CONSTRAINT AND STRUCTURE PRESERVATION IN PDE

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Abstract. In this set of notes we examine numerical techniques for preservation of constraints and (geometric) structures in ODE and PDE systems, with application to the Einstein equations. The techniques are based on explicit enforcement of constraints using Lagrange multiplier methods, and hence involve a type of (controlled) projection onto the constraint manifold. The resulting numerical methods always have the following two properties: 1) they produce solutions which are comparable in accuracy to standard methods which do not enforce the constraints, and 2) they enforce the constraints (exactly). They can sometimes be shown to have an additional property, namely 3) they preserve geometric structure such as time-reversibility and symplecticity. The numerical techniques for the ODE case can be found in the literature on constrained molecular dynamics as far back as the early 1990's, but the PDE case has not been completely developed. We use Lagrangian and Hamiltonian formalism for mechanical (finite-dimensional) and field (infinite-dimensional) systems throughout these notes, but also apply the techniques to more general non-variational problems with constraints. In the last section we consider application to various constrained formulations of the Einstein equations.

Contents

1. Lagrange Functional Theory in Banach Spaces

In this section we assemble some nonlinear functional analysis material for understanding constraints in mechanics and field theory. We outline Lagrange functional theory in Banach spaces, the mathematical framework which justifies the use of Lagrange functionals in field theory (and Lagrange multipliers in mechanics). The material in this section can be found in the combination of [11, 26, 27].

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1.1. **Nonlinear Operators, Functionals, and Differentiation in Banach Spaces.** We very briefly summarize some notation and a few standard concepts which we will need from nonlinear functional analysis. Let X and Y be real Banach spaces (abstract complete normed vector, or linear, spaces over the field $\mathbb{R}$) with norms $\|\cdot\|_X$ and $\|\cdot\|_Y$, respectively. We will at times assume that a particular Banach space X also has Hilbert space structure, meaning that the norm is actually induced by an inner-product, $\|\cdot\|_X = (\cdot,\cdot)_X^{1/2}$. We will assume all Banach spaces we encounter are *separable* (have countable bases). In much of what follows, we will be concerned with linear and nonlinear operators (functions, mappings) between Banach spaces, $F : \mathcal{D}(F) \subseteq X \mapsto \mathcal{R}(F) \subseteq Y$, where $\mathcal{D}(F)$, $\mathcal{R}(F)$, and $\mathcal{N}(F)$ represent the domain, range, and null-space (or kernel) of F, respectively. In the special case that the range space $Y \equiv \mathbb{R}$, we refer to F as a (possibly nonlinear) *functional* on X. The space of all *bounded linear* functionals on X is called the (topological) *dual space* of X, and is denoted X^*. We will assume that all Banach spaces X we encounter are *reflexive*, meaning that $(X^*)^* = X$. The space $\mathcal{R}(F) \subseteq Y$ is called *closed* in Y if for any sequence $v_k \in X$ such that $F(v_k)$ converges in Y, there exists $v \in \mathcal{R}(F)$ such that $\lim_{k\to\infty} F(v_k) = F(v)$. If $\mathcal{R}(F) = Y$ it is then trivially closed. The vector space of linear operators $A : X \mapsto Y$ is denoted $L(X,Y)$. If X and Y are Hilbert spaces, the (Hilbert) adjoint of $A \in L(X,Y)$ is the unique $A^T \in L(Y,X)$ satisfying $(Au,v)_Y = (u, A^T v)_X$, $\forall u \in X$, $\forall v \in Y$. The operator $A \in L(X,X)$ is *self-adjoint* if $A = A^T$.

We now briefly review differentiation of nonlinear operators in Banach spaces (cf. [25]). Let X be a Banach space with norm $\|\cdot\|_X$, and let $F(u) : D \subseteq X \mapsto \mathbb{R}$ be a nonlinear functional on D, where D is a nonempty open set. The *Gateaux variation* of F at $u \in D$ in the direction v, if it exists, is defined as

$$VF(u;v) = \left.\frac{d}{d\epsilon} F(u+\epsilon v)\right|_{\epsilon=0} = \lim_{\epsilon\to 0} \frac{F(u+\epsilon v) - F(v)}{\epsilon}. \tag{1}$$

The *first variation* of F at u in the direction v is defined as

$$\delta F = \frac{\delta F}{\delta u} = \epsilon VF(u;v). \tag{2}$$

It is always the case that $VF(u;v)$ is homogeneous in v, meaning that $VF(u;\epsilon v) = \epsilon VF(u;v)$, but VF may not be linear (homogeneous and additive) in v because it is not always additive: $VF(u;v+w) \neq VF(u;v) + VF(u;w)$. However, if $VF(u;v)$ exists for all $v \in X$, and if $VF(u;v)$ is a bounded and linear functional on X, then $VF(u;v)$ is called the *Gateaux (directional, functional, or variational) derivative* of F at u. Since for each argument $u \in X$, the Gateaux derivative $VF(u;v) : X \mapsto L(X,\mathbb{R})$ lies in the dual space X^* of bounded linear functionals on X, any of the following notation (distinct from $VF(u;v)$) is used to denote the action of the Gateaux derivative on $v \in X$ as a bounded linear functional in X^*:

$$F'(u)v = DF(u)v = F'(u)(v) = DF(u)(v) = \langle F'(u), v\rangle = \langle DF(u), v\rangle, \tag{3}$$

where the last four expressions make explicit that the Gateaux derivative of a nonlinear functional at a point u is a linear functional of v. The angle brackets $\langle y, x\rangle$ in the last two expressions in (3) are standard notation for the "duality pairing" between a function $x \in X$ and a bounded linear functional in the dual space, $y \in X^*$. (The first two expressions in (3) will be used below when F is more general than a functional.) If X has the additional structure of a Hilbert space, then through the Riesz Representation Theorem there exists a unique $z \in X$ such that

$$\langle F'(u), v\rangle = (z, v)_X, \quad \forall v \in X. \tag{4}$$

For this reason it is common notation to write z as $F'(u)$, and to in turn use the notation $(F'(u), v)_X$ involving the inner-product on X in place of the duality pairing notation for the action of F' on $v \in X$. The functional F is the *potential* of F', and F' is the *derivative* (adjoint of the *gradient*) of F.

The Gateaux derivative can be (equivalently) defined directly, which allows for application to more general nonlinear operators $F(u) : X \mapsto Y$, where now X and Y are both general Banach spaces. The *Gateaux derivative* of F at u in the direction v is the unique linear operator $F'(u) : X \mapsto L(X, Y)$, satisfying:

$$\lim_{\epsilon\to 0} \frac{1}{\epsilon} \|F(u + \epsilon v) - F(u) - \epsilon F'(u)v\|_Y = 0. \tag{5}$$

The *Frechet derivative* of F at u is the unique linear operator $F'(u) : X \mapsto L(X, Y)$, satisfying:

$$\lim_{v\to 0} \frac{1}{\|v\|_X} \|F(u + v) - F(u) - F'(u)v\|_Y = 0. \tag{6}$$

Just as the Gateaux variation exists more generally than the Gateaux derivative (but are precisely the same linear operator when they both exist), the Gateaux derivative exists more generally than the Frechet derivative (some interesting examples appear in [20]). When both the Gateaux and Frechet derivatives exist, they are again precisely the same linear operator, and then also the same as the Gateaux variation. Therefore, it is often convenient to compute the Gateaux derivative (and when it also exists, the Frechet derivative) using the expression for the Gateaux variation:

$$F'(u)v = \left.\frac{d}{d\epsilon} F(u + \epsilon v)\right|_{\epsilon=0}. \tag{7}$$

We will use the following notation interchangably for ordinary and partial (Gateaux) derivatives:

$$\dot{F} = F' = \frac{dF}{dt}, \qquad F(t) : [0, T] \subseteq \mathbb{R} \mapsto Y, \tag{8}$$

$$D_{u_k} G = D_k G = \partial_{u_k} G = \partial_k G = \frac{\partial G}{\partial u_k}, \quad G(u) = G(u_1, \ldots, u_n) : X_1 \times X_n \mapsto Y, \tag{9}$$

where $Y, X_1, \ldots, X_n$ are Banach spaces, and where the partial (Gateaux) derivative is defined as:

$$D_{u_k} G(u)v = \left.\frac{d}{d\epsilon} G(u + \epsilon [v]_k)\right|_{\epsilon=0}, \tag{10}$$

with

$$v = \{v_1, \ldots, v_n\}, \qquad [v]_k = \{0, \ldots, 0, v_k, 0, \ldots, 0\}. \tag{11}$$

In the case of $F(u) : X \mapsto Y$ with $X = \mathbb{R}^n$ and $Y = \mathbb{R}^m$, the Gateaux and Frechet derivatives (when they exist) are exactly the Jacobian matrix of partial derivatives (the collection of Gateaux derivatives in the coordinate directions) having m rows and n columns:

$$F'(u) = \partial_j F_i(u) = \frac{\partial F_i(u)}{\partial u_j}, \quad i = 1, \ldots, m, \quad j = 1, \ldots, n. \tag{12}$$

A final comment about notation for derivatives: We will refer to Gateaux (directional, functional, variational) differentiation as simply *differentiation*, since it is always clear from the context when this general notion of differentiation is required, and since it reduces to normal ordinary and partial differentiation. We will also use both DF and F' to denote the derivative in different situations when it simplifies the presentation.

