, and investigate the connections between them. In particular, we utilize techniques from symplectic geometry to provide a precise geometric characterization of when semi-discretization, time integration, and adjoining commute.

1.1. Discretize-then-Optimize versus Optimize-then-Discretize.

There is a vast literature on solving optimization and optimal control problems for differential equations via adjoint methods; we will not provide an exhaustive list but refer the reader to the following references and the references therein. Studies of adjoint systems for ODEs and DAEs are performed in [7; 12; 46; 49], in the context of optimal control in [13; 41; 50], and in the context of neural networks in [9; 15; 31]. For PDEs, adjoint methods for time-dependent PDEs with adaptive mesh refinement is studied in [27], adjoints for specific PDE systems are studied in [26; 35; 39; 43], and *a posteriori* analysis of adjoint systems is reviewed in [17].

One of the major conceptual questions is when to use discretize-then-optimize (DtO) methods versus optimize-then-discretize (OtD) methods and, in particular, what are the discrepancies between the two approaches. It is known that these two different approaches, in general, do not commute, and can lead to different discrete gradients of objective functions.

For ODEs, it is known that DtO recovers the exact discrete gradients, whereas OtD may not (see, for example, [15; 46]). This leads to the result that DtO methods produce gradients that are independent of the error of the forward method [36], and thus produce proper descent directions for discrete objective functions. On the other hand, the exact discrete gradient produced from DtO is not always *adjoint consistent*, i.e., a consistent approximation of the time-continuous gradient, see, for example, [1].

Extending the discussion to PDEs, one also must include the process of spatial discretization which can lead to further discrepancies in DtO and OtD [27; 35]. For Galerkin or Galerkin-like methods (e.g., discontinuous Galerkin methods), there is a similar issue of adjoint consistency for DtO methods [2; 20; 21].

One of the main goals of this paper is to provide a geometric characterization of the discrepancy between DtO versus OtD methods, both for semi-discretization and time integration.

1.2. **Main Results.** In this paper, we perform a systematic study of adjoint systems associated with evolution equations on infinite dimensional Banach spaces at the fully continuous, semi-discrete, and fully discrete levels, and of the relations amongst these levels. Vital to our analysis will be the construction of the infinite-dimensional Hamiltonian structure associated with adjoint systems for evolution equations, which will pave the way to a geometric characterization of the relations between these levels.

In Section 2, we investigate the fully continuous adjoint system associated with semilinear evolution equations. First, in Section 2.2, we recall some basic facts about semilinear evolution equations, their semigroups and associated adjoint semigroups, and in Section 2.3 we review infinite-dimensional Hamiltonian systems. In Section 2.4, we define adjoint systems associated with evolution equations and equip such systems with an infinite-dimensional Hamiltonian structure. We discuss existence and uniqueness of solutions for these systems with Type II boundary conditions, specifying initial conditions for the forward variable and terminal conditions for the adjoint variable and we further show that the adjoint system obeys an adjoint-variational quadratic conservation law given in Proposition 2.1, which is fundamental to adjoint sensitivity analysis.

In Section 3, we explore the discretization of adjoint systems for evolutionary PDEs, both at the semi-discrete and fully discrete levels. In Section 3.1, we study *method-of-lines* semi-discretizations of adjoint systems. In particular, we show that associated with a method-of-lines semi-discretization of the evolution equation, there is an associated dual semi-discretization of the adjoint system such that semi-discretization and adjoining commute (Theorems 3.1 and 3.2). We show how this implies that in order for semi-discretize-then-optimize and optimize-then-semi-discretize to commute, the optimize-then-semi-discretize method must preserve the Hamiltonian structure. We further characterize the associated dual semi-discretization as the unique semi-discretization of the adjoint system which satisfies a semi-discrete analogue of the adjoint-variational quadratic conservation law in Theorem 3.2.

In Section 3.2, we turn our attention to time integration of adjoint systems associated with ODEs via one-step methods. In particular, we show that time integration via one-step methods and adjoining commute precisely when the one-step method for the adjoint system is the cotangent lift of the one-step method for the forward equation (Theorem 3.3). This generalizes the result of [46], where it is shown that time integration via partitioned Runge–Kutta methods and adjoining commute if and only if the method is symplectic; namely, we generalize this result to the class of all one-step methods. In Theorem 3.3, we additionally characterize the cotangent lift of a one-step method as the unique one-step method which covers the forward one-step method and satisfies the discrete adjoint-variational quadratic conservation law. This addresses the question of DtO versus OtD for time integration via one-step methods: an OtD scheme which does not use the cotangent lifted method cannot satisfy the adjoint quadratic conservation law and hence, can lead to the observed defect in the exact discrete gradient of such methods as discussed in Section 1.1. We furthermore show in Proposition 3.3 that the cotangent lifted method is adjoint consistent provided that the underlying one-step method is *variationally equivariant*, which informally is the property that taking variations and discretizing by the one-step method commute.

Finally, in Section 3.3, we combine the previous results for semi-discretization and time integration to discuss the natural relations between the fully continuous, semi-discrete, and fully discrete levels of the adjoint system associated with evolution equations.

2. Adjoint Systems for Evolutionary PDEs

In this section, we investigate adjoint systems associated with semilinear evolution equations and in particular, utilize techniques from infinite-dimensional symplectic geometry [10] to equip such systems with a symplectic structure. This structure will be useful for our investigation of semi-discretization and time integration of these systems. It should be noted that much of our discussion can be applied, at least formally, to more general nonlinear evolution equations, although analytic issues such as existence and uniqueness would be problem dependent. Throughout the paper, we will assume that X is a real reflexive Banach space, $\langle \cdot, \cdot \rangle$ will denote the duality pairing between X^* and X, and B^* will denote the adjoint of an operator B with respect to this duality pairing. We start by recalling some basic facts about adjoint systems in the finite-dimensional (ODE) setting.

2.1. Geometry of Finite-Dimensional Adjoint Systems.

In [49], we provide a systematic study of the geometry of adjoint systems associated with ODEs and DAEs, utilizing tools from symplectic and presymplectic geometry, respectively. This paper extends the results of [49] to the infinite-dimensional setting, where we will consider adjoint systems associated with evolution equations on a Banach space. As a primer, it will be useful to recall some facts on the geometry of adjoint systems in the finite-dimensional setting (for more details, see [49]).

Let M be a finite-dimensional manifold and consider the ODE on M given by

$$\dot{q} = f(q), \tag{2.1}$$

where f is a vector field on M. Letting $\pi : TM \to M$ denote the tangent bundle projection, we recall that a vector field f is a map $f : M \to TM$ which satisfies $\pi \circ f = \mathbf{1}_M$, i.e., f is a section of the tangent bundle.

Consider the Hamiltonian $H : T^*M \to \mathbb{R}$ given by $H(q,p) = \langle p, f(q) \rangle_q$ where $\langle \cdot, \cdot \rangle_q$ is the duality pairing of T_q^*M with T_qM. Recall that the cotangent bundle T^*M possesses a canonical symplectic form $\Omega = -d\Theta$ where Θ is the tautological one-form on T^*M. With coordinates $(q,p) = (q^A, p_A)$ on T^*M, this symplectic form has the coordinate expression $\Omega = dq \wedge dp \equiv dq^A \wedge dp_A$.

We define the adjoint system as the ODE on T^*M given by Hamilton's equations, with the above choice of Hamiltonian H and the canonical symplectic form. Thus, the adjoint system is given by the equation

$$i_{X_H}\Omega = dH,$$

whose solution curves on T^*M are the integral curves of the Hamiltonian vector field X_H. As is well-known, for the particular choice of Hamiltonian $H(q,p) = \langle p, f(q) \rangle_q$, the Hamiltonian vector field X_H is given by the cotangent lift $\widehat{f}$ of f, which is a vector field on T^*M that covers f (for a discussion of the geometry of the cotangent bundle and lifts, see [29; 52]). With coordinates $z = (q,p)$ on T^*M, the adjoint system is the ODE on T^*M given by

$$\dot{z} = \widehat{f}(z). \tag{2.2}$$

To be more explicit, recall that the cotangent lift of f is constructed as follows. Let $\Phi_\epsilon : M \to M$ denote the time-ϵ flow map of f, which generates a one-parameter family of diffeomorphisms. Then, we consider the cotangent lifted diffeomorphisms given by $T^*\Phi_{-\epsilon} : T^*M \to T^*M$. This covers Φ_ϵ

in the sense that $\pi_{T^*M} \circ T^*\Phi_{-\epsilon} = \Phi_\epsilon \circ \pi_{T^*M}$ where $\pi_{T^*M} : T^*M \to M$ is the cotangent bundle projection. The cotangent lift $\widehat{f}$ is then defined to be the infinitesimal generator of the cotangent lifted flow,

$$\widehat{f}(z) = \frac{d}{d\epsilon}\Big|_{\epsilon=0} T^*\Phi_{-\epsilon}(z).$$

We can directly verify that $\widehat{f}$ is the Hamiltonian vector field for H, which follows from

$$i_{\widehat{f}}\Omega = -i_{\widehat{f}}d\Theta = -\mathcal{L}_{\widehat{f}}\Theta + d(i_{\widehat{f}}\Theta) = d(i_{\widehat{f}}\Theta) = dH,$$

where $\mathcal{L}_{\hat{f}}\Theta = 0$ follows from the fact that cotangent lifted flows preserve the tautological one-form and $H = i_{\widehat{f}}\Theta$ follows from a direct computation, where $i_{\widehat{f}}\Theta$ is interpreted as a function on the cotangent bundle which maps (q, p) to $\langle \Theta(q, p), \widehat{f}(q, p)\rangle_q$.

The adjoint system (2.2) covers (2.1) in the following sense.

Proposition (Proposition 2.2 of [49])**.** *Integral curves to the adjoint system* (2.2) *lift integral curves to the system* (2.1)*.*

In coordinates, the adjoint system has the form

$$\begin{aligned}\dot{q} &= f(q),\\ \dot{p} &= -[Df(q)]^*p.\end{aligned}$$

We will often to refer to the variable q as the forward variable and $\dot{q} = f(q)$ as the forward or base equation; we refer to p as the adjoint variable and $\dot{p} = -[Df(q)]^*p$ as the adjoint equation. We refer to both equations together as the adjoint system.

The adjoint system possesses a quadratic invariant associated with the variational equations of (2.1). The variational equation is given by considering the tangent lifted vector field on TM, $\widetilde{f} : TM \to TTM$, which is defined in terms of the flow Φ_ϵ generated by f by

$$\widetilde{f}(q, \delta q) = \frac{d}{d\epsilon}\Big|_{\epsilon=0} T\Phi_\epsilon(q, \delta q),$$

where $(q, \delta q)$ are coordinates on TM. That is, $\widetilde{f}$ is the infinitesimal generator of the tangent lifted flow. The variational equation associated with (2.1) is the ODE associated with the tangent lifted vector field. In coordinates,

$$\frac{d}{dt}(q, \delta q) = \widetilde{f}(q, \delta q). \tag{2.3}$$

Proposition (Proposition 2.3 of [49])**.** *For integral curves* (q, p) *of* (2.2) *and* $(q, \delta q)$ *of* (2.3)*, which cover the same curve* q*,*

$$\frac{d}{dt}\Big\langle p(t), \delta q(t)\Big\rangle_{q(t)} = 0. \tag{2.4}$$

This quadratic invariant is the key to adjoint sensitivity analysis [46] and its invariance is a consequence of symplecticity of the Hamiltonian flow [49].

In moving to the infinite-dimensional setting, we will develop the infinite-dimensional Hamiltonian structure of adjoint systems associated with evolution equations. We will further investigate the reduction of this structure under semi-discretization and its preservation under geometric time integration. As a result, this will allow us to geometrically characterize the discrepancy between DtO and OtD methods.

2.2. **Semilinear Evolutionary PDEs.** We recall some facts about abstract semilinear evolution equations of the following form. Let $A : \mathfrak{D}(A) \subset X \to X$ be a closed densely defined unbounded linear operator, with domain $\mathfrak{D}(A)$. Fix $t_f > 0$ and let $f : [0, t_f] \times X \to X$. We then consider the following evolution problem

$$\dot{q}(t) = Aq(t) + f(t, q(t)), \tag{2.5a}$$
$$q(0) = q_0. \tag{2.5b}$$

Note that we allow f to be a time-dependent and generally nonlinear operator; this includes inhomogeneous source terms of the form $f(t)$, as well as time-independent nonlinearities of the form $f(q)$.

We will assume throughout that A generates a C_0-semigroup $\{e^{tA}\}_{t\geq 0}$. This holds, for example, if A is a maximally contractive operator, by the Hille–Yosida theorem [37]. The C_0-semigroup is characterized by the properties

$$e^{0A} = I_X,$$
$$e^{sA}e^{tA} = e^{(s+t)A}, \text{ for all } s, t \geq 0,$$
$$\lim_{t\searrow 0} \|e^{tA}x - x\|_X = 0, \text{ for all } x \in X.$$

The first two properties are the statement that $\{e^{tA}\}_{t\geq 0}$ generates a semigroup on X and the third property is the statement that the semigroup is strongly continuous (C_0). The generator A is related to its semigroup by

$$Ax = \lim_{t\searrow 0} \frac{e^{tA}x - x}{t},$$

where the domain $\mathfrak{D}(A)$ is the subspace of X where the above limit exists.

Given $q_0 \in \mathfrak{D}(A)$, the curve $q(t) = e^{tA}q_0$ is the unique solution to the evolution equation (2.5) with $f \equiv 0$. For the evolution equation (2.5) with generally nonzero f, there are various assumptions which one can impose on f to ensure that the evolution equation admits a solution, at least locally [33; 37]. For our purposes, we will assume that $f : [0, t_f] \times X \to X$ is Lipschitz continuous in both variables. Then, for $q_0 \in \mathfrak{D}(A)$, (2.5) admits a unique solution which is characterized by Duhamel's principle [37]

$$q(t) = e^{tA}q_0 + \int_0^t e^{(t-s)A} f(s, q(s))ds. \tag{2.6}$$

The solution is strong in the sense that $q \in C^1([0, t_f], X) \cap C^0([0, t_f], D(A))$.