1.2. **Differentiable Manifolds, Submanifolds, and Submersions.** Let $G : X \mapsto Y$, where X and Y are Banach spaces. Consider an implicitly defined *manifold* $\mathcal{M} \subseteq X$, characterized as a the zero level-set of the mapping G:

$$\mathcal{M} = \{ \ u \in \mathcal{D}(G) \subseteq X \mid G(u) = 0 \in \mathcal{R}(G) \subseteq Y \ \} . \tag{13}$$

An *admissible curve* or *admissible path* in $\mathcal{M}$ through $u \in \mathcal{M}$ is a differentiable mapping $\gamma(t) : (-t_0, t_0) \mapsto \mathcal{M}$, for some $t_0 > 0$, with $\gamma(0) = u$. A vector $v \in X$ is called a *tangent vector* to $\mathcal{M}$ at u if there exists an admissible path $\gamma(t)$ to $\mathcal{M}$ at u such that $\gamma'(0) = v$. The set of tangent vectors at a point $u \in \mathcal{M}$ form a vector space $T_u\mathcal{M}$ known as the *tangent space* of $\mathcal{M}$ at u:

$$T_u\mathcal{M} = \{ \ v \in X \mid \dot{\gamma}(0) = v, \text{ with } \gamma(t) \text{ an admissible path in } \mathcal{M} \text{ through } u \ \}. \tag{14}$$

The *tangent bundle* $T\mathcal{M}$ of a manifold $\mathcal{M}$ is the union of the tangent spaces at all points $u \in \mathcal{M}$:

$$T\mathcal{M} = \bigcup_{u \in \mathcal{M}} T_u\mathcal{M}. \tag{15}$$

A particular tangent space $T_u\mathcal{M}$ is called a *fiber* of the tangent bundle $T\mathcal{M}$ at $u \in \mathcal{M}$. The map $\pi_{\mathcal{M}} : T\mathcal{M} \mapsto \mathcal{M}$ which maps tangent vectors to their attachment points on $\mathcal{M}$ is called the *natural projection* operator, and the inverse image $\pi_{\mathcal{M}}^{-1}$ of $\pi_{\mathcal{M}}$ assigns a fiber $T_u\mathcal{M}$ of the tangent bundle $T\mathcal{M}$ to each point $u \in \mathcal{M}$. A *vector field* on $\mathcal{M}$ is a map $V : \mathcal{M} \mapsto T\mathcal{M}$, so that a vector $V(u) \in T_u\mathcal{M}$ is assigned to each $u \in \mathcal{M}$. The vector space of bounded linear functionals on the tangent space $T_u\mathcal{M}$ is the *cotangent space* $T_u^*\mathcal{M}$, and the disjoint union of the cotangent spaces is called the *cotangent bundle* $T^*\mathcal{M}$:

$$T^*\mathcal{M} = \bigcup_{u \in \mathcal{M}} T_u^*\mathcal{M}. \tag{16}$$

Analogously, $T_u^*\mathcal{M}$ is called a fiber of the cotangent bundle $T^*\mathcal{M}$ at $u \in \mathcal{M}$.

A property of nonlinear mappings that we will use repeatedly in these notes in the case of implicitly defined manifolds is *submersion*. A mapping $G : \mathcal{D}(G) \subseteq X \mapsto Y$ is called a *submersion* at u if the following three conditions hold:

1) $G(u)$ is C^1 in a ball around u.
2) $G'(u) : X \mapsto L(X, Y)$ is a surjective linear operator at u (i.e., $\mathcal{R}(G') = Y$).
3) There exists a linear projection operator P which splits X into $\mathcal{N}(G'(u))$ and $\mathcal{N}^{\perp}(G'(u))$.

Note that if $X = \mathbb{R}^n$ and $Y = \mathbb{R}^m$, then 2) is equivalent the assumption that $G'(u)$ has full rank, and then 3) follows from the fact that $\mathcal{N}(G'(u)) \perp \mathcal{R}(G'(u)^T)$, so that $X = \mathbb{R}^n \equiv \mathcal{N}(G'(u)) \oplus \mathcal{R}(G'^T(u))$.

If $G : X \mapsto Y$ is a submersion at $u \in \mathcal{M}$, a classical result due to Ljusternik (cf. Theorem 43.C in [27]) gives a useful alternative characterization of the tangent space $T_u\mathcal{M}$ which will make it possible to develop a very general framework for Lagrange functionals and multipliers in the next section:

$$T_u\mathcal{M} \equiv \mathcal{N}(G'(u)) = \{ \ v \in X \mid G'(u)v = 0 \in Y \ \}. \tag{17}$$

In other words, the tangent space is precisely the null space of the derivative of the operator G implicitly defining the manifold $\mathcal{M}$. Moreover, Ljusternik's result is also that there exists local structure (an atlas of charts), giving $\mathcal{M}$ the mathematical structure of a C^1 manifold (or *differentiable manifold*). The differentiable manifold structure allows for the construction of derivatives, differentials, and directional derivatives of various types of functions having $\mathcal{M}$ is their domain, providing an intrinsic differential calculus on $\mathcal{M}$ that does not depend extrinsically on X through the relationship $\mathcal{M} \subseteq X$. The differentiable manifold structure may be exploited by numerical methods to construct algorithms for solving constrained problems which never depart from $\mathcal{M}$ (see §2.5 and §3.5).

1.3. **Lagrange Functional Theory in Banach Spaces for Constrained Stationarity.** We are interested in the following abstract problem:

$$\text{Find } u \in X \text{ such that}: \quad F(u) = \text{ stationary}, \tag{18}$$

$$\text{Subject to}: \quad G(u) = 0, \tag{19}$$

where $F : \mathcal{D}(F) \subseteq X \mapsto \mathbb{R}$, $G : \mathcal{D}(G) \subseteq X \mapsto Y$, and where X and Y are real Banach spaces. A point $u \in X$ is said to be a *critical point* of F, and F is then said to be *stationary* at u, if the Frechet derivative of F at u vanishes in all directions $v \in X$:

$$\langle F'(u), v\rangle = 0, \quad \forall v \in X. \tag{20}$$

(Much of what follows also makes sense in the more general case of the Gateaux derivative.) The point $u \in X$ may be a local minimizer, maximizer, or saddle point for F.

The (equality) constraint G forces the solution u to lie on a *constraint manifold* $\mathcal{M} \subseteq X$ as defined implicitly in (13) as the zero level-set of G. We will always assume that G is a submersion on all of $\mathcal{M}$, so that the implicitly defined $\mathcal{M}$ has an explicit differentiable manifold structure. (This result is discussed in §1.2.) For example, even in the case of the complex nonlinear constraints in the Einstein equations considered later in these notes, G can be shown to be a C^1 mapping between suitably chosen Sobolev spaces (cf. [9]). A point $u \in \mathcal{M}$ is a called a critical point of F with respect to $\mathcal{M}$, and F is then said to be *stationary* with respect to $\mathcal{M}$ at u, if the Frechet derivative of F at u is zero for all directions $v \in T_u\mathcal{M}$:

$$\langle F'(u), v\rangle = 0, \quad \forall v \in T_u\mathcal{M} \subseteq X. \tag{21}$$

We then regard u as the solution to (18)–(19).

Note that (18)–(19) is a more general version of the following problem:

$$\text{Find } u \in X \text{ such that}: \quad F(u) = \min_{v\in X} F(v), \tag{22}$$

$$\text{Subject to}: \quad G(u) = 0. \tag{23}$$

A standard result in the calculus of variations in Banach spaces is that a necessary (but not sufficient) condition for the solution to (22) is that (18) hold. Therefore, the solution to (18)–(19) is a *necessary condition* for solving (22)–(23). (A *sufficient condition* would also involve a positive spectrum assumption on the second Frechet derivative of F at u.) In either case, a more general framework would allow for inequality constraints of the form $G(u) \geq 0$, but we will restrict ourselves to the case of equality constraints of the form (19). Due to its applicability to the Principle of Least Action (giving rise to a saddle-point problem) in the setting of Lagrangian and Hamiltonian formulations of mechanics and field theory, we will focus entirely on the more general problem (18)–(19).

The following abstract result for linear operators on Banach spaces is the foundation for Lagrange functional and multiplier theory.

Theorem 1.1. *Let X and Y be real Banach spaces, and let $A \in L(X,Y)$ and $B \in L(X,\mathbb{R})$ be bounded linear operators with $\mathcal{R}(A)$ closed. If the following hold:*

$$Bv = 0 \qquad \forall v \in X \qquad \text{such that} \qquad Av = 0, \tag{24}$$

then there exists a bounded linear functional on Y, denoted $\lambda \in Y^*$, such that

$$\lambda_0 Bv + \langle \lambda, Av \rangle = 0, \qquad \forall v \in X, \tag{25}$$

where $\lambda_0 = 1$. If $\mathcal{R}(A) = Y$, then λ is unique. If $\mathcal{R}(A) \neq Y$, then there exists $0 \neq \lambda \in Y^*$ such that (25) holds with $\lambda_0 = 0$. Moreover, λ_0 and λ are never simultaneously zero.

Proof. The closed range assumption on A implies $\mathcal{N}(A) \perp \mathcal{R}(A^T)$; the proof is then quite similar to the finite-dimensional case (cf. Proposition 43.1 in [27]). □

We noted in §1.2 that if the constraint operator G is a submersion at $u \in \mathcal{M}$, the tangent space and the null space of the constraint derivative are precisely the same space: $T_u\mathcal{M} \equiv \mathcal{N}(G'(u))$. Together with Theorem 1.1, this result can be exploited to develop an abstract theory of Lagrange functionals and multipliers, and justifies their use in mechanics and field theory. The following is one version of a Lagrange functional result which follows from Theorem 1.1, where F is thought of as an abstract *Lagrangian*.

Theorem 1.2. *Let X and Y be real Banach spaces, let $F : \mathcal{D}(F) \subseteq X \mapsto \mathbb{R}$ be F-differentiable at $u \in \mathcal{D}(F)$, and let $G : \mathcal{D}(G) \subseteq X \mapsto Y$ be a submersion at u such that $G(u) = 0$. Then F is stationary at $u \in \mathcal{M} \subseteq X$ with respect to $\mathcal{M}$ if and only if the Euler-Lagrange equations hold*

$$\langle F'(u), v \rangle - \langle \lambda, G'(u)v \rangle = 0, \qquad \forall v \in X, \tag{26}$$

for a fixed (Lagrange) bounded linear functional $\lambda \in Y^*$.

Proof. Application of Theorem 1.1 (cf. Proposition 43.21 in [27].) The assumption that G be a submersion provides the closed range assumption for use of Theorem 1.1, and allows the use of the alternative characterization of the tangent space as the nullspace of the constraint derivative. In the finite-dimensional case, the submersion assumption reduces to the standard constraint qualification assumption, where $G'(u)$ becomes the Jacobian matrix at u, and the assumption $\mathcal{R}(G') = Y$ is equivalent to the assumption that the Jacobian matrix has full rank. □

Theorem 1.2 tells us that the solution $u \in \mathcal{M} \subseteq X$ to (18)–(19) is precisely the point of stationarity of the *augmented* functional (or augmented Lagrangian):

$$\bar{F}(u, \lambda) = F(u) - \langle \lambda, G(u) \rangle : X \times Y^* \mapsto \mathbb{R}. \tag{27}$$

Therefore, finding the solution to (18)–(19) is mathematically equivalent to finding the pair $\{u, \lambda\} \in X \times Y^*$ that satisfies the constraint $G(u) = 0$ and solves the Euler-Lagrange equations (26), making the augmented Lagrangian functional (27) stationary. Since differentiation of the augmented Lagrangian functional (27) with respect to λ yields back the constraint $G(u) = 0$, the Euler-Lagrange equations and constraints can be considered together as the following problem:

$$\text{Find } \{u, \lambda\} \in X \times Y^* \text{ such that } \langle D\bar{F}(u, \lambda), (v, \gamma)\rangle = 0, \quad \forall \{v, \gamma\} \in X \times Y^*. \tag{28}$$

Since the chain rule gives

$$\begin{aligned} \langle D\bar{F}(u, \lambda), (v, \gamma)\rangle &= \langle D_u\bar{F}(u, \lambda), v\rangle + \langle D_\lambda\bar{F}(u, \lambda), \gamma\rangle && (29)\\ &= [\langle DF(u), v\rangle - \langle \lambda, DG(u)v\rangle] - \langle \gamma, G(u)\rangle, && (30)\end{aligned}$$

we can also write this as: Find $\{u, \lambda\} \in X \times Y^*$ such that $\forall \{v, \gamma\} \in X \times Y^*$:

$$\begin{aligned} \langle DF(u), v\rangle - \langle \lambda, DG(u)v\rangle &= 0,\\ -\langle \gamma, G(u)\rangle &= 0. \end{aligned} \tag{31}$$

1.3.1. *Example: An Abstract Quadratic Functional with Linear Constraints.* Consider now problem (18)–(19) in the case of a quadratic energy $F : X \mapsto \mathbb{R}$ and a linear constraint $G : X \mapsto Y$ of the form:

$$F(u) = (Au, u)_X - (f, u)_X, \qquad 0 = G(u) = g - Bu, \tag{32}$$

where X and Y are real Hilbert spaces with inner-products $(\cdot, \cdot)_X$ and $(\cdot, \cdot)_Y$, and with $f \in X$, $g \in Y$, $A \in L(X, X)$, $B \in L(X, Y)$. Assume A is self-adjoint on X: $(Au, v) = (u, Av), \forall u, v \in X$. By Theorem 1.2, we know the solution $u \in X$ to problem (18)–(19) is a stationary point of the augmented Lagrangian:

$$\bar{F}(u, \lambda) = F(u) - \langle \lambda, G(u)\rangle = (Au, u)_X - (f, u)_X - (\lambda, g - Bu)_Y, \tag{33}$$

where we have used the Riesz representation theorem to identify a (unique) $\lambda \in Y$ such that

$$\langle \lambda, y\rangle = (\lambda, y)_Y, \quad \forall y \in Y. \tag{34}$$

The Euler-Lagrange equations are then: Find $\{u, \lambda\} \in X \times Y^*$ such that $\forall \{v, \gamma\} \in X \times Y^*$:

$$\begin{aligned} \langle DF(u), v\rangle - \langle \lambda, DG(u)v\rangle &= 0,\\ -\langle \gamma, G(u)\rangle &= 0, \end{aligned} \tag{35}$$

where

$$\begin{aligned} \langle DF(u), v\rangle &= \frac{d}{d\epsilon}F(u + \epsilon v)\bigg|_{\epsilon=0} = (Au, v)_X - (f, v)_X, && (36)\\ \langle \lambda, DG(u)v\rangle &= \langle \lambda, \frac{d}{d\epsilon}G(u + \epsilon v)\bigg|_{\epsilon=0}\rangle = (\lambda, Bv)_Y = \left(B^T\lambda, v\right)_X, && (37)\\ \langle \gamma, G(u)\rangle &= \langle \gamma, g - Bu\rangle = (g - Bu, \gamma)_Y = (g, \gamma)_Y - (Bu, \gamma)_Y, && (38)\end{aligned}$$

where $B^T \in L(Y, X)$ is the adjoint of B. This yields the following abstract linear system for the stationary point $\{u, \lambda\} \in X \times Y^*$:

$$\begin{array}{ccccc} Au & + & B^T\lambda & = & f,\\ Bu & & & = & g. \end{array} \tag{39}$$

As an application, incompressible steady Stokes flow (steady laminar incompressible Navier-Stokes flow) fits precisely into this framework, and numerical schemes focus on the efficient numerical solution of the symmetric indefinite linear system in (39) after discretization by the finite element method or other techniques. Moreover, the most effective numerical techniques for steady incompressible Navier-Stokes flow involve repeated solution of (39) as part of Newton-type iterative methods.

1.3.2. *Example: A Nonlinear Energy on $H^1(\Omega)$ with Nonlinear PDE Constraints.* Consider now problem (18)–(19) in the case of a nonlinear energy functional and nonlinear PDE constraints of the form:

$$F(u) = \int_\Omega \mathcal{L}(x, u, \nabla u)\, dx, \qquad 0 = G(u) = \begin{pmatrix} G_1(x, u, \nabla u, \nabla^2 u) \\ \vdots \\ G_K(x, u, \nabla u, \nabla^2 u) \end{pmatrix}, \tag{40}$$

where $G(u) : X \mapsto Y = Y_1 \times Y_2 \times \cdots \times Y_K$, $u = (u_1, \ldots, u_J) \in X = X_1 \times X_2 \times \cdots \times X_J$, where each X_k and Y_k are suitable Sobolev spaces. Here, each constraint of the form $G_k = 0$ represents a general nonlinear second order boundary value problem:

$$\begin{aligned} -\nabla \cdot a_k(x, u, \nabla u) + b_k(x, u, \nabla u) &= 0 \text{ in } \Omega, && (41) \\ n \cdot a_k(x, u, \nabla u) + c_k(x, u, \nabla u) &= 0 \text{ on } \partial_1\Omega, && (42) \\ u &= 0 \text{ on } \partial_0\Omega, && (43) \end{aligned}$$

where $\Omega \subset \mathbb{R}^d$ is a bounded open subset of $\mathbb{R}^d$, and where $\partial\Omega = \partial_0\Omega \cup \partial_1\Omega$, $\emptyset = \partial_0\Omega \cap \partial_1\Omega$. The *Lagrangian density* $\mathcal{L}$ is a nonlinear function representing an energy principle, such as the elastic energy of a structure modeled with solid mechanics. In this case, the constraints G_k could represent some physical barrier to deformation of the structure.

The problem (18)–(19) with F and G defined as in (40) is general enough to include most time-independent constrained minimization problems arising in mathematical physics, where the objective functional and constraints are second order and arbitrarily nonlinear, with the constraints appearing in divergence form. In the most natural cases, $X_j = H^1_{0,D}(\Omega)$, $j = 1, \ldots J$, and $Y_k = H^{-1}(\Omega)$, $k = 1, \ldots, K$. Since Y is a product space, the Riesz Representation theorem gives the (unique) form of the linear functional as:

$$\begin{aligned} \langle \lambda, G(u) \rangle &= (\lambda, G(u))_{L^2(\Omega)} && (44) \\ &= \sum_{k=1}^K (\lambda_k, G_k)_{L^2(\Omega)} && (45) \\ &= \sum_{k=1}^K \int_\Omega \lambda_k \left(b_k(x, u, \nabla u) - \nabla \cdot a_k(x, u, \nabla u) \right) dx && (46) \\ &= \sum_{k=1}^K \int_\Omega a_k(x, u, \nabla u) \cdot \nabla \lambda_k + b_k(x, u, \nabla u) \lambda_k \, dx && (47) \\ &\quad + \sum_{k=1}^K \int_{\partial_1\Omega} c_k(x, u, \nabla u) \lambda_k \, ds, && (48) \end{aligned}$$

where we have employed the divergence theorem with the natural boundary condition (42), and where $\lambda = (\lambda_1, \ldots, \lambda_K) \in Z = Z_1 \times \cdots \times Z_K$, with $Z_j = H^1(\Omega)$. The essential boundary condition (43) is built into the solution space:

$$H^1_{0,D}(\Omega) = \left\{ \; u \in H^1(\Omega) \mid \text{trace } u = 0 \text{ on } \partial_0\Omega \; \right\}. \tag{49}$$