We will be interested in a dual problem associated with the evolution equation (2.5a). To investigate this dual problem, we will need the notion of the adjoint of the unbounded operator A. We define the associated adjoint operator $A^* : \mathfrak{D}(A^*) \subset X^* \to X^*$ as follows: the domain $\mathfrak{D}(A^*)$ is the set of all $x^* \in X^*$ for which there exists a $y^* \in X^*$ such that

$$\langle y^*, x\rangle = \langle x^*, Ax\rangle, \text{ for all } x \in \mathfrak{D}(A).$$

Since $\mathfrak{D}(A)$ is dense, if such a y^* exists, it is unique, and hence, we define $A^*x^* = y^*$. Note that since A is by assumption closed and densely defined, A^* is weak*-densely defined and weak*-closed [33; 37]. Since, by assumption, X is reflexive, A^* is weak-densely defined and weakly closed. Thus, A^* generates a weakly continuous semigroup on X^*, $\{e^{tA^*}\}_{t\geq 0}$, which is in fact the adjoint of the C_0 semigroup e^{tA}, i.e., $e^{tA^*} = (e^{tA})^*$. By the weak semigroup theorem, $\{e^{tA^*}\}_{t\geq 0}$ is in fact strongly continuous, i.e., it is a C_0 semigroup on X^* [33; 37].

2.3. **Infinite-dimensional Hamiltonian Systems.** Consider the cotangent bundle of a real reflexive Banach space X, $\pi_{T^*X} : T^*X \to X$, where, using the natural identification $T^*X \cong X \times X^*$, the bundle projection is given by $\pi_{T^*X}(q,p) = q$. Define the canonical one-form on T^*X as follows: for $(q,p) \in T^*X$ and $(v,w) \in T_{(q,p)}(T^*X) \cong X \times X^*$,

$$\Theta(q,p) \cdot (v,w) := -\langle p, T\pi_{T^*X}(v,w)\rangle = -\langle p, v\rangle.$$

The canonical symplectic form on T^*X is defined as $\Omega = d\Theta$; for $(v_1,w_1),(v_2,w_2) \in T_{(q,p)}(T^*X)$, we have the expression

$$\Omega(q,p) \cdot ((v_1,w_1),(v_2,w_2)) = \langle w_2, v_1\rangle - \langle w_1, v_2\rangle.$$

Let $\mathfrak{D}^1$ be a dense subspace of X which is additionally a Banach space with respect to a norm $\|\cdot\|_{\mathfrak{D}^1}$ and let $\mathfrak{D}^2$ be a dense subspace of X^* which is additionally a Banach space with respect to a norm $\|\cdot\|_{\mathfrak{D}^2}$. A Hamiltonian is a map $H : \mathfrak{D}^1 \times \mathfrak{D}^2 \to \mathbb{R}$ which is Fréchet differentiable in both arguments. Then, a Hamiltonian system is specified by a triple (T^*X, Ω, H) and associated with a Hamiltonian system is Hamilton's equations

$$i_{X_H}\Omega = dH.$$

Since X is reflexive, Ω is strongly non-degenerate and hence, the Hamiltonian vector field $X_H : \mathfrak{D}^1 \times \mathfrak{D}^2 \to TT^*X$ exists and is uniquely defined (for a detailed discussion of infinite-dimensional Hamiltonian systems, see [10]). The Hamiltonian vector field has the expression

$$\begin{aligned} X_H &: \mathfrak{D}^1 \times \mathfrak{D}^2 \to TT^*X, \\ &(q,p) \mapsto (D_pH(q,p), -D_qH(q,p)) \in T_{(q,p)}T^*X \cong X \times X^*. \end{aligned}$$

We say that a curve (q,p) on T^*X is a solution of Hamilton's equations if it is an integral curve of X_H. Equivalently, such a solution satisfies

$$\begin{aligned} \dot{q} &= D_pH(q,p), \\ \dot{p} &= -D_qH(q,p). \end{aligned}$$

Of course, even though X_H exists and is uniquely defined, this does not necessarily imply the existence or uniqueness of its corresponding integral curves; so one has to proceed with caution. At this point, we cannot say anything regarding the integral curves of X_H without specifying a particular Hamiltonian system; below, we investigate solutions for our particular interest of adjoint systems.

Time-Dependent Hamiltonian Systems To treat time-dependent evolutionary PDEs, we extend the definition of a Hamiltonian system to the case where the Hamiltonian is time-dependent, i.e., $H : (0,t_f) \times \mathfrak{D}^1 \times \mathfrak{D}^2 \to \mathbb{R}$. Let $\tau_t : (0,t_f) \times X \times X^* \to X \times X^*$ denote the canonical projection onto the second and third factors; we identify Θ and Ω with their pullbacks by τ_t. Then, in the time-dependent setting, Hamilton's equations read

$$i_{X_H}(\Omega - dH \wedge dt) = 0,$$

where the time-dependent Hamiltonian vector field has the expression

$$\begin{aligned} X_H &: (0,t_f) \times \mathfrak{D}^1 \times \mathfrak{D}^2 \to T((0,t_f)) \oplus T(T^*X), \\ &(t,q,p) \mapsto \frac{\partial}{\partial t} + (D_pH(t,q,p), -D_qH(t,q,p)). \end{aligned}$$

In this setting, we say that a curve on $(0,t_f) \times T^*X$ is a solution of Hamilton's equations if it is an integral curve of X_H covering the identity on $(0,t_f)$. Equivalently, such a solution curve is of the form $t \mapsto (t, q(t), p(t))$, where

$$\dot{q}(t) = D_p H(t, q, p), \tag{2.7a}$$

$$\dot{p}(t) = -D_q H(t, q, p). \tag{2.7b}$$

2.4. **Adjoint Systems for Evolutionary PDEs.** In this section, we consider a particular class of infinite-dimensional Hamiltonian systems. Namely, we will explore the adjoint system associated with the evolutionary PDE (2.5a). Let $\mathfrak{D}^1 = \mathfrak{D}(A) \subset X$ and $\mathfrak{D}^2 = \mathfrak{D}(A^*) \subset X^*$.

Define the *adjoint Hamiltonian* associated with the evolutionary PDE (2.5a) by

$$H : [0, t_f] \times \mathfrak{D}(A) \times \mathfrak{D}(A^*) \to \mathbb{R}, \tag{2.8a}$$

$$H(t, q, p) = \langle p, Aq + f(t, q) \rangle \tag{2.8b}$$

We will assume that $f : [0, t_f] \times X \to X$ is Lipschitz in both arguments. Furthermore, we assume that f is differentiable in its second argument and that

$$\sup_{q \in X : \|q\|_X \leq R} \|D_q f(t, q)\|_{X^*} < \infty,$$

uniformly in $t \in [0, t_f]$, for any $R > 0$. Compute

$$D_q H(t, q, p) = A^* p + [D_q f(t, q)]^* p,$$
$$D_p H(t, q, p) = Aq + f(t, q).$$

Thus, Hamilton's equations (2.7) for the adjoint Hamiltonian are

$$\dot{q}(t) = Aq(t) + f(t, q(t)), \tag{2.9a}$$

$$\dot{p}(t) = -A^* p(t) - [D_q f(t, q(t))]^* p(t). \tag{2.9b}$$

We refer to equations (2.9) as the adjoint system associated with the evolutionary PDE (2.5a). To solve the adjoint system, we have to specify appropriate boundary conditions for the problem. We will consider Type II boundary conditions $q(0) = q_0 \in \mathfrak{D}(A)$, $p(t_f) = p_f \in \mathfrak{D}(A^*)$, which specifies an initial condition for the forward variable q and a terminal condition for the adjoint variable p. As motivation for these boundary conditions, let us consider as an example the linear case, $f \equiv 0$.

Example 2.1 (Linear Case)**.** *In the linear case $f \equiv 0$, the semilinear evolution PDE is simply $\dot{q} = Aq$; the associated adjoint system is*

$$\dot{q} = Aq,$$
$$\dot{p} = -A^* p.$$

We would like to use the semigroups $\{e^{tA}\}_{t \geq 0}$ and $\{e^{tA^*}\}_{t \geq 0}$ generated by A and A^*, respectively, to construct solutions of the adjoint system. First note that we cannot, in general, use the semigroups to solve the adjoint system as an initial value problem, $(q(0), p(0)) = (q_0, p_0) \in \mathfrak{D}(A) \times \mathfrak{D}(A^*)$, due to the minus sign appearing in the second equation, i.e., the relevant operator to consider is $-A^*$, which may not generate a semigroup, without further assumptions [33]. However, $-A^*$ does generate a semigroup in reverse time, $\{e^{(t_f - t)A^*}\}_{t \leq t_f}$. To see this, define a reverse time parameter $s := t_f - t$. Then, the equation $\dot{p} = -A^* p$ with condition $p(t_f) = p_f$ can be equivalently expressed as

$$\frac{d}{ds} p = A^* p,$$
$$p\Big|_{s=0} = p_f.$$

Thus, this equation can be solved via the semigroup $\{e^{sA^*}\}_{s\geq 0}$ in the reverse time variable s, which is equivalent to using the semigroup $\{e^{(t_f-t)A^*}\}_{t\leq t_f}$ in the standard time variable t.

We can then solve the adjoint system if we place Type II boundary conditions $(q(0), p(t_f)) = (q_0, p_f) \in \mathfrak{D}(A) \times \mathfrak{D}(A^*)$ with $t_f > 0$. Thus, we can define a solution of Hamilton's equations with Type II boundary conditions by

$$\begin{aligned}(q, p) &: [0, t_f] \to X \times X^*,\\ (q(t), p(t)) &= (e^{tA}q_0, e^{(t_f-t)A^*}p_f).\end{aligned}$$

By the properties of the semigroups discussed previously, we have that this curve is a solution of Hamilton's equations with Type II boundary conditions, i.e.,

$$\begin{aligned}\dot{q}(t) &= Aq \textit{ for all } t \in (0, t_f),\\ \dot{p}(t) &= -A^*p \textit{ for all } t \in (0, t_f),\\ q(0) &= q_0 \in \mathfrak{D}(A),\\ p(t_f) &= p_f \in \mathfrak{D}(A^*),\end{aligned}$$

where the last two equations are interpreted in the strong C_0 sense as $t \searrow 0$ and $t \nearrow t_f$, respectively. These are the natural boundary conditions to consider for adjoint sensitivity analysis, where the adjoint equation for p is interpreted as evolving backward or "backpropagating" in time.

Returning to the general case, we consider the adjoint system (2.9) with boundary conditions $q(0) = q_0 \in \mathfrak{D}(A)$, $p(t_f) = p_f \in \mathfrak{D}(A^*)$. Note that the first equation (2.9a) admits a unique solution $q \in C^1([0, t_f], X) \cap C^0([0, t_f], \mathfrak{D}(A^*))$ with $q(0) = q_0$, as discussed in (2.2). In particular, $\sup_{t\in[0,t_f]} \|q(t)\|_X < \infty$. Thus, with this solution curve $q(t)$ fixed, we have that the map $(t, p) \mapsto -[D_q f(t, q(t))]^*p$ is Lipschitz in both arguments. Hence, by the theory discussed in Section 2.2, there exists a unique solution $p \in C^1([0, t_f], X^*) \cap C^0([0, t_f], \mathfrak{D}(A^*))$ to the second Hamilton's equation above with $p(t_f) = p_f$.

Now, we show that the adjoint system admits an *adjoint-variational* quadratic invariant. To do this, we define the variational equation as the linearization of $\dot{q}(t) = Aq(t) + f(t, q(t))$ about the solution curve $q(t)$, i.e.,

$$\begin{aligned}\dot{\delta q}(t) &= A\delta q(t) + D_q f(t, q(t))\delta q(t),\\ \delta q(0) &= \delta q_0 \in \mathfrak{D}(A).\end{aligned}$$

Again, by the assumptions on f, there exists a unique solution $\delta q \in C^1([0, t_f], X) \cap C^0([0, t_f], \mathfrak{D}(A))$ to the above variational equation. We can now state an adjoint sensitivity analysis result.

Proposition 2.1. *Let the solution curves q, p, and δq be as above. Then, for any $t \in (0, t_f)$,*

$$\frac{d}{dt}\langle p(t), \delta q(t)\rangle = 0. \tag{2.10}$$

Proof. Since $p \in C^1([0, t_f], X^*) \cap C^0([0, t_f], \mathfrak{D}(A^*))$ and $\delta q \in C^1([0, t_f], X) \cap C^0([0, t_f], \mathfrak{D}(A))$, we can directly compute

$$\begin{aligned}\frac{d}{dt}\langle p(t), \delta q(t)\rangle &= \langle \dot{p}(t), \delta q(t)\rangle + \langle p(t), \dot{\delta q}(t)\rangle\\ &= \langle -A^*p(t) - [D_q f(t, q(t))]^*p(t), \delta q(t)\rangle + \langle p(t), A\delta q(t) + D_q f(t, q(t))\delta q(t)\rangle = 0.\end{aligned}$$

□

Remark 2.1. *The quadratic invariant in Proposition 2.1 is fundamental to adjoint sensitivity analysis for evolutionary PDEs. Although the main purpose of this paper is to investigate the structure of adjoint systems and their discretization, we will briefly outline the concept of adjoint sensitivity analysis here.*

Formally, for a minimization problem

$$\min_{q_0 \in X} C(q(t_f)) \text{ such that } \dot{q}(t) = Aq(t) + f(t, q(t)),\ \dot{q}(0) = q_0,$$

the gradient of the cost function with respect to q_0 *in a direction* δq_0 *is given by* $\langle DC(q(t_f)), \delta q(t_f)\rangle$*, where* $\delta q(t)$ *solves the variational equation with* $\delta q(0) = \delta q_0$*. If we want to express this quantity in terms of the initial perturbation* δq_0 *instead of the perturbation propagated to the terminal time* $\delta q(t_f)$*, we can do this through the solution* $p(t)$ *of the adjoint equation by setting* $p(t_f) = DC(q(t_f))$ *and applying the previous proposition, which yields*

$$\langle DC(q(t_f)), \delta q(t_f)\rangle = \langle p(t_f), \delta q(t_f)\rangle = \langle p(0), \delta q(0)\rangle.$$

The gradient can then be computed by solving the variational equation forward in time or the adjoint equation backward in time. See for example [17; 26; 35; 39; 43; 46].