By Theorem 1.2, we know that the solution $u \in X$ to problem (18)–(19) is a stationary point of the augmented Lagrangian:

$$\bar{F}(u,\lambda) = F(u) - \langle \lambda, G(u) \rangle = \int_\Omega \mathcal{L}(x,u,\nabla u)\ dx - \langle \lambda, G(u) \rangle. \tag{50}$$

The Euler-Lagrange equations are then: Find $\{u,\lambda\} \in X \times Y^*$ such that $\forall \{v,\gamma\} \in X \times Y^*$:

$$\begin{aligned} \langle DF(u), v \rangle - \langle \lambda, DG(u)v \rangle &= 0, \\ -\langle \gamma, G(u) \rangle &= 0, \end{aligned} \tag{51}$$

where

$$\langle DF(u), v \rangle = \frac{d}{d\epsilon} F(u+\epsilon v)\bigg|_{\epsilon=0} = \int_\Omega \left(\frac{\partial \mathcal{L}}{\partial u} v + \frac{\partial \mathcal{L}}{\partial [\nabla u]} \nabla v \right) dx, \tag{52}$$

$$\langle \lambda, DG(u)v \rangle = \langle \lambda, \frac{d}{d\epsilon} G(u+\epsilon v)\bigg|_{\epsilon=0} \rangle = (\lambda, \frac{\partial G}{\partial u} v)_{L^2(\Omega)} = \int_\Omega \lambda^T \frac{\partial G}{\partial u} v\ dx, \tag{53}$$

$$\langle \gamma, G(u) \rangle = (\gamma, G(u))_{L^2(\Omega)} = \int_\Omega \gamma^T G\ dx. \tag{54}$$

The final form of the Euler-Lagrange equations now depends on the particular form of the Lagrange density $\mathcal{L}$ in (40), and on the details on the nonlinear functions a_k, b_k, and c_k appearing in (41)–(43) defining G.

2. Constraint and Structure Preservation in ODE

We briefly review Lagrangian and Hamiltonian formalism for finite-dimensional mechanical systems modeled by ordinary differential equations (ODE). This material can be found in e.g. [1, 7]. We then consider the inclusion of constraints into the formalism using Lagrange multipliers, following e.g. [12]. The use of Lagrange multipliers is then considered for the more general case of constrained non-variational equations which do not arise as conditions for stationarity of action integrals. We then examine structure-preserving numerical integrators for unconstrained and constrained Lagrangian and Hamiltonian ODE, as well as unconstrained and constrained non-variational ODE which do not arise from an action principle.

2.1. **Lagrangian and Hamiltonian ODE formalism.** Consider now a finite-dimensional mechanical system with configuration space Q and coordinates (or positions) $\{q_i(t)\}_{i=1}^n$ describing the configuration of the system at any time t. We will often refer to the entire set of positions $\{q_i(t)\}_{i=1}^n$ simply as $q_i(t)$, where the index is assumed to range from 1 to n, or simply as $q(t)$. In other words, $q_i(t) : [0,T] \mapsto \mathbb{R}$ (or $\mathbb{R}^n$), $q(t) : [0,T] \mapsto \mathbb{R}^n$, and for fixed $t_0 \in [0,T]$, the set of coordinates $q_i(t_0)$ represents a particular configuration (or point) in Q. A remarkable fact is that the equations of motion for a finite-dimensional mechanical system can be derived variationally from a Lagrangian of the form:

$$L(q_i, \dot{q}_i) : Q \times Q \mapsto \mathbb{R}, \tag{55}$$

where $\dot{q}_i = dq_i/dt$ are referred to as velocities. (The dependence of L on t is often only implicitly through q_i.) The equations of motion arise as the stationary point of an action integral $\mathcal{S}(q_i)$ built from the Lagrangian, expressing the Principle of Least Action (or Hamilton's Principle). Let $q_i(0)$ and $q_i(T)$ be arbitrary fixed points in Q. The set of permissible variations from $q_i(t)$ are those which satisfy

$v_i(0) = v_i(T) = 0$, so that $q(0)+v(0) = q(0)$ and $q(T)+v(T) = q(T)$. The Principle of Least Action can then be written as

$$\langle D\mathcal{S}(q_i), v_i\rangle = \frac{d}{d\epsilon}\mathcal{S}(q_i + \epsilon v_i)\Big|_{\epsilon=0} = 0 \quad \forall v_i, \quad \mathcal{S}(q_i) = \int_0^T L(q_i, \dot{q}_i)\ dt. \tag{56}$$

In other words, we obtain the equations of motion by setting to zero the derivative of $\mathcal{S}$, computed as:

$$\begin{aligned}
\langle D\mathcal{S}(q_i), v_i\rangle &= \frac{d}{d\epsilon}\mathcal{S}(q_i + \epsilon v_i)\Big|_{\epsilon=0} && (57)\\
&= \int_0^T \frac{d}{d\epsilon}L(q_i + \epsilon v_i, \dot{q}_i + \epsilon \dot{v}_i)\Big|_{\epsilon=0}\ dt && (58)\\
&= \int_0^T \left(\sum_{i=1}^n \frac{\partial L}{\partial q_i} v_i + \sum_{i=1}^n \frac{\partial L}{\partial \dot{q}_i}\dot{v}_i\right)\ dt && (59)\\
&= \sum_{i=1}^n \int_0^T \left(\frac{\partial L}{\partial q_i} - \frac{d}{dt}\frac{\partial L}{\partial \dot{q}_i}\right) v_i\ dt, && (60)
\end{aligned}$$

where we have employed the chain rule and integration by parts. The boundary terms have been dropped due to v_i being permissible. Since this holds for arbitrary permissible v_i, we are left with the Euler-Lagrange equations of motion for the n positions $q_i(t)$:

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{q}_i} = \frac{\partial L}{\partial q_i}, \quad i = 1, \ldots, n. \tag{61}$$

The appropriate side conditions which would allow for (61) to be well-posed are values for $q_i(0)$ and $\dot{q}_i(0)$.

A Hamiltonian formulation can be obtained from a Lagrangian formulation by introducing conjugate momenta through the Legendre transformation:

$$p_i = \frac{\partial L}{\partial \dot{q}_i}, \quad i = 1, \ldots, n, \tag{62}$$

and then by changing variables from $(q_i, \dot{q}_i)$ to (q_i, p_i). The equations of motion in the new variables can be obtained by defining a Hamiltonian of the form

$$H(q_i, p_i) = \sum_{j=1}^n p_j \dot{q}_j - L(q_i, \dot{q}_i), \tag{63}$$

and then by differentiation of the Hamiltonian with respect to the new position and momenta variables:

$$\begin{aligned}
\frac{\partial H}{\partial p_i} &= \dot{q}_i + \sum_{j=1}^n \left(p_j \frac{\partial \dot{q}_j}{\partial p_i} - \frac{\partial L}{\partial q_j}\frac{\partial q_j}{\partial p_i} - \frac{\partial L}{\partial \dot{q}_j}\frac{\partial \dot{q}_j}{\partial p_i}\right) && (64)\\
&= \dot{q}_i + \sum_{j=1}^n \left(p_j \frac{\partial \dot{q}_j}{\partial p_i} - p_j \frac{\partial \dot{q}_j}{\partial p_i}\right) = \dot{q}_i, && (65)\\
\frac{\partial H}{\partial q_i} &= \sum_{j=1}^n \frac{\partial p_i}{\partial q_j}\dot{q}_j + \sum_{j=1}^n p_j \frac{\partial \dot{q}_j}{\partial q_i} - \frac{\partial L}{\partial q_i} - \sum_{j=1}^n \frac{\partial L}{\partial \dot{q}_j}\frac{\partial \dot{q}_j}{\partial q_i} && (66)\\
&= -\frac{\partial L}{\partial q_i} = -\frac{d}{dt}\frac{\partial L}{\partial \dot{q}_i} = -\dot{p}_i, && (67)
\end{aligned}$$

where we have used (62) and (61), and the fact that p_i and q_i are independent. This then gives Hamilton's equations of motion for the $2n$ positions and momenta $\{q_i(t), p_i(t)\}$:

$$\dot{q}_i = \frac{\partial H}{\partial p_i}, \qquad \dot{p}_i = -\frac{\partial H}{\partial q_i}, \qquad i = 1, \ldots, n. \tag{68}$$

The appropriate side conditions which would allow for (68) to be well-posed are values for $q_i(0)$ and $p_i(0)$.

It is interesting to note (cf. [17]) that the equations of motion (68) also arise directly as a stationary point of an action integral built from the Hamiltonian rather than the Lagrangian:

$$D\mathcal{S}(q_i, p_i) = 0, \qquad \text{where} \ \ \mathcal{S}(q_i, p_i) = \int_0^T \sum_{j=1}^n p_j \dot{q}_j - H(q_i, p_i)\, dt, \tag{69}$$

where the derivative is computed in the natural way:

$$\begin{aligned} \big\langle D\mathcal{S}(q_i, p_i), (v_i, w_i) \big\rangle &= \big\langle D_{q_i}\mathcal{S}(q_i, p_i), v_i \big\rangle + \big\langle D_{p_i}\mathcal{S}(q_i, p_i), w_i \big\rangle && (70) \\ &= \frac{d}{d\epsilon}\mathcal{S}(q_i + \epsilon v_i, p_i)\bigg|_{\epsilon=0} + \frac{d}{d\epsilon}\mathcal{S}(q_i, p_i + \epsilon w_i)\bigg|_{\epsilon=0}, && (71) \end{aligned}$$

and where the appropriate conditions on v_i are now $p_i(0)v_i(0) = p_i(T)v_i(T) = 0$. This fact will be useful for constrained Hamiltonian formulations in §2.2, allowing for the introduction of Lagrange multipliers directly into the action integral (69) rather than first going through (56).