3. Discretization of Adjoint Systems

In this section, we investigate the semi-discretization and time integration of the adjoint system associated with an evolutionary PDE. We show that associated with semi-discretization in space and time integration of an evolutionary PDE, there are naturally associated dual methods such that adjoining and discretization commute, and characterize these uniquely in terms of semi-discrete and fully discrete analogues of the adjoint-variational quadratic conservation law (2.10).

Recall that for a linear operator B, we denote its adjoint with respect to a duality pairing $\langle\cdot,\cdot\rangle$ as B^*. As we will see, when we discuss discretization in the subsequent sections, several duality pairings arise. To avoid ambiguity, we introduce some extra notation. Let V be a finite-dimensional vector space, V^* its dual. For a duality pairing $\langle\cdot,\cdot\rangle_M : V^* \times V \to \mathbb{R}$, we will denote the adjoint of an operator B with respect to this pairing as B^{*M}. When $V = \mathbb{R}^N$, we denote $\langle\cdot,\cdot\rangle_S$ as the standard duality pairing, and thus, the adjoint with respect to the standard duality pairing is just given by the transpose, $B^{*S} = B^T$.

Now, consider two duality pairings $\langle\cdot,\cdot\rangle_L$ and $\langle\cdot,\cdot\rangle_R$ on $V^* \times V$, related by an invertible operator $P : V \to V$ such that

$$\langle \mathbf{p}, \mathbf{v}\rangle_L = \langle \mathbf{p}, P\mathbf{v}\rangle_R \text{ for all } \mathbf{p} \in V^*, \mathbf{v} \in V.$$

Then, the adjoint of an operator B with respect to $\langle\cdot,\cdot\rangle_L$ is related to its adjoint with respect to $\langle\cdot,\cdot\rangle_R$ by

$$B^{*L} = P^{-*R} B^{*R} P^{*R}. \tag{3.1}$$

Note in particular that $P^{*L} = P^{*R}$.

Now, consider an ODE on V of the form $\dot{\mathbf{q}} = K\mathbf{q} + \mathbf{f}(t, \mathbf{q})$ where K is a linear operator (of course, by letting $K = 0$, this encompasses a fully nonlinear ODE as well), and let $\langle\cdot,\cdot\rangle_M$ be a duality pairing on $V \times V^*$. Then, we define the adjoint Hamiltonian associated with the pairing $\langle\cdot,\cdot\rangle_M$ as

$$H^M(t, \mathbf{q}, \mathbf{p}) = \langle \mathbf{p}, K\mathbf{q} + \mathbf{f}(t, \mathbf{q})\rangle_M.$$

The adjoint system *induced* by the pairing $\langle\cdot,\cdot\rangle_M$ is given by Hamilton's equations

$$\dot{\mathbf{q}} = \frac{\delta}{\delta \mathbf{p}} H^M(t, \mathbf{q}, \mathbf{p}) = K\mathbf{q} + \mathbf{f}(t, \mathbf{q}), \tag{3.2a}$$

$$\dot{\mathbf{p}} = \frac{\delta}{\delta \mathbf{q}} H^M(t, \mathbf{q}, \mathbf{p}) = -K^{*M}\mathbf{p} - [D_{\mathbf{q}}\mathbf{f}(t,\mathbf{q})]^{*M}\mathbf{p}, \tag{3.2b}$$

where the above variational derivatives of a real-valued function G of $\mathbf{q}$ and $\mathbf{p}$ are defined by

$$\left\langle \delta\mathbf{p}, \frac{\delta G}{\delta \mathbf{q}} \right\rangle_M = \frac{d}{d\epsilon}\Big|_{\epsilon=0} G(\mathbf{q}, \mathbf{p} + \epsilon\delta\mathbf{p}) \text{ for all } \delta\mathbf{p} \in V^*,$$
$$\left\langle \frac{\delta G}{\delta \mathbf{q}}, \delta\mathbf{q} \right\rangle_M = \frac{d}{d\epsilon}\Big|_{\epsilon=0} G(\mathbf{q} + \epsilon\delta\mathbf{q}, \mathbf{p}) \text{ for all } \delta\mathbf{q} \in V.$$

3.1. **Semi-Discretization of Adjoint Systems.** We now introduce the notion of a Galerkin semi-discretization of the evolution equation (2.5a) on X into a finite-dimensional subspace X_h. We will subsequently drop the subspace requirement to allow for more general semi-discretizations.

Let X_h be a finite-dimensional subspace of X, where as before $\langle \cdot, \cdot \rangle$ denotes the duality pairing on $X \times X^*$, and let $\{\varphi_i\}_{i=1}^{\dim(X_h)}$ be a basis for X_h. Let $\{l_j\}_{j=1}^{\dim(X_h)}$ be a set of degrees of freedom for X_h, i.e., a basis for X_h^*. A *Galerkin semi-discretization* of (2.5a) is specified by an approximation $q(t) \approx \sum_i \mathbf{q}^i(t)\varphi_i$ satisfying the evolution equation on the degrees of freedom, i.e.,

$$\left\langle l_j, \dot{\mathbf{q}}^i(t)\varphi_i - \mathbf{q}^i(t)A\varphi_i - f(t, \mathbf{q}^k(t)\varphi_k) \right\rangle = 0, \; j = 1, \dots, \dim(X_h),$$

where we adopt the Einstein summation convention that repeated upper and lower indices are summed over.

Let M and K denote mass and stiffness matrices, respectively, with entries

$$M_{ji} = \langle l_j, \varphi_i \rangle,$$
$$K_{ji} = \langle l_j, A\varphi_i \rangle.$$

Let $\mathbf{q}(t)$ denote the vector with components $\mathbf{q}^i(t)$, and let the semi-discretized semilinear term be denoted by the vector $\mathbf{f}(t, \mathbf{q})$ with entries

$$\mathbf{f}^j(t, \mathbf{q}) = \langle l_j, f(t, \mathbf{q}^k\varphi_k) \rangle.$$

Then, the semi-discretization can be expressed as

$$M\frac{d}{dt}\mathbf{q} = K\mathbf{q} + \mathbf{f}(t, \mathbf{q}). \tag{3.3}$$

Now, we form the adjoint system [49] for the semi-discrete system (3.3). First, since M is invertible, we express the above as a standard ODE,

$$\frac{d}{dt}\mathbf{q} = M^{-1}K\mathbf{q} + M^{-1}\mathbf{f}(t, \mathbf{q}).$$

Note that the adjoint system depends on the duality pairing on $X_h \times X_h^*$ by equations (3.2). There are two immediately obvious choices of duality pairing. First, since we identify $X_h \cong \mathbb{R}^N$, $N = \dim(X_H)$, where the identification is $Q^i\varphi_i \cong \mathbf{q}$, an obvious choice of duality pairing is just the standard duality pairing on $\mathbb{R}^N$, $\langle \cdot, \cdot \rangle_S$. The adjoint system induced by the standard duality pairing, via equations (3.2), is given by

$$\frac{d}{dt}\mathbf{q} = M^{-1}K\mathbf{q} + M^{-1}\mathbf{f}(t, \mathbf{q}), \tag{3.4a}$$

$$\frac{d}{dt}\mathbf{z} = -K^T M^{-T}\mathbf{z} - [D_{\mathbf{q}}\mathbf{f}(t, \mathbf{q})]^T M^{-T}\mathbf{z}, \tag{3.4b}$$

where $D_{\mathbf{q}}\mathbf{f}$ is the usual Jacobian of $\mathbf{f}$ with respect to the argument $\mathbf{q}$. Alternatively, we can consider the duality pairing on $\mathbb{R}^N$ naturally induced by the mass matrix, i.e.,

$$\langle \mathbf{p}, \mathbf{v}\rangle_M = \mathbf{p}^T M \mathbf{v}.$$

The adjoint system induced by the mass matrix is given by

$$\frac{d}{dt}\mathbf{q} = M^{-1}K\mathbf{q} + M^{-1}\mathbf{f}(t,\mathbf{q}), \tag{3.5a}$$

$$\frac{d}{dt}\mathbf{p} = -(K^{*M}M^{-*M} + [D_{\mathbf{q}}\mathbf{f}(t,\mathbf{q})]^{*M}M^{-*M})\mathbf{p}. \tag{3.5b}$$

By equation (3.1), the second equation can equivalently be written as

$$M^T\frac{d}{dt}\mathbf{p} = -K^T\mathbf{p} - [D_{\mathbf{q}}\mathbf{f}(t,\mathbf{q})]^T\mathbf{p}.$$

Note that the above adjoint systems were formed by first semi-discretizing the evolution equation and subsequently forming the adjoint system. We will now reverse this process: we will first form the adjoint system at the continuous level and subsequently semi-discretize. Recall the continuous adjoint system is given by

$$\begin{aligned} \dot{q} &= Aq + f(t,q), \\ \dot{p} &= -A^*p - [Df(t,q)]^*p. \end{aligned}$$

To semi-discretize this system, we discretize the q variable as before, $q(t) \approx \sum_i \mathbf{q}^i(t)\varphi_i$ with degrees of freedom given by $\{l_j\}$. For $p \in X^*$, we semi-discretize by using the basis $\{l_j\}$ of X_h^* via $p(t) \approx \sum_j \mathbf{p}^j(t) l_j$ and degrees of freedom given by $\{\varphi_i\}$ (since X is reflexive, we have $X^{**} = X$). As we will see, this is a natural choice of semi-discretization for p since the resulting system is equivalent to (3.4) and (3.5). Furthermore, we will see in Theorem 3.2 that it is the unique semi-discretization of the adjoint system covering the base semi-discretization and satisfying a semi-discrete analogue of equation (2.10).

Proposition 3.1. *With the above choice of semi-discretization for the continuous adjoint system, we have the semi-discrete adjoint system*

$$M\frac{d}{dt}\mathbf{q} = K\mathbf{q} + \mathbf{f}(t,\mathbf{q}), \tag{3.6a}$$

$$M^T\frac{d}{dt}\mathbf{p} = -K^T\mathbf{p} - [D_{\mathbf{q}}\mathbf{f}(t,\mathbf{q})]^T\mathbf{p}. \tag{3.6b}$$

Note that this is equivalent to the mass-matrix-induced semi-discrete adjoint system in (3.5)*.*

Proof. The semi-discretization of the evolution equation (3.6a) is the same as before, so we only have to verify (3.6b). The semi-discretization of the adjoint equation is given by

$$\langle \dot{\mathbf{p}}^j l_j, \varphi_i\rangle = \langle -A^*\mathbf{p}^j l_j, \varphi_i\rangle - \langle [D_q f(t, \mathbf{q}^k\varphi_k)]^*\mathbf{p}^j l_j, \varphi_i\rangle,\ i = 1,\dots,\dim(X_h).$$

We consider each term in the above equation. The first term is the i^{th} component of the vector $M^T d\mathbf{p}/dt$. The second term can be expressed as $\langle -A^*\mathbf{p}^j l_j, \varphi_i\rangle = -\mathbf{p}^j\langle l_j, A\varphi_i\rangle$, which is the i^{th} component of $-K^T\mathbf{p}$. To see that the third term corresponds to the i^{th} component of $-[D_{\mathbf{q}}\mathbf{f}(t,\mathbf{q})]^T\mathbf{p}$, we explicitly compute the Jacobian

$$\begin{aligned} [D_{\mathbf{q}}\mathbf{f}(t,\mathbf{q})]_{ij} &= \frac{\partial}{\partial \mathbf{q}^j}\mathbf{f}^i(t,\mathbf{q}) = \frac{\partial}{\partial \mathbf{q}^j}\langle l_i, f(t,\mathbf{q}^k\varphi_k)\rangle \\ &= \langle l_i, D_q f(t,\mathbf{q}^k\varphi_k)\varphi_j\rangle = \langle [D_q f(t,\mathbf{q}^k\varphi_k)]^* l_i, \varphi_j\rangle. \end{aligned}$$

Thus, we see that the third term is the i^{th} component of $-[D_{\mathbf{q}}\mathbf{f}(t,\mathbf{q})]^T\mathbf{p}$.

□

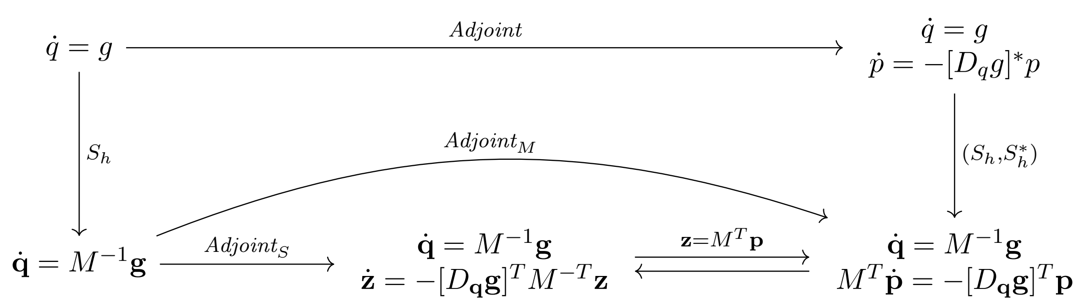
Let us formally denote the semi-discretization procedures on X as S_h and the dual semi-discretization on X^* as S_h^*. For brevity, we denote the right hand side of the continuous and semi-discrete evolution equations as

$$g = Aq + f(t, q),$$
$$\mathbf{g} = K\mathbf{q} + \mathbf{f}(t, \mathbf{q}).$$

We denote the procedures of forming the adjoints with respect to the standard duality pairing and the mass matrix induced duality pairing as Adjoint_S and Adjoint_M, respectively. Then the preceding discussion can be summarized in the following result.