2.1.1. *Example: A system of particles.* Consider a system of N particles in $\mathbb{R}^d$ with positions $\{x_1^i(t), \ldots, x_d^i(t)\}$, $i = 1, \ldots, N$, with corresonding masses $\bar{m}_i$ in a potential field $V(x_j^i) : \mathbb{R}^{dN} \mapsto \mathbb{R}$. Defining the $n = dN$ generalized coordinates and corresponding masses as: $q_{d(i-1)+j}(t) = x_j^i(t)$, $m_{d(i-1)+j} = \bar{m}_i$, $i = 1, \ldots, N$, $j = 1, \ldots, d$, gives rise to the Lagrangian

$$L(q_i, \dot{q}_i) = \frac{1}{2}\sum_{j=1}^n m_j (\dot{q}_j)^2 - V(q_i) = T(\dot{q}_i) - V(q_i), \tag{72}$$

where T and V represent kinetic and potential energy of the mechanical system. The Euler-Lagrange equations produce Newton's equations of motion:

$$m_i \ddot{q}_i = -\frac{\partial V}{\partial q_i}, \quad i = 1, \ldots n. \tag{73}$$

The Hamiltonian formulation of the system arises from the Legendre transformation: $p_i = \partial L / \partial \dot{q}_i = m_i \dot{q}_i$, $i = 1, \ldots, n$, giving a Hamiltonian of the form:

$$\begin{aligned} H(q_i, p_i) &= \sum_{j=1}^n p_j \dot{q}_j - L(q_i, \dot{q}_i) = \frac{1}{2}\sum_{j=1}^n m_j (\dot{q}_j)^2 + V(q_i) && (74) \\ &= \frac{1}{2}\sum_{j=1}^n m_j^{-1} p_j^2 + V(q_i) = T(p_i) + V(q_i). && (75) \end{aligned}$$

The equations of motion are then:

$$\dot{q}_i = \frac{\partial H}{\partial p_i} = m_i^{-1} p_i, \qquad \dot{p}_i = -\frac{\partial H}{\partial q_i} = -\frac{\partial V}{\partial q_i}, \qquad i = 1, \ldots, n. \tag{76}$$

2.2. **Constrained Lagrangian and Hamiltonian ODE formalism.** Consider now an n-dimensional mechanical system with Lagrangian $L(q_i, \dot{q}_i)$, subject to a set of $m < n$ constraints:

$$G_j(q_i, \dot{q}_i) = 0, \quad j = 1, \ldots, m. \tag{77}$$

One can view the constraints as defining a manifold $\mathcal{M}$ in configuration space:

$$\mathcal{M} = \{ \ q \mid G_j(q_i, \dot{q}_i) = 0, \ \ j = 1, \ldots, m \ \}. \tag{78}$$

By Theorem 1.2 in §1, we know that making the Lagrangian L stationary with respect to the constraint manifold $\mathcal{M}$ is mathematically equivalent to making a new action integral $\bar{\mathcal{S}}$ stationary, where $\bar{\mathcal{S}}$ is built from an augmented Lagrangian $\bar{L}$ of the form:

$$\bar{L}(q_i, \dot{q}_i, \lambda_i) = L(q_i, \dot{q}_i) - \sum_{j=1}^{m} \lambda_j G_j(q_i, \dot{q}_i). \tag{79}$$

The additional degrees of freedom $\lambda_i \in \mathbb{R}$ are referred to as Lagrange multipliers. The equations of motion for the constrained mechanical system are then produced by making the corresponding augmented action integral $\bar{\mathcal{S}}$ stationary with respect to both the configuration variables and the Lagrange multipliers, producing the Euler-Lagrange equations for the augmented Lagrangian:

$$\langle D\bar{\mathcal{S}}(q_i, \lambda_i), (v_i, \nu_i) \rangle = 0, \tag{80}$$

where

$$\bar{\mathcal{S}}(q_i, \lambda_i) = \int_0^T \bar{L}(q_i, \dot{q}_i, \lambda_i) \ dt = \int_0^T L(q_i, \dot{q}_i) - \sum_{j=1}^{m} \lambda_j G_j(q_i, \dot{q}_i) \ dt. \tag{81}$$

The derivative is computed as

$$\begin{aligned}
\big\langle D\bar{\mathcal{S}}(q_i, \lambda_i), (v_i, \nu_i) \big\rangle &= \big\langle D_{q_i}\bar{\mathcal{S}}(q_i, \lambda_i), v_i) \big\rangle + \big\langle D_{\lambda_i}\bar{\mathcal{S}}(q_i, \lambda_i), \nu_i) \big\rangle && (82) \\
&= \frac{d}{d\epsilon}\bar{\mathcal{S}}(q_i + \epsilon v_i, \lambda_i)\bigg|_{\epsilon=0} + \frac{d}{d\epsilon}\bar{\mathcal{S}}(q_i, \lambda_i + \epsilon \nu_i)\bigg|_{\epsilon=0}, && (83)
\end{aligned}$$

where

$$\begin{aligned}
\frac{d}{d\epsilon}\bar{\mathcal{S}}(q_i + \epsilon v_i, \lambda_i)\bigg|_{\epsilon=0} &= \int_0^T \frac{d}{d\epsilon} \Big(L(q_i + \epsilon v_i, \dot{q}_i + \epsilon \dot{v}_i) && (84) \\
&\quad - \sum_{j=1}^{m} \lambda_j G_j(q_i + \epsilon v_i, \dot{q}_i + \epsilon \dot{v}_i) \Big)\bigg|_{\epsilon=0} dt && (85) \\
&= \int_0^T \left(\sum_{i=1}^{n} \left(\frac{\partial L}{\partial q_i} - \frac{d}{dt}\frac{\partial L}{\partial \dot{q}_i} \right) v_i \right. && (86) \\
&\quad \left. - \sum_{j=1}^{m} \lambda_j \sum_{i=1}^{n} \left(\frac{\partial G_j}{\partial q_i} - \frac{d}{dt}\frac{\partial G_j}{\partial \dot{q}_i} \right) v_i \right) dt, && (87)
\end{aligned}$$

and

$$\begin{aligned}
\frac{d}{d\epsilon}\bar{\mathcal{S}}(q_i, \lambda_i + \epsilon\nu_i)\bigg|_{\epsilon=0} &= -\int_0^T \frac{d}{d\epsilon}\bigg(L(q_i, \dot{q}_i) &(88)\\
&\qquad - \sum_{j=1}^m (\lambda + \epsilon\nu)_j G_j(q_i, \dot{q}_i)\bigg)\bigg|_{\epsilon=0} dt &(89)\\
&= -\int_0^T \left(\sum_{j=1}^m G_j(q_i, \dot{q}_i)\nu_j\right) dt, &(90)
\end{aligned}$$

and where we have recalled (57). We now identify the derivative of $\bar{\mathcal{S}}$ and force it to vanish, giving the $n+m$ Euler-Lagrange equations for the $n+m$ degrees of freedom $\{q_i, \lambda_i\}$:

$$\begin{aligned}
\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_i} - \sum_{j=1}^m \frac{\partial G_j}{\partial \dot{q}_i}\lambda_j\right) &= \frac{\partial L}{\partial q_i} - \sum_{j=1}^m \frac{\partial G_j}{\partial q_i}\lambda_j, \quad i = 1, \ldots, n, &(91)\\
G_j(q_i, \dot{q}_i) &= 0, \quad j = 1, \ldots, m. &(92)
\end{aligned}$$

The appropriate side conditions which would allow for (91)–(92) to be well-posed are values for $q_i(0)$ and $\dot{q}_i(0)$ such that $G_j(q_i(0), \dot{q}_i(0)) = 0$. In the case that the constraints are holonomic with $G_j(q_i, \dot{q}_i) = G_j(q_i)$, the Euler-Lagrange equations reduce to

$$\begin{aligned}
\frac{d}{dt}\frac{\partial L}{\partial \dot{q}_i} &= \frac{\partial L}{\partial q_i} - \sum_{j=1}^m \frac{\partial G_j}{\partial q_i}\lambda_j, \quad i = 1, \ldots, n, &(93)\\
G_j(q_i) &= 0, \quad j = 1, \ldots, m. &(94)
\end{aligned}$$

A constrained Hamiltonian formulation can be derived in a similar way, by introducing an augmented Hamiltonian:

$$\bar{H}(q_i, p_i, \lambda_i, \pi) = H(q_i, p_i) + \sum_{j=1}^m \lambda_j G_j(q_i, p_i), \tag{95}$$

where the constraints are now $G_j(q_i, p_i) = 0$. Hamilton's equations of motion for the $2n+m$ degrees of freedom $\{q_i, p_i, \lambda_i\}$ are then produced using the augmented Hamiltonian:

$$\dot{q}_i = \frac{\partial \bar{H}}{\partial p_i} = \frac{\partial H}{\partial p_i} + \sum_{j=1}^m \frac{\partial G_j}{\partial p_i}\lambda_j, \qquad \dot{p}_i = -\frac{\partial \bar{H}}{\partial q_i} = -\left(\frac{\partial H}{\partial q_i} + \sum_{j=1}^m \frac{\partial G_j}{\partial q_i}\lambda_j\right), \tag{96}$$

$$i = 1, \ldots, n, \qquad 0 = \frac{\partial \bar{H}}{\partial \lambda_j} = G_j(q_i, p_i), \quad j = 1, \ldots, m. \tag{97}$$

The appropriate side conditions which would allow for (96)–(97) to be well-posed are values for $q_i(0)$ and $p_i(0)$ such that $G_j(q_i(0), p_i(0)) = 0$. Again, in the case that the constraints are holonomic with $G_j(q_i, p_i) = G_j(q_i)$, Hamilton's equations reduce to

$$\dot{q}_i = \frac{\partial H}{\partial p_i}, \qquad \dot{p}_i = -\left(\frac{\partial H}{\partial q_i} + \sum_{j=1}^m \frac{\partial G_j}{\partial q_i}\lambda_j\right), \qquad i = 1, \ldots, n, \tag{98}$$

$$G_j(q_i) = 0, \quad j = 1, \ldots, m. \tag{99}$$

2.2.1. *Example: The pendulum problem.* A pendulum in the plane is a classical example of a mechanical system with a (holonomic) constraint. The planar pendulum is characterized by the position $q_i(t) = (q_1(t), q_2(t))$ and velocity $\dot{q}_i(t) = (\dot{q}_1(t), \dot{q}_2(t))$ of the pendulum "bob", modeled as a point with mass m, and the fixed length l of the pendulum rod. The kinetic energy, potential energy, and constraint of the mechanical system are respectively

$$T(\dot{q}_i) = \frac{m}{2}(\dot{q}_1^2 + \dot{q}_2^2), \qquad V(q_i) = mgq_2, \qquad G(q_i) = (q_1^2 + q_2^2) - l^2 = 0, \tag{100}$$

where g is the acceleration due to gravity. The constraint is simply that the pendulum bob must always be a distance l from the center of the pendulum (taken to be at the origin for simplicity). The Lagrangian and Hamiltonian then have the form

$$L(q_i, \dot{q}_i) = T(\dot{q}_i) - V(q_i) = \frac{m}{2}(\dot{q}_1^2 + \dot{q}_2^2) - mgq_2, \tag{101}$$

$$H(q_i, p_i) = T(p_i) + V(q_i) = \frac{1}{2m}(p_1^2 + p_2^2) + mgq_2, \tag{102}$$

where we have employed the Legendre transformation $p_i = \partial L / \partial \dot{q}_i = m\dot{q}_i$. To incorporate the single constraint, we follow §2.2 and form the augmented Lagrangian and Hamiltonian:

$$\bar{L}(q_i, \dot{q}_i) = L(q_i, \dot{q}_i) - \lambda G(q_i) = \frac{m}{2}(\dot{q}_1^2 + \dot{q}_2^2) - mgq_2 - \lambda G(q_i), \tag{103}$$

$$\bar{H}(q_i, p_i) = H(q_i, p_i) + \lambda G(q_i) = \frac{1}{2m}(p_1^2 + p_2^2) + mgq_2 + \lambda G(q_i). \tag{104}$$

The Euler-Lagrange equations and Hamilton's equations are then respectively

$$\begin{bmatrix} m\ddot{q}_1 \\ m\ddot{q}_2 \\ 0 \end{bmatrix} = \begin{bmatrix} -2q_1\lambda \\ -mg - 2q_2\lambda \\ q_1^2 + q_2^2 - l^2 \end{bmatrix}, \qquad \begin{bmatrix} \dot{q}_1 \\ \dot{q}_2 \\ \dot{p}_1 \\ \dot{p}_2 \\ 0 \end{bmatrix} = \begin{bmatrix} m^{-1}p_1 \\ m^{-1}p_2 \\ -2q_1\lambda \\ -mg - 2q_2\lambda \\ q_1^2 + q_2^2 - l^2 \end{bmatrix}, \tag{105}$$

which are second- and first-order (ordinary) differential algebraic equations (DAE) for the pendulum configuration over time.

2.3. **Constrained non-variational ODE systems.** Consider now a general constrained dynamical ODE system of the form:

$$\dot{y} = F(y), \tag{106}$$

$$0 = G(y). \tag{107}$$

where $y(t) = \{y_i(t)\} : \mathbb{R} \mapsto \mathbb{R}^n$, $F(y) = \{F_i(y)\} : \mathbb{R}^n \mapsto \mathbb{R}^n$, $G(y) = \{G_j(y)\} : \mathbb{R}^n \mapsto \mathbb{R}^m$, and where $y(0)$ is given with $G(y(0)) = 0 \in \mathbb{R}^m$. We will assume that this system does not arise as the Euler-Lagrange equations or as Hamilton's equations from a known Lagrangian or Hamiltonian, and such ODE systems are referred to as *non-variational* or *non-cannonical.* A method-of-lines discretization (a spatial semi-discretization) of an arbitrary hyperbolic or parabolic PDE system which is first-order in time, and which has time-independent (e.g., elliptic or algebraic) constraints, will produce a constrained ODE system having the form (106)–(107). Even if the original PDE system had Lagrangian or Hamiltonian structure, the resulting

ODE system will generally not have any structure unless special spatial discretizations are used (see §3.4). In any event, one can still apply Lagrange multiplier techniques to (106)–(107) to explicitly enforce the constraints during evolution, as we will now explain. The following discussion also applies to variational (Lagrangian and Hamiltonian) formulations, where this additional structure is simply ignored.

A non-constant functional $I(y) : \mathbb{R}^n \mapsto \mathbb{R}$ is called a *first integral* (invariant, constant of motion, conserved quantity) of (106) if (cf. [8])

$$I'(y)F(y) = \sum_{i=1}^{n} \frac{\partial I(y)}{\partial y_i} F_i(y) = 0 \in \mathbb{R}, \qquad \forall y(t) \in \mathbb{R}^n. \tag{108}$$

In this case, every solution $y(t)$ of (106) has the property that $I(y(t)) = I(y(0)) =$ constant, since

$$\frac{d}{dt} I(y(t)) = \sum_{i=1}^{n} \frac{\partial I(y)}{\partial y_i} \dot{y}_i = I'(y)F(y) = 0 \in \mathbb{R}, \qquad \forall y(t) \in \mathbb{R}^n. \tag{109}$$

Note that while the constraint function G defines an obvious constraint manifold

$$\mathcal{M} = \{ \ y \in \mathbb{R}^n \ | \ G(y) = 0 \in \mathbb{R}^m \ \}, \tag{110}$$

the connection to the ODE gives a second, hidden constraint, that can be revealed by differentiation:

$$0 = \frac{d}{dt} G(y(t)) = \sum_{i=1}^{n} \frac{\partial G_j}{\partial y_i} \dot{y}_i = G'(y)F(y) \in \mathbb{R}^m, \ \forall y(t) \in \mathcal{M}, \ \text{s.t. } \dot{y} = F(y). \tag{111}$$

Since this holds only for $y(t) \in \mathcal{M}$ such that $\dot{y} = F(y)$, *each* scalar constraint $G_j : \mathbb{R}^n \mapsto \mathbb{R}$ is referred to as a *weak invariant* of (106). Thus, if $y(t)$ satisfies the ODE (106) as well as the constraint (107), then $F(y)$ must lie in the null space of $G'(y)$. Recall now the Ljusternik result from §1.3 that if G is a submersion on $\mathcal{M}$, then (17) holds. Therefore, the constraint (sub)manifold $\mathcal{M}_F \subseteq \mathcal{M}$ for the solution to (106)–(107) can be then characterized equivalently as any of:

$$\begin{aligned} \mathcal{M}_F &= \{ \ y \in \mathcal{M} \ | \ G'(y)F(y) = 0 \ \} & (112)\\ &= \{ \ y \in \mathcal{M} \ | \ F(y) \in T_y\mathcal{M} \ \} & (113)\\ &= \{ \ y \in \mathbb{R}^n \ | \ G(y) = 0, \ F(y) \in T_y\mathcal{M} \ \} & (114)\\ &= \{ \ y \in \mathbb{R}^n \ | \ G(y) = 0, \ G'(y)F(y) = 0 \ \}. & (115) \end{aligned}$$

This characterization motivates the use of Lagrange multipliers even in the absense of an action integral whose stationarity generates (106). This is due to the fact that one can show quite easily (cf. [8]) that the solution to (106) satisfies $y(t) \in \mathcal{M} \ \forall t > 0$ whenever $y(0) \in \mathcal{M}$ if and only if $F(y) \in T_y\mathcal{M}, \ \forall y \in \mathcal{M}$. In this case, one can view $\dot{y} = F(y)$ as a differential equation on the manifold $\mathcal{M}$ (or rather, on $\mathcal{M}_F \subseteq \mathcal{M}$).