Theorem 3.1. *The system* (3.6) *arising from forming the continuous adjoint equation and semi-discretizing is equivalent to the systems* (3.4) *and* (3.5) *that arise from semi-discretizing the forward equation and forming a discrete adjoint under the appropriate duality pairing and inner product. That is, semi-discretization and forming the adjoint commute, with the above choices of semi-discretization, once composed with the appropriate transformations, as summarized in the commutative diagram* (3.7)*.*

(3.7)



Although these two systems are equivalent via the coordinate transformation $\mathbf{p} = M^{-T}\mathbf{z}$, we note that each represent a canonical Hamiltonian system on T^*X_h with different coordinate representations and duality pairings. The system (3.4) can be interpreted as a Hamiltonian system on $T^*X_h \cong X_h \times X_h^*$ with duality pairing given by the standard duality pairing on $\mathbb{R}^n$, $\langle \mathbf{x}, \mathbf{y}\rangle = \mathbf{x}^T\mathbf{y}$, canonical symplectic form given by $\Omega_h^S = \langle d\mathbf{q} \wedge d\mathbf{z}\rangle_S = d\mathbf{q}^{\,T} \wedge d\mathbf{z}$, and Hamiltonian

$$H_h^S(t, \mathbf{q}, \mathbf{z}) = \mathbf{z}^T M^{-1} K\mathbf{q} + \mathbf{z}^T M^{-1}\mathbf{f}(t, \mathbf{q}).$$

On the other hand, (3.5) and (3.6) can be interpreted as a Hamiltonian system on T^*X_h with duality pairing $\langle \mathbf{x}, \mathbf{y}\rangle_M = \mathbf{x}^T M\mathbf{y}$, with symplectic form $\Omega_h^M = \langle d\mathbf{q} \wedge d\mathbf{p}\rangle_M = (M d\mathbf{q})^T \wedge d\mathbf{p}$, and Hamiltonian

$$H_h^M(t, \mathbf{q}, \mathbf{p}) = \mathbf{p}^{\,T} K\mathbf{q} + \mathbf{p}^T\mathbf{f}(t, \mathbf{q}).$$

That (3.4) is equivalent to (3.6) can be expressed as the fact that the mapping $\Theta_M : (t, \mathbf{q}, \mathbf{z}) \mapsto (t, \mathbf{q}, M^{-*}\mathbf{z})$ pulls back the associated time-dependent contact structures as

$$\Theta_M^*(\Omega_h^M - dH^M \wedge dt) = \Omega_h^S - dH^S \wedge dt.$$

In the autonomous case, i.e., where f does not depend explicitly on t, this can be expressed as the fact that $\Theta_M : (\mathbf{q}, \mathbf{z}) \mapsto (\mathbf{q}, M^{-*}\mathbf{z})$ is a symplectomorphism

$$\Theta_M^*\Omega_h^M = \Omega_h^S,$$

and pulls back the Hamiltonian as

$$\Theta_M^* H_h^M = H_h^S.$$

From a finite element and discretization perspective, the formulation of (3.5) and (3.6) is more natural, as the duality pairing on T^*X_h is induced from the duality pairing on T^*X. In particular, with $p = \mathbf{p}^j l_j$ and $q = \mathbf{q}^i \varphi_i$, we have

$$\langle \mathbf{p}, \mathbf{q} \rangle_M = \mathbf{p}^j M_{ji} \mathbf{q}^i = \mathbf{p}^j \langle l_j, \varphi_i \rangle \mathbf{q}^i = \langle p, q \rangle.$$

From this observation, it is straightforward to verify that if $\Pi_h : X \to X_h$ denotes the Galerkin projection, where $\Pi_h(q) \in X_h$ is defined by

$$\langle \Pi_h(q), l_j \rangle = \langle q, l_j \rangle \text{ for all } j,$$

then the semi-discrete Hamiltonian and semi-discrete symplectic structure are related to their infinite-dimensional counterparts as

$$\Pi_h^{**}\Omega = \Omega_h^M, \quad \Pi_h^{**}H = H_h^M,$$

where Π_h^{**} is the twice-iterated pullback of Π_h. The above equation is the statement that the semi-discrete Hamiltonian structure is the Galerkin restriction of the infinite-dimensional Hamiltonian structure.

Remark 3.1. *In the commutative diagram* (3.7)*, we utilize two choices of duality pairings* $\langle \cdot, \cdot \rangle_M$ *and* $\langle \cdot, \cdot \rangle_S$*. We include the standard duality pairing as it is the usual duality pairing used to form adjoint systems. We include the mass matrix induced duality pairing since the OtD method given by the dual semi-discretization* (S_h, S_h^*) *is naturally equivalent to a DtO method with respect to the mass matrix, whereas it is only equivalent to the DtO method with respect to the standard duality pairing once composed with the appropriate transformation. Note also that a diagram analogous to* (3.7) *holds with replacing the standard duality pairing with an arbitrary duality pairing.*

Remark 3.2 (Equilibrium preservation)**.** *In non-dissipative PDEs, often one is interested in preservation of equilibria (also known as well-balanced schemes), e.g., [14], such that physical equilibria are maintained post spatial and temporal discretization. Consider laminar flow through a domain with constant inflow (Dirichlet) boundary conditions: if initial conditions are in equilibrium (in this case constant and equal to inflow boundary conditions), discretization in space and time should maintain equilibrium for arbitrarily long time. For this example, the spatial discretization would typically have zero row-sums (e.g., consider finite-difference discretizations of advection), wherein the constant vector (laminar flow) is in the nullspace of* $M^{-1}K$*, and any one-step explicit integration scheme has solution update* $\mathbf{g}_{n+1} = \mathbf{g}_n + \Delta t p(M^{-1}K)\mathbf{g}_n = \mathbf{g}_n$*, for some polynomial* $p(M^{-1}K)$*. However, in the standard duality adjoint* (3.4)*, the resulting scheme is unlikely to preserve equilibria, as* $K^T M^{-T}$ *will have zero column sums rather than row sums, and constant vectors will no longer be invariant under explicit integration schemes. In contrast, the mass-induced duality pairing* (3.6) *will facilitate equilbiria preservation in this case, as the natural discretization of* K^T *will maintain the constant nullspace of* K*, invariant to nonuniform scaling by the mass matrix. General equilibria preservation is more complex, but we believe the mass-induced duality pairing is the most natural way to maintain equilbrium preservation in the adjoint equation, while also maintaining discrete symplectic structure of the full adjoint system.*

Note that both systems satisfy a semi-discrete adjoint-variational conservation law.

Proposition 3.2. *The mass matrix induced adjoint system* (3.6) *admits a quadratic adjoint-variational conservation law. For a solution* $\mathbf{p}(t)$ *of the adjoint equation* (3.6b) *and a solution* $\delta\mathbf{q}(t)$ *of the variational equation associated with* (3.3)*, covering the same solution* $\mathbf{q}(t)$ *of* (3.3)*,*

$$\frac{d}{dt}\langle \mathbf{p}(t), \delta\mathbf{q}(t) \rangle_M = 0. \tag{3.8}$$

Similarly, the standard duality pairing induced adjoint system (3.4) *admits a quadratic adjoint-variational conservation law. For a solution* $\mathbf{z}(t)$ *of the adjoint equation* (3.4b) *and a solution* $\delta\mathbf{q}(t)$ *of the variational equation covering the same solution* $\mathbf{q}(t)$ *of the semi-discrete evolution equation,*

$$\frac{d}{dt}\langle \mathbf{z}(t), \delta\mathbf{q}(t)\rangle_S = 0. \tag{3.9}$$

Proof. This follows from Proposition 2.1 in the standard adjoint theory for ODEs. □

As we will see shortly when discussing more general semi-discretizations, once the semi-discretization S_h for the forward variable is fixed, and a duality pairing is chosen, then the full semi-discretization on $X_h \times X_h^*$ is the unique semi-discretization of the fully continuous adjoint system such that the conservation law, (3.8) or (3.9), corresponding to the choice of duality pairing holds.

More general semi-discretizations. Note that we made a particular choice of semi-discretization of the Banach space X. When X is a function space, it can be thought of as a spatial discretization via a subspace method, such as the finite element method. Once this semi-discretization of X is fixed, there is a natural dual choice of semi-discretization for the adjoint system on $X \times X^*$ such that it arises as the adjoint system of the semi-discretized evolution equation on X. Also, note that this notion of semi-discretization is fairly general. X need not be an infinite-dimensional function space; it applies to sequence spaces such as $l^2(\mathbb{R})$ or even cases where X is finite-dimensional (in which case, a semi-discretization of X can be seen as a dimensional reduction to a "lower order" space).

However, more general semi-discretizations are possible. For example, X_h need not be chosen as a subspace but is more generally an approximating space that one can define an approximation of A on. This allows more flexibility in the choice of semi-discretization, such as mixed methods and DG methods. Furthermore, this allows for more freedom in treating the semilinear term, e.g., by quadrature. In essence, as before, once a semi-discretization of the evolution equation is fixed, there is a natural dual choice of semi-discretization of the adjoint system such that the corresponding diagram of adjoining and semi-discretization commute. Abstractly, such a semi-discretization and its dual semi-discretization reduce the adjoint Hamiltonian system on T^*X to an adjoint Hamiltonian system on T^*X_h.

To be more precise, we introduce the following more general notion of semi-discretization: a *method-of-lines semi-discretization* of an evolution equation on a Banach space X is a procedure for mapping the evolution equation into an ODE on a finite-dimensional vector space X_h (of course, one wants that the solution to the semi-discrete problem converges as $h \to 0$, in some sense, to a solution of the continuous problem but we will not discuss this here as it will depend generally on the choice of semi-discretization). Associated with an evolution equation of the form (2.5a), we denote the semi-discretization as an ODE

$$\frac{d}{dt}\mathbf{q} = K_h[A, f](\mathbf{q}), \tag{3.10}$$

where $K_h[A, f]$ is generally a time-dependent nonlinear operator on X_h constructed from A and f. We will assume that $K_h[A, f](\mathbf{q})$ is differentiable in $\mathbf{q}$ given that $f(t, q)$ is differentiable in q. We will assume that any method-of-lines semi-discretization admits a solution on the interval $[0, t_f]$ where the semilinearity f and its derivative are uniformly bounded as discussed in Section 2.4 (which is the case for Galerkin semi-discretization, since the associated semi-discrete semilinear term $\mathbf{f}$ enjoys the same bounds).

Now, we can state the following very general result regarding adjoining and semi-discretization.

Theorem 3.2. *A method-of-lines semi-discretization of the adjoint system* (2.9) *on* $X \times X^*$ *into a vector space* P_h *commutes with the process of semi-discretization of the evolution equation* (2.5a) *into* X_h *followed by adjoining if and only if it is equivalent to the adjoint system on* $X_h \times X_h^*$*, equipped with a duality pairing* $\langle \cdot, \cdot \rangle_h$*, formed from the semi-discrete ODE* (3.10)*; namely,*

$$\frac{d}{dt}\mathbf{q} = K_h[A, f](\mathbf{q}), \tag{3.11a}$$

$$\frac{d}{dt}\mathbf{z} = -[D_{\mathbf{q}} K_h[A, f](\mathbf{q})]^{*h}\mathbf{z}. \tag{3.11b}$$

Furthermore, given a method-of-lines semi-discretization (3.10) *of the evolution equation, the dual semi-discretization* (3.11) *is the unique method-of-lines semi-discretization into* $X_h \times X_h^*$*, equipped with the duality pairing* $\langle \cdot, \cdot \rangle_h$*, of the adjoint system covering* (3.10) *on the interval* $[0, t_f]$ *such that the adjoint-variational conservation law holds,*

$$\frac{d}{dt}\langle \mathbf{z}(t), \delta\mathbf{q}(t)\rangle_h = 0,$$

where $\delta\mathbf{q}(t)$ *is the solution of the variational equation associated with* (3.10)*,*

$$\frac{d}{dt}\delta\mathbf{q} = [D_{\mathbf{q}} K_h[A, f](\mathbf{q})]\delta\mathbf{q},$$

with arbitrary but fixed initial condition $\delta\mathbf{q}(t_0) = \delta\mathbf{q}_0$ *for any* $t_0 \in [0, t_f)$ *and terminal condition* $\mathbf{z}(t_f) = \mathbf{z}_f$*.*

Proof. The first statement of the theorem simply follows from the definitions and a direct calculation that (3.11b) is the adjoint equation associated with (3.11a).

For the second statement, clearly (3.11) satisfies the above adjoint-variational conservation law by Proposition 2.1.

To show that it is unique, suppose we have another method-of-lines semi-discretization of the adjoint system covering the semi-discretization of the evolution equation, i.e., we have a semi-discretization of the continuous adjoint system of the form

$$\frac{d}{dt}\mathbf{q} = K_h[A, f](\mathbf{q}),$$
$$\frac{d}{dt}\mathbf{z}' = L_h(\mathbf{q}, \mathbf{z}'),$$

satisfying

$$\frac{d}{dt}\langle \mathbf{z}'(t), \delta\mathbf{q}(t)\rangle_h = 0.$$

Since both semi-discretizations satisfy the Type II boundary conditions fixing $\delta\mathbf{q}(t_0) = \delta\mathbf{q}_0$ and $\mathbf{z}(t_f) = \mathbf{z}_f = \mathbf{z}'(t_f)$, we have by integrating their respective quadratic conservation laws from t_0 to t_f,

$$\langle \mathbf{z}'(t_0), \delta\mathbf{q}_0\rangle_h = \langle \mathbf{z}'(t_f), \delta\mathbf{q}(t_f)\rangle_h = \langle \mathbf{z}_f, \delta\mathbf{q}(t_f)\rangle_h = \langle \mathbf{z}(t_f), \delta\mathbf{q}(t_f)\rangle_h = \langle \mathbf{z}(t_0), \delta\mathbf{q}_0\rangle_h.$$

In particular, since $\delta\mathbf{q}_0$ is arbitrary, we have

$$\mathbf{z}'(t_0) = \mathbf{z}(t_0).$$

Since $t_0 \in [0, t_f)$ is arbitrary, we have $\mathbf{z}(t) = \mathbf{z}'(t)$ for all $t \in [0, t_f]$. Thus,

$$L_h(\mathbf{q}(t), \mathbf{z}(t)) = L_h(\mathbf{q}(t), \mathbf{z}'(t)) = \frac{d}{dt}\mathbf{z}'(t) = \frac{d}{dt}\mathbf{z}(t) = -[D_{\mathbf{q}} K_h[A, f](\mathbf{q}(t))]^{*h}\mathbf{z}(t),$$

i.e., they are the same semi-discretization. □

Remark 3.3. *Note that in the above theorem, we allow the semi-discretization of the adjoint system to map into a vector space P_h, not necessarily $X_h \times X_h^*$, and it suffices to require that the semi-discretization of the adjoint system on P_h is equivalent to the adjoint system on $X_h \times X_h^*$ formed from* (3.10)*, i.e., there exists an invertible transformation $\Phi_{P_h} : P_h \to X_h \times X_h^*$ mapping the corresponding semi-discrete adjoint systems to each other. More precisely, P_h must have a Hamiltonian structure given by pulling back the Hamiltonian structure on $X_h \times X_h^*$,*

$$\Omega_{P_h} = \Phi_{P_h}^* \Omega_h,$$
$$H_{P_h} = \Phi_{P_h}^* H_h,$$

where Ω_h is the canonical symplectic form on $X_h \times X_h^*$ and $H_h = \langle \mathbf{z}, K_h[A, f](\mathbf{q})\rangle_h$ is the adjoint Hamiltonian associated with the system (3.11)*.*

In the literature, it is often the case that the semi-discretization of the adjoint system is not formulated from the cotangent bundle $X \times X^*$ to $X_h \times X_h^*$. For example, when X is a Hilbert space, often the identification of X^* with X via the Riesz representation theorem is utilized to write the adjoint system as a system on $X \times X$. For example, this is done in [35] for the adjoint system associated with Burgers' equation, where the same (piecewise linear finite element) method-of-lines semi-discretization is used for both the forward evolution equation in the variable y and the adjoint equation in the variable p, resulting in a semi-discrete ODE on $X_h \times X_h$. Thus, in terms of the notation introduced in the above theorem, the semi-discretization used in [35] utilizes $P_h = X_h \times X_h$.