To understand why this is the case, let $y \in \mathcal{M}$ be arbitrary but fixed, and assume that $G(y)$ is a submersion at y. Since $G : \mathbb{R}^n \mapsto \mathbb{R}^m$, we can guarantee that G is a submersion at y simply by assuming that G is C^1 in a ball around y in $\mathbb{R}^n$, and that the $m \times n$ Jacobian matrix $G' = \partial G_j / \partial y_i \in L(\mathbb{R}^n, \mathbb{R}^m)$ has full rank at y. Consider now (106)–(107), where in general $F(y) \notin T_y\mathcal{M} \equiv \mathcal{N}(G'(y))$. We denote the $n \times m$ transpose matrix of G' as $G'^T = L(\mathbb{R}^m, \mathbb{R}^n)$. Since $\mathbb{R}^n$ may be equipped with an inner-product, and since it is complete in the corresponding induced norm (it has finite dimension), so-equipped it is a Hilbert space. Therefore, the Hilbert space Projection Theorem ensures that $\mathbb{R}^n$ may be orthogonally decomposed into the direct sum

$$\mathbb{R}^n \equiv \mathcal{N}(G') \oplus \mathcal{R}(G'^T). \tag{116}$$

In fact, this can be accomplished using orthogonal projectors $Q : \mathbb{R}^n \mapsto \mathcal{R}(G'^T)$ and $P : \mathbb{R}^n \mapsto \mathcal{N}(G')$ defined explicitly as

$$Q = G'^T \left(G'G'^T\right)^{-1} G', \qquad P = I - Q, \qquad \text{so that } P + Q = I. \tag{117}$$

The projectors Q and P are well-defined, since the full-rank assumption guarantees that $G'G'^T$ is nonsingular. It is easy to verify that if $u \in \mathcal{R}(G'^T)$, then $Qu = u$, and $Pu = 0$. Consider now

$$F = (P + Q)F = PF + QF = PF + G'^T\lambda, \tag{118}$$

where $PF \in \mathcal{N}(G')$ and $QF = G'^T\lambda \in \mathcal{R}(G'^T)$ for some $\lambda \in \mathbb{R}^m$. Therefore, if we form

$$G'^T\lambda = Qf = G'^T \left(G'G'^T\right)^{-1} G'F, \quad \text{or simply} \quad \lambda = \left(G'G'^T\right)^{-1} G'F, \tag{119}$$

then we can formally project $F(y)$ onto $T_y\mathcal{M}$ as follows:

$$F - G'^T\lambda = (P + Q)F - G'^T\lambda = PF \in \mathcal{N}(G'(y)) = T_y\mathcal{M}. \tag{120}$$

Therefore, the following augmented problem:

$$\dot{y} = F(y) - G'^T\lambda, \tag{121}$$

$$0 = G(y), \tag{122}$$

is now a differential equation on the manifold $\mathcal{M}$. Since the expression for λ in (119) depends on $y(t)$, the equations (121)–(122) must be solved simultaneously for $\{y, \lambda\}$. The Lagrange multipliers λ are viewed as adjusting in response to $y(t)$ so that $F - G'^T\lambda \in T_y\mathcal{M}$ continues to hold, allowing the trajectory of $y(t)$ to remain on $\mathcal{M}$, thereby allowing for the simultaneous solution of (121)–(122).

We will give an alternative derivation of (121)–(122) below in the discretized setting, where the augmented problem arises naturally as the Euler-Lagrange equations for the solution to a constrained minimization problem, characterizing the projection of a constraint-violating approximate solution back onto the constraint manifold.

2.4. **Structure-preserving time discretizations.** There has been much work in this area at least as far back as 1983, and even as early as the 1950's; cf. [23, 5, 3, 13, 24, 8]. One can look up both explicit and implicit numerical integrators in the literature which preserve various geometric properties from the original ODE system.

2.5. **ODE integrators with exact constraint preservation.** Numerical integrators for (ordinary) differential algebraic equations (DAE) which exactly enforce algebraic constraints are typically based on Lagrange multipliers. This leads to numerical methods which 1) are comparable in accuracy to standard methods, and 2) enforce the constraints exactly. There has been much activity on numerical integrators that also 3) preserve geometric structure (time-reversibility, symplectivity, etc) as far back as the early 1990's [2, 14, 15, 6]. One can look up both explicit and implicit numerical integrators in the literature which preserve both the constraints and various geometric properties from the original ODE system, although constraint preservation always requires the solution of some (generally nonlinear) algebraic system at each time step.

3. Constraint and Structure Preservation in PDE

We first briefly review Lagrangian and Hamiltonian formalism for fields modeled by partial differential equations (PDE), following e.g. [16, 28]. To establish the notation for relativistic formulations, in this section we assume that spacetime has the topology $\Omega \times \mathbb{R}$, where Ω is a fixed Riemannian d-manifold. We then develop Lagrangian and Hamiltonian mechanics for time-dependent tensor fields living on this fixed d-manifold. Constraints are then incorporated into the formalism using the Lagrange functional theory from §1. Following this we consider constrained non-variational PDE which do not arise from a Least Action Principle. We then consider structure preserving space and time discretizations for PDE, and outline some techniques for constraint preservation based on Lagrange functional formulations. The PDE case requires much closer attention be paid to the function spaces in which the fields live than the ODE case requires; we will punt on this for the moment and refer to e.g. [16, 28] for the details for the particular examples we consider.

3.1. **Lagrangian and Hamiltonian PDE formalism.** Consider a field system with configuration space Q and (scalar or tensor) field(s) $\phi(x^k, t)$ describing the configuration of the system at any time $t \in [0, T]$. For fixed $t_0 \in [0, T]$, the "field" $\phi(x^k, t_0)$ is a configuration (or point) in Q, and will represent one or more scalar or tensors fields over a Riemannian d-manifold Ω, with $x^k = (x^1, \ldots, x^d) \in \Omega$. ($\Omega$ may simply be a single open set $\Omega \subseteq \mathbb{R}^d$.) In other words, at any fixed time $t_0 \in [0, T]$, $\phi(x^k, t_0) \in Q$, and $\phi(x^k, t) : \Omega \times [0, T] \mapsto V$, where V is the corresponding space of point tensors at x^k. We supress all indices on the tensor field(s) represented by ϕ. Here, $\dot{\phi} = \partial\phi/\partial t$, and $\partial_k \phi$ will represent covariant partial differentiaion of (each tensor field in) ϕ with respect to x^k (or the entire set of derivatives over all indices), defined using the connection provided by the Riemannian metric on Ω. We will use Einstein summation convention for repeated up and down indices in products.

The field equations for many infinite-dimensional (or field) systems in physics can be derived variationally from a Lagrangian functional L of the form:

$$L(\phi, \dot{\phi}) : Q \times Q \mapsto \mathbb{R}, \ L(\phi, \dot{\phi}) = \int_\Omega \mathcal{L}(x^k, \phi, \dot{\phi}, \partial_j \phi) \, dx, \tag{123}$$

where $\mathcal{L}$ is a Lagrangian density of the fields ϕ, $\dot{\phi}$, and $\partial_j \phi$ over Ω. The field equations arise as the stationary point of an action integral $\mathcal{S}(\phi)$ built from the Lagrangian, expressing the Principle of Least Action. Let $\phi(x^k, 0)$ and $\phi(x^k, T)$ be arbitrary fixed points in Q; directions (variations) ψ will be referred to as "permissible" if $\psi(x^k, 0) = \psi(x^k, T) = 0$, so that $\phi(x^k, 0) + \psi(x^k, 0) = \phi(x^k, 0)$ and $\phi(x^k, T) + \psi(x^k, T) = \phi(x^k, T)$. We also assume that permissible directions satisfy $\psi(x^k, t) = 0$ on the spatial boundary $\partial\Omega \times [0, T]$, so that $\phi(x^k, t) + \psi(x^k, t) = \phi(x^k, t)$ on $\partial\Omega \times [0, T]$. The Principle of Least Action then takes the form

$$\langle D\mathcal{S}(\phi), \psi \rangle = 0, \ \forall \text{ permissible } \psi, \text{ where } \mathcal{S}(\phi) = \int_0^T L(\phi, \dot{\phi}) \, dt. \tag{124}$$

Thus, we set to zero the derivative of $\mathcal{S}$, computed as the following linear functional of ψ:

$$\begin{aligned}
\langle D\mathcal{S}(\phi), \psi \rangle &= \frac{d}{d\epsilon}\mathcal{S}(\phi+\epsilon\psi)\Big|_{\epsilon=0} && (125)\\
&= \int_0^T \frac{d}{d\epsilon} L(\phi+\epsilon\psi, \dot\phi+\epsilon\dot\psi)\Big|_{\epsilon=0}\, dt && (126)\\
&= \int_0^T \langle D_\phi L, \psi\rangle + \langle D_{\dot\phi} L, \dot\psi\rangle\, dt && (127)\\
&= \int_0^T \langle D_\phi L, \psi\rangle - \frac{d}{dt}\langle D_{\dot\phi} L, \psi\rangle\, dt, && (128)
\end{aligned}$$

where we have employed the chain rule and integration by parts in time. The boundary terms have been dropped due to ψ being permissible. The equations for the field(s) ϕ are then obtained by forcing the quantity (126)–(128) to vanish for all permissible directions ψ, which will hold if and only if ϕ solves the following problem involving the *Euler-Lagrange equations*:

$$\text{Find } \phi \text{ such that} : \frac{d}{dt}\langle D_{\dot\phi} L, \psi\rangle = \langle D_\phi L, \psi\rangle, \ \forall \text{ permissible } \psi. \qquad (129)$$

The appropriate side conditions which would allow for (129) to be well-posed are values for $\phi(x^k, 0)$ and $\dot\phi(x^k, 0)$.

It remains now to compute the derivatives of L appearing in (129). These are just

$$\begin{aligned}
\langle D_\phi L, \psi\rangle &= \frac{d}{d\epsilon} L(\phi+\epsilon\psi, \dot\phi)\Big|_{\epsilon=0} && (130)\\
&= \frac{d}{d\epsilon}\int_\Omega \mathcal{L}(x^k, [\phi+\epsilon\psi], \dot\phi, \partial_j[\phi+\epsilon\psi])\Big|_{\epsilon=0}\, dx && (131)\\
&= \int_\Omega \left(\frac{\partial\mathcal{L}}{\partial\phi}\psi + \frac{\partial\mathcal{L}}{\partial[\partial_j\phi]}\partial_j\psi\right)\, dx, && (132)
\end{aligned}$$

and

$$\begin{aligned}
\frac{d}{dt}\langle D_{\dot\phi} L, \psi\rangle = \langle D_{\dot\phi} L, \dot\psi\rangle &= \frac{d}{d\epsilon} L(\phi, \dot\phi+\epsilon\dot\psi)\Big|_{\epsilon=0} && (133)\\
&= \frac{d}{d\epsilon}\int_\Omega \mathcal{L}(x^k, \phi, [\dot\phi+\epsilon\dot\psi], \partial_j\phi)\Big|_{\epsilon=0}\, dx && (134)\\
&= \int_\Omega \frac{\partial\mathcal{L}}{\partial\dot\phi}\dot\psi\, dx = \frac{d}{dt}\int_\Omega \frac{\partial\mathcal{L}}{\partial\dot\phi}\psi\, dx, && (135)
\end{aligned}$$

where the boundary terms have been dropped due to ψ being permissible. Since these expressions hold for an arbitrary permissible direction ψ, we view the following as expressing the *weak form* of the Euler-Lagrange equations in terms of the Lagrangian density $\mathcal{L}$: Find ϕ such that $\forall$ permissible ψ,

$$\frac{d}{dt}\int_\Omega \frac{\partial\mathcal{L}}{\partial\dot\phi}\psi\, dx = \int_\Omega \frac{\partial\mathcal{L}}{\partial\phi}\psi\, dx + \int_\Omega \frac{\partial\mathcal{L}}{\partial[\partial_j\phi]}\partial_j\psi\, dx. \qquad (136)$$

With enough differentiability, we may use the divergence theorem on the third integral in (136) together with the arbitrariness of ψ to obtain the *strong form* of the Euler-Lagrange equations in terms of the Lagrangian density $\mathcal{L}$:

$$\partial_t \left(\frac{\partial \mathcal{L}}{\partial \dot{\phi}}\right) = \frac{\partial \mathcal{L}}{\partial \phi} - \partial_j \left(\frac{\partial \mathcal{L}}{\partial [\partial_j \phi]}\right). \tag{137}$$

A Hamiltonian formulation can be obtained from a Lagrangian formulation by introducing conjugate momenta through the Legendre transformation (also called the fiber derivative): $\pi = L_{\dot{\phi}}$, and then by changing variables from $(\phi, \dot{\phi})$ to (ϕ, π). Note that

$$\begin{aligned}
\langle \pi, \dot{\psi} \rangle &= \langle D_{\dot{\phi}} L, \dot{\psi} \rangle = \frac{d}{d\epsilon} L(\phi, \dot{\phi} + \epsilon \dot{\psi}) \Big|_{\epsilon=0} && (138) \\
&= \int_\Omega \frac{d}{d\epsilon} \mathcal{L}(x^k, \phi, [\dot{\phi} + \epsilon \dot{\psi}], \partial_j \phi) \Big|_{\epsilon=0} \ dx && (139) \\
&= \int_\Omega \frac{\partial \mathcal{L}}{\partial \dot{\phi}} \dot{\psi} \ dx = \langle \frac{\partial \mathcal{L}}{\partial \dot{\phi}}, \dot{\psi} \rangle, && (140)
\end{aligned}$$

so that in the case of the particular form of the Lagrangian we are considering here, we have simply

$$\pi = \frac{\partial \mathcal{L}}{\partial \dot{\phi}}. \tag{141}$$

The field equations in the new variables can be obtained by defining a Hamiltonian of the form

$$\begin{aligned}
H(\phi, \pi) &= \int_\Omega \pi \dot{\phi} \ dx - L(\phi, \dot{\phi}) && (142) \\
&= \int_\Omega \left(\frac{\partial \mathcal{L}}{\partial \dot{\phi}} \dot{\phi} - \mathcal{L}(x^k, \phi, \dot{\phi}, \partial_j \phi) \right) \ dx && (143) \\
&= \int_\Omega \mathcal{H}(\phi, \pi) \ dx, && (144)
\end{aligned}$$

where $\mathcal{H}(\phi, \pi) = \pi \dot{\phi} - \mathcal{L}(x^k, \phi, \dot{\phi}, \partial_j \phi)$ is the Hamiltonian density, and then by differentiating the Hamiltonian with respect to the new position and momenta variables:

$$\begin{aligned}
\langle D_\pi H, \kappa \rangle &= \frac{d}{d\epsilon} H(\phi, \pi + \epsilon \kappa) \Big|_{\epsilon=0} && (145) \\
&= \int_\Omega \left(\dot{\phi} \kappa + \pi \frac{\partial \dot{\phi}}{\partial \pi} \kappa - \frac{\partial \mathcal{L}}{\partial \phi} \frac{\partial \phi}{\partial \pi} \kappa - \frac{\partial \mathcal{L}}{\partial \dot{\phi}} \frac{\partial \dot{\phi}}{\partial \pi} \kappa \right) dx && (146) \\
&= \int_\Omega \dot{\phi} \kappa \ dx = \langle \dot{\phi}, \kappa \rangle, && (147)
\end{aligned}$$

$$\begin{aligned}
\langle D_\phi H, \psi \rangle &= \frac{d}{d\epsilon} H(\phi + \epsilon \psi, \pi) \Big|_{\epsilon=0} && (148) \\
&= \int_\Omega \left(\frac{\partial \pi}{\partial \phi} \dot{\phi} \psi + \pi \frac{\partial \dot{\phi}}{\partial \phi} \psi - \frac{\partial \mathcal{L}}{\partial \phi} \psi - \frac{\partial \mathcal{L}}{\partial [\partial_j \phi]} \partial_j \psi - \frac{\partial \mathcal{L}}{\partial \dot{\phi}} \frac{\partial \dot{\phi}}{\partial \phi} \psi \right) dx && (149) \\
&= -\int_\Omega \left(\frac{\partial \mathcal{L}}{\partial \phi} \psi + \frac{\partial \mathcal{L}}{\partial [\partial_j \phi]} \partial_j \psi \right) dx && (150) \\
&= -\frac{d}{dt} \int_\Omega \frac{\partial \mathcal{L}}{\partial \dot{\phi}} \psi \ dx = -\int_\Omega \dot{\pi} \psi \ dx = -\langle \dot{\pi}, \psi \rangle, && (151)
\end{aligned}$$

where we have used (141) and (136), and the fact that π and ϕ are independent. This is then simply

$$\dot{\phi} = D_\pi H, \;\; \dot{\pi} = -D_\phi H. \tag{152}$$

As in the ODE case (cf. [17]), the field equations (152) also arise as a stationary point of an action integral built from the Hamiltonian rather than the Lagrangian:

$$\langle D\mathcal{S}(\phi,\pi),(\psi,\kappa)\rangle = \frac{d}{d\epsilon}\mathcal{S}(\phi+\epsilon\psi,\pi+\epsilon\kappa)\bigg|_{\epsilon=0} = 0, \tag{153}$$

where

$$\mathcal{S}(\phi,\pi) = \int_0^T \int_\Omega \pi\dot{\phi}\; dx - H(\phi,\pi)\; dt, \tag{154}$$

where now $\pi(x^k,0)\psi^i(x^k,0) = \pi(x^k,T)\psi^i(x^k,T) = 0$ are the appropriate boundary conditions. This fact will be useful for constrained Hamiltonian formulations in §3.2, allowing for the introduction of Lagrange functionals directly into the action integral (153) rather than first going through (124).

3.1.1. *Example: Linear elastodynamics.*

3.2. **Constrained Lagrangian and Hamiltonian PDE formalism.**

3.2.1. *Example: Maxwell's equations.*

3.3. **Constrained non-variational PDE systems.**

3.3.1. *Example: Incompressible Navier-Stokes.*

3.4. **Structure-preserving space and time discretizations.** If space is semi-discretized to reduce a PDE system to an ODE system, and if the resulting ODE system retains Lagrangian or Hamiltonian structure, then the geometric (structure-preserving) time discretizations for Lagrangian and Hamiltonian ODE systems described in §2.4 immediately apply. Semi-discretizations of space for various PDE systems which preserve Lagrangian or Hamiltonian structure in the original PDE have been examined e.g. in [10]. Alternatively, one can consider spacetime discretizations of the PDE system which directly produce structure-preserving discrete dynamical systems; cf. [4, 22, 21, 18, 19].

3.4.1. *Spatial finite element discretizations.*

3.4.2. *Spacetime finite element discretizations.*

3.5. **PDE integrators with exact constraint preservation.** If space is semi-discretized to reduce a constrained PDE system to a constrained ODE system, and if the resulting ODE system retains constrained Lagrangian or Hamiltonian structure, then the geometric (structure-preserving) time discretizations for constrained Lagrangian and Hamiltonian ODE systems described in §2.5 immediately apply. Alternatively, one can attempt to construct spacetime discretizations of the PDE system which directly produce structure-preserving discrete constrained dynamical systems.

4. Constraint & Structure Preservation in the Einstein Equations

4.1. Constrained Lagrangian and Hamiltonian formulations.

4.2. Constrained non-variational formulations.

4.3. Integrators with exact constraint preservation.

4.4. Implementation based on finite element methods and FEtk.

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