As an immediately corollary to Theorem 3.2, we have that any method-of-lines semi-discretization of an infinite-dimensional adjoint system which corresponds to the adjoint of a method-of-lines semi-discretization of the evolution equation must necessarily have a Hamiltonian structure on P_h, since it must be equivalent to the Hamiltonian structure on $X_h \times X_h^*$. Heuristically, for semi-discretize-then-optimize and optimize-then-semi-discretize methods to commute, the optimize-then-semi-discretize method must necessarily preserve the Hamiltonian structure.

Note that the above uniqueness depends on the choice of the duality pairing; for example, as we have seen explicitly in the Galerkin semi-discretization case, there are two semi-discretizations on $X_h \times X_h^*$ (which we identified with $\mathbb{R}^N \times \mathbb{R}^{N*}$ using a basis) which satisfy the adjoint quadratic conservation law; namely, one with respect to the standard duality pairing on $\mathbb{R}^N$ and one with respect to the duality pairing $\langle \cdot, \cdot \rangle_M$. Although the two systems arising from different duality pairings are equivalent via a similarity transformation, this subtle distinction becomes important when moving to the fully discrete setting by incorporating time integration, as we will explain in Section 3.3.

3.2. **Time Integration.** To completely discretize a semi-discrete system, we have to further integrate the system in time. Note that the results of this section hold for general adjoint systems for ODEs, not just those that arise from semi-discretization. To begin, we will recall some facts about maps and time integration for ODEs.

Consider an ODE $\dot{\mathbf{y}} = \mathbf{g}(t, \mathbf{y})$ on a vector space V. We will denote the duality pairing on $V \times V^*$ as $\langle \cdot, \cdot \rangle$ and the adjoint of an operator B as B^*.

Let $\Phi : V \to V$ be a (local) diffeomorphism. Recall that the *tangent lift* of Φ, denoted $T\Phi : TV \to TV$, is defined by

$$T\Phi(\mathbf{v_y}) = T_\mathbf{y}\Phi(\mathbf{v_y}) \in T_{\Phi(\mathbf{y})}V \text{ for } \mathbf{v_y} \in T_\mathbf{y}V,$$

where $T_\mathbf{y}\Phi(\mathbf{v_y})$ is the linearization of Φ at $\mathbf{y}$, which is represented as the Jacobian of Φ in a local chart. This induces a dual map on the cotangent spaces, for $\mathbf{a} \in T^*_{\Phi(\mathbf{y})}V$, by

$$\langle T^*_\mathbf{y}\Phi(\mathbf{a}), \mathbf{v_y}\rangle = \langle \mathbf{a}, T_\mathbf{y}\Phi(\mathbf{v_y})\rangle \text{ for all } \mathbf{v_y} \in T_\mathbf{y}V. \tag{3.12}$$

We then define the cotangent lift of Φ to be $T^*\Phi^{-1}$, which is a (local) vector bundle morphism $T^*\Phi^{-1} : T^*V \to T^*V$. Furthermore, it is a (local) symplectomorphism, with T^*V equipped with its canonical symplectic form.

Now, consider a one-step method for the ODE $\dot{\mathbf{y}} = \mathbf{g}(t, \mathbf{y})$, which is specified by a generally nonlinear map

$$\Phi_{\Delta t}[n, \mathbf{g}] : V \to V$$

which depends on the current time step t^n (in the non-autonomous setting) and the vector field $\mathbf{g}$ defining the ODE. The one-step method is given by

$$\mathbf{y}_{n+1} = \Phi_{\Delta t}[n, \mathbf{g}](\mathbf{y}_n).$$

We will assume that $\Phi_{\Delta t}[n, \mathbf{g}]$ is a local diffeomorphism, which is generally true by an implicit function argument, given differentiability of $\mathbf{g}$ in its second argument and a sufficiently small time step. Thus, we can define its cotangent lift $T^*\Phi^{-1}_{\Delta t}[n, \mathbf{g}]$. As the cotangent lift is a symplectomorphism, we have that the method

$$\begin{aligned} \mathbf{y}_{n+1} &= \Phi_{\Delta t}[n, \mathbf{g}](\mathbf{y}_n), \\ \mathbf{p}_{n+1} &= T^*\Phi^{-1}_{\Delta t}[n, g]\mathbf{p}_n, \end{aligned}$$

is a symplectic method on $T^*V \cong V \times V^*$, i.e., $\langle d\mathbf{y}_{n+1} \wedge d\mathbf{p}_{n+1} \rangle = \langle d\mathbf{y}_n \wedge d\mathbf{p}_n \rangle$. With the solution curve $\{y_n\}$ for the forward variable fixed, we interpret the cotangent lift as a one-step map $T^*\Phi^{-1}_{\Delta t}[n, g] : V^* \to V^*$. Note that this method can be thought of as a one-step approximation of the adjoint system, since the continuous-time flow of the adjoint system is given by the cotangent lift of the flow of the forward ODE (as discussed in Section 2.1). Also note that for backpropagation where the terminal value for the adjoint variable is specified, the second equation above is more naturally expressed as a map $\mathbf{p}_{n+1} \mapsto \mathbf{p}_n$ given by $\mathbf{p}_n = T^*\Phi_{\Delta t}[n, \mathbf{g}]\mathbf{p}_{n+1}$.

Remark 3.4. *We will refer to the cotangent lifted one-step method as the combined integrator in both the y and p variables, as well as just the integrator in the p variable (which depends on the y variable); it will be clear in context which is meant.*

It is well-known that integration of the forward ODE by a Runge–Kutta (RK) method and then adjoining is equivalent to first adjoining and then integrating by the associated symplectic partitioned RK method (see [4; 46; 49]). We extend this result to all one-step time integration methods.

Theorem 3.3. *Time integration by a one-step method and adjoining commute, where time integration of the base ODE is given by a one-step method $\Phi_{\Delta t}[n, \mathbf{g}]$, time integration of the adjoint system is given by the cotangent lift of the one-step method, adjoining the ODE is given by the usual adjoint ODE system [49], and the adjoint of the discrete system is as defined in [49]. That is, the following diagram commutes.*

$$\begin{array}{ccc} \dot{\mathbf{y}} = \mathbf{g}(t, \mathbf{y}) & \xrightarrow{\textit{Adjoint}} & \begin{array}{c} \dot{\mathbf{y}} = \mathbf{g}(t, \mathbf{y}) \\ \dot{\mathbf{p}} = -[D_{\mathbf{y}}\mathbf{g}(t, \mathbf{y})]^*\mathbf{p} \end{array} \\ \Big\downarrow {\scriptstyle \Phi_{\Delta t}[n,\mathbf{g}]} & & \Big\downarrow {\scriptstyle (\Phi_{\Delta t}[n,\mathbf{g}], T^*\Phi^{-1}_{\Delta t}[n,\mathbf{g}])} \\ \mathbf{y}_{n+1} = \Phi_{\Delta t}[n, \mathbf{g}](\mathbf{y}_n) & \xrightarrow{\textit{Adjoint}} & \begin{array}{c} \mathbf{y}_{n+1} = \Phi_{\Delta t}[n, \mathbf{g}](\mathbf{y}_n) \\ \mathbf{p}_{n+1} = T^*\Phi^{-1}_{\Delta t}[n, \mathbf{g}](\mathbf{p}_n) \end{array} \end{array} \tag{3.13}$$

Furthermore, the cotangent lifted method is the unique one-step method $\mathbf{p}_n \mapsto \mathbf{p}_{n+1}$ satisfying

$$\langle \mathbf{p}_{n+1}, \delta\mathbf{y}_{n+1} \rangle = \langle \mathbf{p}_n, \delta\mathbf{y}_n \rangle, \tag{3.14}$$

where $\delta \mathbf{y}_{n+1}$ solves the variational equation associated with the one-step method

$$\delta \mathbf{y}_{n+1} = T_{\mathbf{y}_n}\Phi_{\Delta t}[n,\mathbf{g}]\delta \mathbf{y}_n,$$

for arbitrary $\delta\mathbf{y}_n$ and arbitrary right-hand-side of the ODE g. Furthermore, an alternative representation of the cotangent lifted one-step method is

$$\mathbf{p}_n = \left(\frac{\delta \mathbf{y}_{n+1}}{\delta \mathbf{y}_n}\right)^* \mathbf{p}_{n+1}. \tag{3.15}$$

Proof. To prove the first statement, we have to show that the discrete adjoint system $\mathbf{y}_{n+1} = \Phi_{\Delta t}[n,\mathbf{g}](\mathbf{y}_n)$ yield the method given by the cotangent lift of $\Phi_{\Delta t}[n,\mathbf{g}]$ applied to the continuous adjoint system. To each $\mathbf{y}_n$, we define an associated adjoint variable $\mathbf{p}_n$. Define the discrete action by

$$\mathbb{S}(\mathbf{y}_n,\mathbf{p}_{n+1}) = \langle \mathbf{p}_{n+1}, \Phi_{\Delta t}[n,\mathbf{g}](\mathbf{y}_n)\rangle.$$

The discrete adjoint system is then given by [49]

$$\mathbf{y}_{n+1} = \frac{\delta}{\delta \mathbf{p}_{n+1}}\mathbb{S}(\mathbf{y}_n,\mathbf{p}_{n+1}),$$
$$\mathbf{p}_{n} = \frac{\delta}{\delta \mathbf{y}_{n}}\mathbb{S}(\mathbf{y}_n,\mathbf{p}_{n+1}).$$

The first equation is simply the one-step method for the base ODE,

$$\mathbf{y}_{n+1} = \frac{\delta}{\delta \mathbf{p}_{n+1}}\mathbb{S}(\mathbf{y}_n,\mathbf{p}_{n+1}) = \Phi_{\Delta t}[n,\mathbf{g}](\mathbf{y}_n).$$

The second equation can be computed, for an arbitrary variation $\delta\mathbf{y}$,

$$\begin{aligned}\langle \mathbf{p}_n, \delta\mathbf{y}\rangle &= \frac{d}{d\epsilon}\Big|_{\epsilon=0}\mathbb{S}(\mathbf{y}_n+\epsilon\delta\mathbf{y},\mathbf{p}_{n+1}) = \left\langle \mathbf{p}_{n+1}, \frac{d}{d\epsilon}\Big|_{\epsilon=0}\Phi_{\Delta t}[n,\mathbf{g}](\mathbf{y}_n+\epsilon\delta\mathbf{y})\right\rangle \\ &= \langle \mathbf{p}_{n+1}, T_{\mathbf{y}_n}\Phi_{\Delta t}[n,\mathbf{g}]\delta\mathbf{y}\rangle = \langle T^*_{\mathbf{y}_n}\Phi_{\Delta t}[n,\mathbf{g}]]\mathbf{p}_{n+1}, \delta\mathbf{y}\rangle.\end{aligned}$$

Since this holds for any $\delta\mathbf{y}$, the second equation is

$$\mathbf{p}_n = T^*\Phi_{\Delta t}[n,\mathbf{g}]\mathbf{p}_{n+1},$$

or, equivalently,

$$\mathbf{p}_{n+1} = T^*\Phi^{-1}_{\Delta t}[n,g]\mathbf{p}_n,$$

as was to be shown.

For the second statement of the theorem that the cotangent lift of the one-step method satisfies equation (3.14), we use that the cotangent lifted method is given by $\mathbf{p}_n = T^*_{\mathbf{y}_n}\Phi_{\Delta t}[n,\mathbf{g}]\mathbf{p}_{n+1}$, from which,

$$\langle \mathbf{p}_n, \delta\mathbf{y}_n\rangle = \langle T^*_{\mathbf{y}_n}\Phi_{\Delta t}[n,\mathbf{g}]\mathbf{p}_{n+1}, \delta\mathbf{y}_n\rangle = \langle \mathbf{p}_{n+1}, T_{\mathbf{y}_n}\Phi_{\Delta t}[n,\mathbf{g}]\delta\mathbf{y}_n\rangle = \langle \mathbf{p}_{n+1}, \delta\mathbf{y}_{n+1}\rangle.$$

For uniqueness, suppose there are two one-step methods $\mathbf{p}_n \mapsto \mathbf{p}_{n+1}$ and $\mathbf{p}_n \mapsto \tilde{\mathbf{p}}_{n+1}$ satisfying (3.14), i.e.,

$$\langle \mathbf{p}_{n+1}, \delta\mathbf{y}_{n+1}\rangle = \langle \mathbf{p}_n, \delta\mathbf{y}_n\rangle = \langle \tilde{\mathbf{p}}_{n+1}, \delta\mathbf{y}_{n+1}\rangle.$$

Using $\delta\mathbf{y}_{n+1} = T_{\mathbf{y}_n}\Phi_{\Delta t}[n,\mathbf{g}]\delta\mathbf{y}_n$, we have

$$\langle \mathbf{p}_{n+1}, T_{\mathbf{y}_n}\Phi_{\Delta t}[n,\mathbf{g}]\delta\mathbf{y}_n\rangle = \langle \tilde{\mathbf{p}}_{n+1}, T_{\mathbf{y}_n}\Phi_{\Delta t}[n,\mathbf{g}]\delta\mathbf{y}_n\rangle.$$

Equivalently,

$$\langle (T^*_{\mathbf{y}_n}\Phi_{\Delta t}[n,\mathbf{g}])(\mathbf{p}_{n+1}-\tilde{\mathbf{p}}_{n+1}), \delta\mathbf{y}_n\rangle = 0.$$

Since $\delta\mathbf{y}_n$ is arbitrary, we have $(T^*_{\mathbf{y}_n}\Phi_{\Delta t}[n,\mathbf{g}])(\mathbf{p}_{n+1}-\tilde{\mathbf{p}}_{n+1}) = 0$. Finally, since the one-step method is a local diffeomorphism, the operator $T^*_{\mathbf{y}_n}\Phi_{\Delta t}[n,\mathbf{g}]$ has trivial kernel, and hence, $\mathbf{p}_{n+1} = \tilde{\mathbf{p}}_{n+1}$.

Finally, the representation (3.15) follows from observing that since $\mathbf{y}_{n+1}$ is a function of $\mathbf{y}_n$, their variations are related by

$$\delta \mathbf{y}_{n+1} = \frac{\delta \mathbf{y}_{n+1}}{\delta \mathbf{y}_n} \delta \mathbf{y}_n. \tag{3.16}$$

Substituting this into (3.14) yields

$$\langle \mathbf{p}_n, \delta \mathbf{y}_n \rangle = \langle \mathbf{p}_{n+1}, \delta \mathbf{y}_{n+1} \rangle = \left\langle \mathbf{p}_{n+1}, \frac{\delta \mathbf{y}_{n+1}}{\delta \mathbf{y}_n} \delta \mathbf{y}_n \right\rangle = \left\langle \left(\frac{\delta \mathbf{y}_{n+1}}{\delta \mathbf{y}_n} \right)^* \mathbf{p}_{n+1}, \delta \mathbf{y}_n \right\rangle.$$

Again, $\delta \mathbf{y}_n$ is arbitrary and thus, equation (3.15) holds. □

Analogous to the discussion of semi-discretization in Section 3.1, this commutative diagram leads to a non-trivial structural condition that an OtD method (where here discretize refers to one-step time integration) must satisfy in order to be equivalent to a DtO method; namely, the one-step method used in the OtD method must be a symplectic integrator and, in particular, equivalent to the cotangent lift of a one-step method (here, by equivalent, we mean that we are allowing for equivalent representations of the same time integration scheme, such as the concept of reducibility in the context of Runge–Kutta methods [19]).

The previous theorem shows that the cotangent lifted method is the unique one-step method covering the forward one-step method and satisfying the adjoint quadratic conservation law (3.14). This explains the observed discrepancy in the literature for discrete gradients produced by DtO and OtD methods for ODEs, as discussed in Section 1.1, since utilizing a time integration scheme in an OtD method which is not the cotangent lifted method cannot satisfy the discrete adjoint quadratic conservation law and hence, cannot produce exact discrete gradients.

Order of the Cotangent Lifted Method. In the context of adjoint sensitivity analysis, since the conservation law (3.14) holds, the cotangent lifted method produces the exact discrete gradient [46] for the discrete minimization problem

$$\min_{\mathbf{y}^*} C(\mathbf{y}_N) \text{ such that } \mathbf{y}_{n+1} = \Phi_{\Delta t}[n, \mathbf{g}](\mathbf{y}_n), n = 0, \dots, N-1, \ \mathbf{y}_0 = \mathbf{y}^*,$$

where N is the index corresponding to t_f. We now address the question of adjoint consistency, i.e., how well the discrete gradient produced from the cotangent lifted method approximates the time-continuous gradient, corresponding to the time-continuous minimization problem

$$\min_{\mathbf{y}^*} C(\mathbf{y}(t_f)) \text{ such that } \dot{\mathbf{y}}(t) = \mathbf{g}(t, \mathbf{y}), \mathbf{y}(0) = \mathbf{y}^*.$$

In essence, we would like to transfer the order of accuracy of the one-step method to the order of accuracy of its cotangent lift. To do this, we will need an additional assumption on the one-step method; namely, that taking variations and applying the one-step method commute. To be more precise, we introduce the following definitions.

The *variational system* associated with the ODE $\dot{\mathbf{y}} = \mathbf{g}(t, \mathbf{y})$ on V is given by the ODE together with its variational equation, i.e.,

$$\frac{d}{dt} \begin{pmatrix} \mathbf{y} \\ \delta \mathbf{y} \end{pmatrix} = \begin{pmatrix} \mathbf{g}(t, \mathbf{y}) \\ D_{\mathbf{y}} \mathbf{g}(t, \mathbf{y}) \delta \mathbf{y} \end{pmatrix} =: \widetilde{\mathbf{g}} \left(t, \begin{pmatrix} \mathbf{y} \\ \delta \mathbf{y} \end{pmatrix} \right). \tag{3.17}$$

We denote the right hand side of the variational system as $\widetilde{g}$, viewed as an ODE on $V \times V$.

Let $\Phi_{\Delta t}[\cdot, \cdot]$ be a one-step method. The *variational system* associated with the one-step method is given by the one-step method together with its variational equation, i.e.,

$$\mathbf{y}_{n+1} = \Phi_{\Delta t}[n, \mathbf{g}](\mathbf{y}_n), \tag{3.18a}$$

$$\delta \mathbf{y}_{n+1} = T_{\mathbf{y}_n} \Phi_{\Delta t}[n, \mathbf{g}] \delta \mathbf{y}_n. \tag{3.18b}$$

We say that the one-step method is *variationally equivariant* if the one-step method applied to the variational system associated with the ODE (3.17) is the same as the variational system associated with the one-step method (3.18). That is,

$$\Phi_{\Delta t}[n, \widetilde{\mathbf{g}}] \begin{pmatrix} \mathbf{y}_n \\ \delta \mathbf{y}_n \end{pmatrix} = \begin{pmatrix} \Phi_{\Delta t}[n, \mathbf{g}](\mathbf{y}_n) \\ T_{\mathbf{y}_n} \Phi_{\Delta t}[n, \mathbf{g}] \delta \mathbf{y}_n \end{pmatrix}.$$

Informally, a one-step method is variationally equivariant if applying the one-step method and taking variations commute. For example, this is true for Runge–Kutta methods (RK) [19], more generally for Generalized Additive Runge–Kutta methods (GARK) [32], and exponential Runge–Kutta methods.

We can now relate the order of accuracy for the discrete gradients obtained from the cotangent lifted method to the order of accuracy of the forward method. The following analysis closely mirrors the corresponding result for RK and GARK schemes [32; 44].

Define the *solution sensitivity matrix* associated with an ODE $\dot{\mathbf{y}} = \mathbf{g}(t, \mathbf{y})$ on V as

$$S_{t_2,t_1}(\mathbf{y}(t_1)) = \frac{\delta \mathbf{y}(t_2)}{\delta \mathbf{y}(t_1)}, \ t_2 \geq t_1,$$

where $\mathbf{y}(t)$ is the exact solution of the ODE. Note we view the solution sensitivity matrix as a linear mapping $S_{t_2,t_1}(\mathbf{y}(t_1)) : V \to V$.

Proposition 3.3. *Let $\Phi_{\Delta t}$ be a variationally equivariant one-step method. Assume that the ODE $\dot{\mathbf{y}} = \mathbf{g}(t, \mathbf{y})$ is smooth and has a smooth solution. Furthermore, assume sufficient regularity such that the solution sensitivity matrix and the derivative of the cost function are Lipschitz,*

$$\|S_{t_2,t_1}(\mathbf{y}) - S_{t_2,t_1}(\mathbf{y}')\|_{op} \leq c \|\mathbf{y} - \mathbf{y}'\|_V, \tag{3.19}$$

$$\|DC(\mathbf{y}) - DC(\mathbf{y}')\|_{V^*} \leq c \|\mathbf{y} - \mathbf{y}'\|_V, \tag{3.20}$$

for all $\mathbf{y}, \mathbf{y}' \in V$ and $t_2 \geq t_1$ (where $\|\cdot\|_V$ denotes a norm on V, $\|\cdot\|_{V^*}$ the associated dual norm, and $\|\cdot\|_{op}$ the operator norm; this result is independent of the norm since V is finite-dimensional.) Assume that the one-step method $\mathbf{y}_{n+1} = \Phi_{\Delta t}[n, \mathbf{g}](\mathbf{y}_n)$ converges with order r,

$$\mathbf{y}_n - \mathbf{y}(t_n) = \mathcal{O}(\Delta t^r).$$

Then, the cotangent lifted method $\mathbf{p}_n = T^*_{\mathbf{y}_n} \Phi_{\Delta t}[n, \mathbf{g}] \mathbf{p}_{n+1}$ with terminal condition $\mathbf{p}_n = DC(\mathbf{y}_n)$ approximates the solution of the time-continuous adjoint equation with order r

$$\mathbf{p}_n - \mathbf{p}(t_n) = \mathcal{O}(\Delta t^r),$$

where $\mathbf{p}(t)$ is the exact solution of

$$\dot{\mathbf{p}} = -[D\mathbf{g}(t, \mathbf{y})] \mathbf{p}, \ \mathbf{p}(t_f) = DC\left(\mathbf{y}(t_f)\right).$$

Proof. The solution $\delta \mathbf{y}(t)$ for the second component of the time-continuous variational system (3.17) is simply propagated by the solution sensitivity matrix, $\delta \mathbf{y}(t_2) = S_{t_2,t_1}(\mathbf{y}(t_1)) \delta \mathbf{y}(t_1)$ [32].

At the discrete level, the solution of the variational equation associated with the one-step method $\delta \mathbf{y}_{n+1} = T_{\mathbf{y}_n} \Phi_{\Delta t}[n, \mathbf{g}] \delta \mathbf{y}_n = \delta \mathbf{y}_{n+1} / \delta \mathbf{y}_n$, from equation (3.16), can be represented $\delta \mathbf{y}_{n_2} = S^{\Delta t}_{n_2,n_1}(\mathbf{y}_{n_1}) \delta \mathbf{y}_{n_1}$, where $S^{\Delta t}_{n_2,n_1}$ is the numerical solution sensitivity matrix

$$S^{\Delta t}_{n_2,n_1}(\mathbf{y}_{n_1}) = \frac{\delta \mathbf{y}_{n_2}}{\delta \mathbf{y}_{n_1}}.$$

By assumption, the one-step method is variationally equivariant, so the solution $\{\mathbf{y}_n, \delta \mathbf{y}_n\}$ of the variational system associated with the one-step method is equivalently given by the one-step method applied to the time-continuous variational system. In particular, this solution then inherits the order of accuracy of the one-step method. Furthermore, the stability for $\{\delta \mathbf{y}_n\}$ is precisely the linear stability of the one-step method. Thus, we have convergence of order r for $\{\delta \mathbf{y}_n\}$,

$$\delta \mathbf{y}_n = \delta \mathbf{y}(t_n) + \mathcal{O}(\Delta t^r).$$

In particular, this implies that the numerical sensitivity matrix approximates the continuous sensitivity matrix to order r, since for arbitrary $\mathbf{v} \in V$ and initial condition $\delta \mathbf{y}_{n_1} = \mathbf{v} = \delta \mathbf{y}(t_1)$, we have

$$\mathcal{O}(\Delta t^r) = \delta \mathbf{y}(t_2) - \delta \mathbf{y}_{n_2} = \Big(S_{t_2,t_1}(\mathbf{y}(t_1)) - S^{\Delta t}_{n_2,n_1}(\mathbf{y}(t_1))\Big)\mathbf{v}.$$

Thus,

$$S_{t_2,t_1}(\mathbf{y}) - S^{\Delta t}_{n_2,n_1}(\mathbf{y}) = \mathcal{O}(\Delta t^r).$$

From Theorem (3.3), we know that

$$\mathbf{p}_n = \left(\frac{\delta \mathbf{y}_{n+1}}{\delta \mathbf{y}_n}\right)^* \mathbf{p}_{n+1},$$

and hence

$$\mathbf{p}_n = \left(S^{\Delta t}_{N,n}\right)^* \mathbf{p}_n = \left(S^{\Delta t}_{N,n}(\mathbf{y}_n)\right)^* DC(\mathbf{y}_n),$$

whereas the time-continuous adjoint variable similarly satisfies

$$\mathbf{p}(t_n) = \frac{\delta C(\mathbf{y}(t_f))}{\delta \mathbf{y}(t_n)} = \Big(S^{\Delta t}_{t_f,t_n}(\mathbf{y}(t_n))\Big)^* DC(\mathbf{y}(t_f)).$$

Combining the above, we obtain

$$\begin{aligned}
\mathbf{p}_n - \mathbf{p}(t_n) &= \left(S^{\Delta t}_{N,n}(\mathbf{y}_n)\right)^* DC(\mathbf{y}_n) - \Big(S^{\Delta t}_{t_f,t_n}(\mathbf{y}(t_n))\Big)^* DC(\mathbf{y}(t_f)) \\
&= \left(S^{\Delta t}_{N,n}(\mathbf{y}_n)\right)^* \left(DC(\mathbf{y}_n) - DC(\mathbf{y}(t_f))\right) \\
&\quad + \left(S^{\Delta t}_{N,n}(\mathbf{y}_n) - S_{t_f,t_n}(\mathbf{y}_n)\right)^* DC(\mathbf{y}(t_f)) + (S_{t_f,t_n}(\mathbf{y}_n) - S_{t_f,t_n}(\mathbf{y}(t_n)))^* DC(\mathbf{y}(t_f)).
\end{aligned}$$

The result now immediately follows. □

To prove the above proposition, we used variational equivariance to transfer the order of the one-step method to the order of the linearization of the one-step method, which is equivalently the one-step method of the linearization. Note that variational equivariance is a sufficient condition to be able to transfer the order, i.e., variational equivariance is a sufficient condition for adjoint consistency of the cotangent lifted method. However, even without a variationally equivariant method, if one knows that the linearization of the one-step method retains the order of the one-step method, then the preceding result still follows. The contrapositive implies that if we do not have adjoint consistency, then the one-step method is not variationally equivariant, as the following example shows.

Example 3.1. *As a counterexample of where the above proposition fails without variational equivariance, in [1], it is shown that discrete adjoints for adaptive time-stepping methods do not retain the consistency order of the forward method, leading in the worst case to $\mathcal{O}(1)$ errors in the gradient, i.e., the discrete adjoint of an adaptive time-stepping method is not adjoint consistent. From our perspective, we can understand this from the fact that an adaptive time-stepping method is not variationally equivariant, even if the underlying one-step method is.*

To see this explicitly, consider the time-independent ODE $\dot{\mathbf{y}}(t) = \mathbf{g}(t, \mathbf{y}(t)), \mathbf{y}(t_0) = \mathbf{y}_0$ expressed in time-independent form as

$$\frac{d}{dt}\begin{pmatrix}\mathbf{y}(t)\\ s(t)\end{pmatrix} = \begin{pmatrix}\mathbf{g}(s(t), \mathbf{y}(t))\\ 1\end{pmatrix}, \quad \begin{pmatrix}\mathbf{y}(t_0)\\ s(t_0)\end{pmatrix} = \begin{pmatrix}\mathbf{y}_0\\ t_0\end{pmatrix}. \tag{3.21}$$

For simplicity in presentation, we consider an adaptive forward Euler method applied to the above system, although a similar discussion follows similarly for other one-step methods. Note that the underlying forward Euler method is variationally equivariant, but, as we will see, the adaptive method is not. Applied to the above system, the adaptive forward Euler method is

$$\begin{pmatrix} \mathbf{y}_{n+1} \\ s_{n+1} \end{pmatrix} = \begin{pmatrix} \mathbf{y}_n \\ s_n \end{pmatrix} + h_n \begin{pmatrix} \mathbf{g}(s_n, \mathbf{y}_n) \\ 1 \end{pmatrix}, \tag{3.22a}$$

$$h_{n+1} = S(\mathbf{y}_n, h_n, s_n), \tag{3.22b}$$

where S is a step-size controller, which we assume to be differentiable. The linearization of this method is then

$$\begin{pmatrix} \delta\mathbf{y}_{n+1} \\ \delta s_{n+1} \end{pmatrix} = \begin{pmatrix} \delta\mathbf{y}_n \\ \delta s_n \end{pmatrix} + h_n \begin{pmatrix} D_1\mathbf{g}(s_n, \mathbf{y}_n)\delta s_n + D_2\mathbf{g}(s_n, \mathbf{y}_n)\delta\mathbf{y}_n \\ 0 \end{pmatrix} + \delta h_n \begin{pmatrix} \mathbf{g}(s_n, \mathbf{y}_n) \\ 1 \end{pmatrix}, \tag{3.23a}$$

$$\delta h_{n+1} = D_1 S(\mathbf{y}_n, h_n, s_n)\delta\mathbf{y}_n + D_2 S(\mathbf{y}_n, h_n, s_n)\delta h_n + D_3 S(\mathbf{y}_n, h_n, s_n)\delta s_n. \tag{3.23b}$$

Equations (3.22) *and* (3.23) *form the variational system associated with the adaptive Euler method. To see that the method is not variationally equivariant, we reverse this process; we first linearize* (3.21) *and subsequently, apply the adaptive time-stepping method. The linearization of* (3.21) *is*

$$\frac{d}{dt}\begin{pmatrix} \delta\mathbf{y}(t) \\ \delta s(t) \end{pmatrix} = \begin{pmatrix} D_1\mathbf{g}(s(t), \mathbf{y}(t))\delta s(t) + D_2\mathbf{g}(s(t), y(t))\delta\mathbf{y}(t) \\ 0 \end{pmatrix}. \tag{3.24}$$

We then apply the adaptive Euler method to the time-continuous variational system (3.21), (3.24), *which yields*

$$\begin{pmatrix} \mathbf{y}_{n+1} \\ s_{n+1} \\ \delta\mathbf{y}_{n+1} \\ \delta s_{n+1} \end{pmatrix} = \begin{pmatrix} \mathbf{y}_n \\ s_n \\ \delta\mathbf{y}_n \\ \delta s_n \end{pmatrix} + h_n \begin{pmatrix} \mathbf{g}(s_n, \mathbf{y}_n) \\ 1 \\ D_1\mathbf{g}(s_n, \mathbf{y}_n)\delta s_n + D_2\mathbf{g}(s_n, \mathbf{y}_n)\delta\mathbf{y}_n \\ 0 \end{pmatrix}, \tag{3.25a}$$

$$h_{n+1} = S(\mathbf{y}_n, h_n, s_n). \tag{3.25b}$$

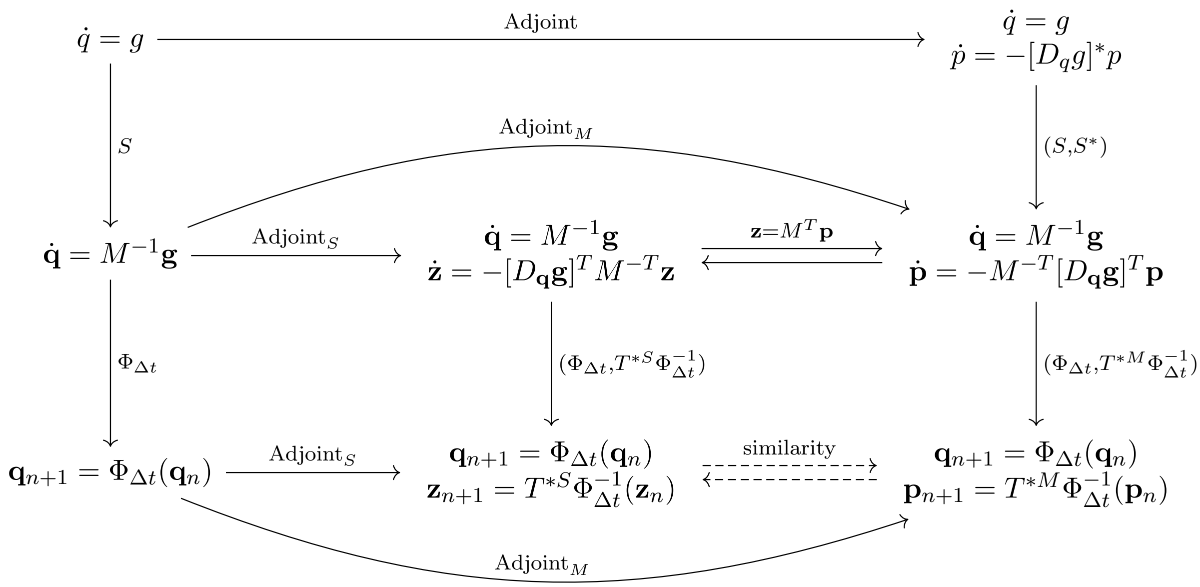
Comparing the variational system of the adaptive method, (3.22) *and* (3.23)*, to the adaptive method applied to the time-continuous variational system,* (3.25)*, we see that these are not equivalent and hence, the adaptive method is not variationally equivariant. More precisely, the lack of variational equivariance arises from the δh_n term in equation* (3.23a)*. We only have variational equivariance when $\delta h_n = 0$, i.e., when $D_1 S = 0, D_2 S = 0, D_3 S = 0$, i.e., there is no adaptive time-stepping. The terms which break the variational equivariance, namely, the derivatives of S, are precisely the terms which lead to adjoint inconsistency as shown in [1].*

In this section, we considered one-step methods and their associated cotangent lifts. One can ask what happens in the case of multi-step methods. In [45], it was shown that the discrete adjoint associated with a multistep method does not generally retain the consistency order of the forward method, both due to error in the backpropagation as well as initialization error for the terminal condition. From our geometric perspective, one-step methods are natural to consider since, at each time-step, a one-step method defines a map $V \to V$ and hence, one can naturally define its cotangent lift. On the other hand, for a multistep method, at each time step, it defines a map $V \times \cdots \times V \to V$ for which there is no immediately obvious notion of cotangent lift. We will now combine the discussions of semi-discretization and time integration together.

3.3. **Naturality of the Full Discretization.** As we have seen, semi-discretization of the evolution equation induces a dual semi-discretization for the corresponding adjoint equation. Furthermore, time integration of the semi-discrete evolution equation induces a dual time integration of the semi-discrete adjoint equation.

Consider the case of Galerkin semi-discretization. We would like to connect the semi-discretization and time integration commutative diagrams together. To do this, first note, as alluded to in Section 3.1, the process of adjoining at the semi-discrete level depends on the (representation of the) duality pairing. This is of course also true for adjoining at the fully discrete level, since the cotangent lift of a map depends on the duality pairing, equation (3.12).

Combining the discussions of Section 3.1 and Section 3.2, we arrive at the following commutative diagram.
(3.26)



In the above diagram, we again denote for brevity

$$g = Aq + f(t, q),$$
$$\mathbf{g} = K\mathbf{q} + \mathbf{f}(t, \mathbf{q}),$$

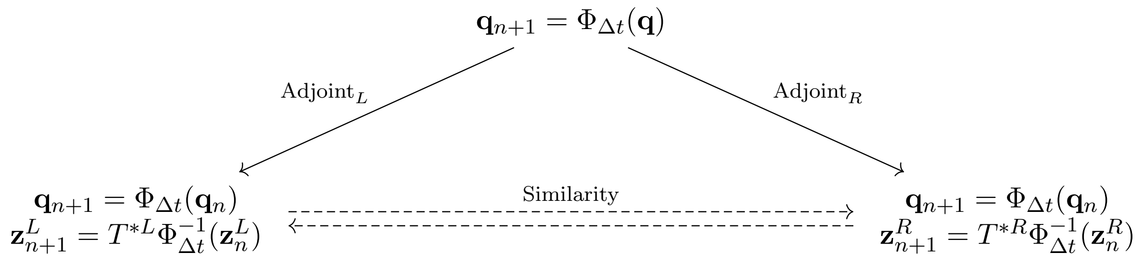
and have suppressed the additional arguments of the one-step method, but they are given by the corresponding semi-discrete ODE. Other than the dashed arrows in the above diagram, we have already explained all of the elements of the diagram. The equivalence of the two vertices connected by the dashed arrows is the statement that they are related by a similarity transformation $T^{*M}\Phi_{\Delta t}^{-1} = M^{-T}T^{*S}\Phi_{\Delta t}^{-1}M^T$ which immediately follows from the definition of the cotangent lift, equation (3.12). Finally, note that we depict these arrows are dashed, not solid, because they represent a weaker version of equivalence. Namely, although they are equivalent assuming exact arithmetic, they will in general not be equivalent with floating point arithmetic; in particular, if M is poorly conditioned or solved indirectly, e.g. using iterative methods as is standard in non-DG FEM discretizations, the two fully discrete methods may produce different results. Also, as noted in Remark 3.2, time integration of the semi-discrete adjoint system induced by different duality pairings may lead to different equilibriium characteristics of the discrete solution.

To elaborate further on this discrepancy, let us focus on the bottom loop of the above diagram and consider a more general method-of-lines semi-discretization, as defined in Section 3.1, and ask generally what is the result of using two different duality pairings. Consider two duality pairings $\langle \cdot, \cdot \rangle_L$ and $\langle \cdot, \cdot \rangle_R$ on $X_h \times X_h^*$ which are related by an invertible operator P via

$$\langle \mathbf{w}, \mathbf{v} \rangle_L = \langle \mathbf{w}, P\mathbf{v} \rangle_R.$$

Now, consider a method-of-lines semi-discretization $\dot{\mathbf{q}} = K_h(\mathbf{q})$ and its time integration by a one-step method $\mathbf{q}_{n+1} = \Phi_{\Delta t}(\mathbf{q})$, where for brevity we denote $K_h = K_h[A, f]$ and $\Phi_{\Delta t} = \Phi_{\Delta t}[n, K_h[A, f]]$. The bottom loop of diagram (3.26) is a special case of the following commutative diagram,

(3.27)



,

where the similarity transformation is given by $T^{*L}\Phi^{-1}_{\Delta t} = P^{-*R}(T^{*R}\Phi^{-1}_{\Delta t})P^{*R}$. Substituting this similarity transformation into the bottom left vertex of diagram (3.27), we have

$$\mathbf{z}^L_{n+1} = T^{*L}\Phi^{-1}_{\Delta t}(\mathbf{z}^L_n) = P^{-*R}(T^{*R}\Phi^{-1}_{\Delta t})P^{*R}\mathbf{z}^L_n.$$

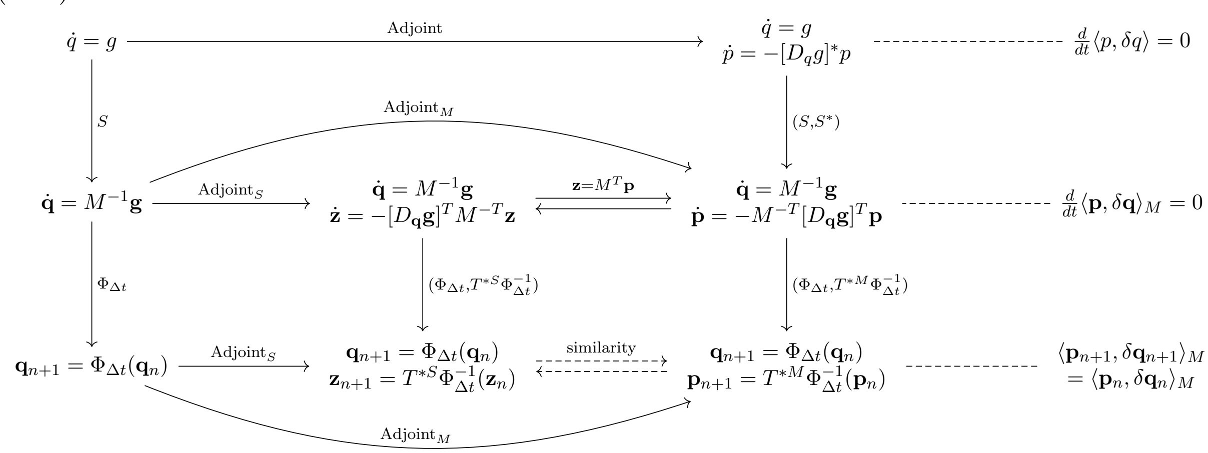
Equivalently,

$$P^{*R}\mathbf{z}^L_{n+1} = T^{*R}\Phi^{-1}_{\Delta t}(P^{*R}\mathbf{z}^L_n). \tag{3.28}$$

Taking $\mathbf{z}^R_{n+1} = P^{*R}\mathbf{z}^L_{n+1}$ of course reproduces the bottom right vertex of diagram (3.27), but note that in general these can produce different numerical results with floating point arithmetic. In particular, if the linear system associated with computing $\mathbf{z}^R_{n+1} = T^{*R}\Phi^{-1}_{\Delta t}(\mathbf{z}^R_n)$ is poorly conditioned, we can instead utilize the formulation (3.28) and view P^{*R} as a preconditioner.

Returning to the full diagram (3.26), we also note that by Theorems 3.1 and 3.3, the semi-discretization and time integration of adjoint systems are uniquely characterized by their respective conservation properties. Thus, to concisely summarize the results derived in this paper, we append these to the diagram.

(3.29)



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Conclusion

In this paper, we developed a Hamiltonian formulation of the adjoint system associated with an evolutionary partial differential equation. This led to natural geometric characterizations of structure-preserving semi-discretization and time integration in terms of semi-discrete and fully discrete adjoint-variational quadratic conservation laws. In particular, the commutativity of DtO with OtD can be uniquely characterized by these adjoint-variational quadratic conservation laws.

For future research, we plan to explore applications of this geometric framework in constructing robust geometric discretizations of adjoint systems for evolutionary PDEs. An interesting related direction would be to combine semi-discretization and time integration procedures into a single space-time discretization procedure and analogously examine the question of DtO versus OtD in this more general setting. It is plausible that this question could be analogously characterized in terms of multisymplectic geometry, which is the space-time generalization of symplectic geometry, and multisymplectic discretizations [5; 8; 30; 48]. Viewing the adjoint system as an equation in space-time instead of as an evolution equation could lead to efficient methods for structure-preserving space-time adjoint sensitivity analysis, utilizing unified space-time discretization methods, e.g.,[23; 40], and parallel all-at-once space-time solvers, e.g., [11; 22].

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References

[1] M. Alexe and A. Sandu. On the discrete adjoints of adaptive time stepping algorithms. *Journal of Computational and Applied Mathematics*, 233(4):1005–1020, 2009. ISSN 0377-0427. doi: https://doi.org/10.1016/j.cam.2009.08.109. (Page 3, 22, 23)

[2] D. N. Arnold, F. Brezzi, B. Cockburn, and L. D. Marini. Unified analysis of discontinuous Galerkin methods for elliptic problems. *SIAM Journal on Numerical Analysis*, 39(5):1749–1779, 2002. doi: 10.1137/S0036142901384162. (Page 3)

[3] M. Benning, E. Celledoni, M. J. Ehrhardt, B. Owren, and C.-B. Schönlieb. Deep learning as optimal control problems: Models and numerical methods. *J. Comput. Dyn.*, 6(2):171–198, 2019. (Page 2)

[4] J. F. Bonnans and J. Laurent-Varin. Computation of order conditions for symplectic partitioned Runge–Kutta schemes with application to optimal control. *Numerische Mathematik*, 103:1–10, 2006. doi: 10.1007/s00211-005-0661-y. (Page 18)

[5] T. J. Bridges and S. Reich. Multi-symplectic integrators: numerical schemes for Hamiltonian PDEs that conserve symplecticity. *Physics Letters A*, 284(4):184 – 193, 2001. (Page 26)

[6] D. G. Cacuci. Sensitivity theory for nonlinear systems. I. Nonlinear functional analysis approach. *J. Math. Phys.*, 22(12):2794–2802, 1981. (Page 2)

[7] Y. Cao, S. Li, L. Petzold, and R. Serban. Adjoint sensitivity analysis for differential-algebraic equations: The adjoint DAE system and its numerical solution. *SIAM J. Sci. Comput.*, 24(3): 1076–1089 (14 pages), 2003. (Page 2)

[8] J. Chen. Variational formulation for the multisymplectic Hamiltonian systems. *Lett. Math. Phys.*, 71(3):243–253, 2005. (Page 26)

[9] R. T. Q. Chen, Y. Rubanova, J. Bettencourt, and D. Duvenaud. Neural ordinary differential equations. In *Proceedings of the 32nd International Conference on Neural Information Processing Systems*, NIPS'18, page 6572–6583, Red Hook, NY, USA, 2018. Curran Associates Inc. (Page 2)

[10] P. R. Chernoff and J. E. Marsden. *Properties of Infinite Dimensional Hamiltonian Systems*. Springer Berlin, Heidelberg, 1974. doi: 10.1007/BFb0073665. (Page 4, 7)

[11] F. Danieli, B. S. Southworth, and A. J. Wathen. Space-time block preconditioning for incompressible flow. *SIAM Journal on Scientific Computing*, 44(1):A337–A363, 2022. (Page 26)

[12] D. Dopico, Y. Zhu, A. Sandu, and C. Sandu. Direct and Adjoint Sensitivity Analysis of Ordinary Differential Equation Multibody Formulations. *Journal of Computational and Nonlinear Dynamics*, 10(1):7 pages, 2014. ISSN 1555-1415. doi: 10.1115/1.4026492. (Page 2)

[13] P. Eichmeir, T. Lauß, S. Oberpeilsteiner, K. Nachbagauer, and W. Steiner. The Adjoint Method for Time-Optimal Control Problems. *Journal of Computational and Nonlinear Dynamics*, 16(2):021003, 2020. ISSN 1555-1415. doi: 10.1115/1.4048808. (Page 2)

[14] U. S. Fjordholm, S. Mishra, and E. Tadmor. Well-balanced and energy stable schemes for the shallow water equations with discontinuous topography. *Journal of Computational Physics*, 230(14):5587–5609, 2011. (Page 14)

[15] A. Gholaminejad, K. Keutzer, and G. Biros. Anode: Unconditionally accurate memory-efficient gradients for neural odes. In *Proceedings of the Twenty-Eighth International Joint Conference on Artificial Intelligence, IJCAI-19*, pages 730–736. IJCAI, 2019. doi: 10.24963/ijcai.2019/103. (Page 2)

[16] M. B. Giles and N. A. Pierce. An introduction to the adjoint approach to design. *Flow, Turbulence and Combustion*, 65:393–415, 2000. (Page 2)

[17] M. B. Giles and E. Süli. Adjoint methods for PDEs: a posteriori error analysis and postprocessing by duality. *Acta Numerica*, 11:145–236, 2002. doi: 10.1017/S096249290200003X. (Page 2, 10)

[18] A. Griewank. A mathematical view of automatic differentiation. In *Acta Numer.*, volume 12, pages 321–398. Cambridge University Press, 2003. (Page 2)

[19] E. Hairer, G. Wanner, and C. Lubich. *Geometric Numerical Integration, Structure-Preserving Algorithms for Ordinary Differential Equations*. Springer Series in Computational Mathematics. Springer Berlin, Heidelberg, 2006. doi: 10.1007/3-540-30666-8. (Page 20, 21)

[20] R. Hartmann. Adjoint consistency analysis of discontinuous Galerkin discretizations. *SIAM Journal on Numerical Analysis*, 45(6):2671–2696, 2007. doi: 10.1137/060665117. (Page 3)

[21] J. E. Hicken, J. Li, O. Sahni, and A. A. Oberai. Adjoint consistency analysis of residual-based variational multiscale methods. *Journal of Computational Physics*, 255:396–406, 2013. ISSN 0021-9991. doi: https://doi.org/10.1016/j.jcp.2013.07.039. (Page 3)

[22] G. Horton and S. Vandewalle. A space-time multigrid method for parabolic partial differential equations. *SIAM Journal on Scientific Computing*, 16(4):848–864, 1995. (Page 26)

[23] G. M. Hulbert and T. J. R. Hughes. Space-time finite element methods for second-order hyperbolic equations. *Computer methods in applied mechanics and engineering*, 84(3):327–348, 1990. (Page 26)

[24] N. H. Ibragimov. Integrating factors, adjoint equations and Lagrangians. *Journal of Mathematical Analysis and Applications*, 318(2):742–757, 2006. (Page 2)

[25] N. H. Ibragimov. A new conservation theorem. *J. Math. Anal. Appl.*, 333(1):311–328, 2007. (Page 2)

[26] M. D. Kulkarni, D. M. Cross, and R. A. Canfield. Discrete adjoint formulation for continuum sensitivity analysis. *AIAA Journal*, 54(2):758–766, 2016. doi: 10.2514/1.J053827. (Page 2, 10)

[27] S. Li and L. Petzold. Adjoint sensitivity analysis for time-dependent partial differential equations with adaptive mesh refinement. *Journal of Computational Physics*, 198(1):310–325, 2004. doi: 10.1016/j.jcp.2003.01.001. (Page 2, 3)

[28] S. Li and L. R. Petzold. Solution adapted mesh refinement and sensitivity analysis for parabolic partial differential equation systems. In L. T. Biegler, M. Heinkenschloss, O. Ghattas, and B. van Bloemen Waanders, editors, *Large-Scale PDE-Constrained Optimization*, pages 117–132. Springer, Berlin, 2003. (Page 2)

[29] J. E. Marsden and T. S. Ratiu. *Introduction to Mechanics and Symmetry.* Texts in Applied Mathematics. Springer New York, NY, 2 edition, 1999. doi: 10.1007/978-0-387-21792-5. (Page 4)

[30] J. E. Marsden and S. Shkoller. Multisymplectic geometry, covariant Hamiltonians, and water waves. *Mathematical Proceedings of the Cambridge Philosophical Society*, 125(3):553–575, 1999. (Page 26)

[31] T. Matsubara, Y. Miyatake, and T. Yaguchi. The symplectic adjoint method: Memory-efficient backpropagation of neural-network-based differential equations. *IEEE Transactions on Neural Networks and Learning Systems*, pages 1–13, 2023. doi: 10.1109/TNNLS.2023.3242345. (Page 2)

[32] M. Narayanamurthi, U. Römer, and A. Sandu. Goal-oriented a posteriori estimation of numerical errors in the solution of multiphysics systems. *arXiv preprint arXiv:2001.08824*, 2020. (Page 21)

[33] J. Neerven. *The Adjoint of a Semigroup of Linear Operators.* Springer Berlin, Heidelberg, 1992. doi: 10.1007/BFb0085008. (Page 6, 8)

[34] V. T. Nguyen, D. Georges, and G. Besançon. State and parameter estimation in 1-D hyperbolic PDEs based on an adjoint method. *Automatica*, 67(C):185–191, May 2016. ISSN 0005-1098. (Page 2)

[35] A. Noack and A. Walther. Adjoint concepts for the optimal control of Burgers equations. *Comput Optim Applic*, 36:109–133, 2007. doi: 10.1007/s10589-006-0393-7. (Page 2, 3, 10, 17)

[36] D. Onken and L. Ruthotto. Discretize-optimize vs. optimize-discretize for time-series regression and continuous normalizing flows. *arXiv preprint arXiv:2005.13420*, 2020. (Page 2)

[37] A. Pazy. *Semigroups of Linear Operators and Applications to Partial Differential Equations.* Springer New York, New York, NY, 1983. doi: 10.1007/978-1-4612-5561-1. (Page 6)

[38] N. A. Pierce and M. B. Giles. Adjoint recovery of superconvergent functionals from PDE approximations. *SIAM Rev.*, 42(2):247–264, 2000. (Page 2)

[39] J. O. Pralits, C. Airiau, A. Hanifi, and D. S. Henningson. Sensitivity analysis using adjoint parabolized stability equations for compressible flows. *Flow, Turbulence and Combustion*, 65: 321–346, 2000. doi: 10.1023/A:1011434805046. (Page 2, 10)

[40] S. Rhebergen, B. Cockburn, and J. J. W. Van Der Vegt. A space–time discontinuous galerkin method for the incompressible navier–stokes equations. *Journal of computational physics*, 233: 339–358, 2013. (Page 26)

[41] I. M. Ross. A roadmap for optimal control: The right way to commute. *Ann. NY Acad. Sci.*, 1065(1):210–231, 2005. (Page 2)

[42] M. Ross and F. Fahroo. A pseudospectral transformation of the convectors of optimal control systems. *IFAC Proc. Ser.*, 34(13):543–548, 2001. (Page 2)

[43] B. F. Sanders and N. D. Katopodes. Adjoint sensitivity analysis for shallow-water wave control. *Journal of Engineering Mechanics*, 126(9):909–919, 2000. doi: 10.1061/(ASCE) 0733-9399(2000)126:9(909). (Page 2, 10)

[44] A. Sandu. On the properties of Runge-Kutta discrete adjoints. In *Computational Science – ICCS 2006*, page 550–557, Berlin, Heidelberg, 2006. Springer-Verlag. (Page 21)

[45] A. Sandu. On consistency properties of discrete adjoint linear multistep methods. *Tech. Rep. TR-07-40*, 2007. (Page 23)

[46] J. M. Sanz-Serna. Symplectic Runge–Kutta schemes for adjoint equations, automatic differentiation, optimal control, and more. *SIAM Review*, 58(1):3–33, 2016. (Page 2, 3, 5, 10, 18, 20)

[47] Z. Sirkes and E. Tziperman. Finite difference of adjoint or adjoint of finite difference? *Mon. Weather Rev.*, 125(12):3373–3378, 1997. (Page 2)

[48] B. Tran and M. Leok. Multisymplectic Hamiltonian variational integrators. *International Journal of Computer Mathematics (Special Issue on Geometric Numerical Integration, Twenty-Five Years Later)*, 99(1):113–157, 2022. (Page 26)

[49] B. K. Tran and M. Leok. Geometric methods for adjoint systems. *J Nonlinear Sci*, 34(25), 2024. doi: 10.1007/s00332-023-09999-7. (Page 2, 4, 5, 11, 18, 19)

[50] A. Walther. Automatic differentiation of explicit Runge–Kutta methods for optimal control. *Comput Optim Applic*, 36:83–108, 2007. doi: 10.1007/s10589-006-0397-3. (Page 2)

[51] Q. Wang, K. Duraisamy, J. J. Alonso, and G. Iaccarino. Risk assessment of scramjet unstart using adjoint-based sampling. *AIAA J.*, 50(3):581–592, 2012. (Page 2)

[52] K. Yano and S. Ishihara. *Tangent and cotangent bundles: differential geometry*. Pure Appl. Math., No. 16. Marcel Dekker, Inc., New York, 1973. (Page 4)