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# Variational integrators for nonvariational partial differential equations

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## HIGHLIGHTS

- Combination of Ibragimov's theory of formal Lagrangians with variational integrators.
- Significant extension of the applicability of variational integrators.
- Numerical schemes for the 2D vorticity equation preserving circulation, enstrophy and energy.
- Covariant generalisation of Arakawa's discretisation of the Jacobian.

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## ABSTRACT

Variational integrators for Lagrangian dynamical systems provide a systematic way to derive geometric numerical methods. These methods preserve a discrete multisymplectic form as well as momenta associated to symmetries of the Lagrangian via Noether's theorem. An inevitable prerequisite for the derivation of variational integrators is the existence of a variational formulation for the considered problem. Even though for a large class of systems this requirement is fulfilled, there are many interesting examples which do not belong to this class, e.g., equations of advection–diffusion type frequently encountered in fluid dynamics or plasma physics.

On the other hand, it is always possible to embed an arbitrary dynamical system into a larger Lagrangian system using the method of formal (or adjoint) Lagrangians. We investigate the application of the variational integrator method to formal Lagrangians, and thereby extend the application domain of variational integrators to include potentially all dynamical systems.

The theory is supported by physically relevant examples, such as the advection equation and the vorticity equation, and numerically verified. Remarkably, the integrator for the vorticity equation combines Arakawa's discretisation of the Poisson brackets with a symplectic time stepping scheme in a fully covariant way such that the discrete energy is exactly preserved. In the presentation of the results, we try to make the geometric framework of variational integrators accessible to non specialists.



## 1. Introduction

In recent years, the field of structure-preserving or geometric discretisation [1–3] has become a flourishing discipline of numerical analysis and scientific computing. One particular family of geometric discretisation methods is that of variational integrators [4–10], which are based on the discretisation of Hamilton's principle of stationary action [11–15]. Variational integrators preserve a discrete multisymplectic form and have good longtime energy behaviour. As we will see, they can be designed to preserve energy even exactly, which in practice means up to machine precision. Furthermore, they preserve momenta associated to symmetries of the discrete equations of motion via a discrete version of Noether's theorem [16,17].

While in most standard discretisation techniques for dynamical systems the equations of motion are directly discretised, the basic idea of variational integrators is to construct a discrete counterpart to the considered system. This means that the fundamental building blocks

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of classical mechanics and field theory, namely the action functional, the Lagrangian, the variational principle, and the Noether theorem, all have discrete equivalents. The application of the discrete variational principle to the discrete action then leads to discrete Euler–Lagrange equations. The evolution map that corresponds to the discrete Euler–Lagrange equations is what is called a variational integrator. The discrete Noether theorem can be used to relate symmetries of the discretised system to discrete momenta that are exactly preserved by this integrator. Whereas most standard techniques put emphasis on the minimisation of local errors, for variational integrators the focus is rather on the preservation of global or geometric properties of the system.

An obvious limitation of the variational integrator method is its applicability to Lagrangian systems only. This excludes a large class of interesting systems, for example the problems of advection–diffusion type often found in fluid dynamics and plasma physics. We propose here that the method of formal (or adjoint) Lagrangians [18] can be used as an expedient to avoid this limitation. More specifically, formal Lagrangians allow us to embed any given system into a larger system which, in turn, admits a Lagrangian formulation. To obtain a formal Lagrangian $L$, the equation at hand, say $\mathcal{F}[u] = 0$, is multiplied by an adjoint variable $v$, giving $L = v \cdot \mathcal{F}[u]$. Variation of the resulting action functional, $\mathcal{A} = \int L\, d^{n+1}\mathrm{x}$, with respect to $v$ gives the original equation $\mathcal{F}[u] = 0$. Variation of the action functional with respect to the physical variable $u$ gives an additional equation that determines the evolution of the adjoint variable $v$.

At first sight one might be tempted to regard the formal Lagrangian formalism as merely a method for obtaining a weak formulation of the problem at hand. Then, if our goal is to obtain an integrator, the details of the dynamics of the adjoint variable $v$ would seem irrelevant. However, it turns out that the dynamics of $v$ play a key role in relating symmetries of the formal Lagrangian to conservation laws satisfied by $u$. Ibragimov [19–21] developed a theory for the analysis of conservation laws of arbitrary differential equations by extending the Noether theorem to formal Lagrangians. This leads to conservation laws for the extended system $(u, v)$, which can be restricted to the original system provided that it is possible to express the solution of the adjoint variable $v$ in terms of $u$.

In this work, we propose the combination of the discrete variational principle with Ibragimov's theory in order to derive variational integrators for systems without a natural Lagrangian formulation and to determine the associated discrete conservation laws. Thereby we extend significantly the applicability of the variational integrator method. The goal of this approach is to design numerical schemes which respect certain conservation laws of a given system in a rather systematic way.

We proceed as follows. In Section 2, we present the theory of variational integrators in simple terminology. To set the stage and fix notation we review the continuous action principle for field theories and the corresponding Noether theorem before passing over to the discrete theory, which is extended to account for discrete divergence symmetries. The style of presentation is chosen to make the theory accessible to a wide audience without extensive background in modern differential geometry. This implies some loss of generality, but hopefully not too much of the geometric beauty of the original work is lost. In Section 3, we recall the inverse problem of the calculus of variations, review the theory of formal Lagrangians and explain the derivation of conserved quantities in this setting. We also provide a geometric formulation of the theory, which to our knowledge has not been presented, yet. Finally, in Section 4, we apply the method to some prototypical examples, including the advection equation and the vorticity equation, and verify the theoretical properties in numerical experiments. More elaborate numerical examples for the Vlasov–Poisson system as well as ideal and reduced magnetohydrodynamics will be presented elsewhere [22–24]. The examples we provide here can be seen as building blocks for these more complicated systems.

## 2. Variational integrators

### 2.1. Geometry and notation

In this work, we are concerned with the discretisation of partial differential equations (PDEs) of evolution type. A field is a map $u : X \to F$ from a bounded domain $X \subset \mathbb{R}^{n+1}$ taking values in an open set $F \subseteq \mathbb{R}^m$. Most often, $X$ corresponds to some region of spacetime with coordinates

$$\mathrm{x} = (\mathrm{x}^\mu) = (\mathrm{x}^0, \mathrm{x}^i) = (t, x, y, z) \quad \text{with } 0 \le \mu \le n,\ 1 \le i \le n,$$

and $n = \dim X - 1$ being the number of space-like dimensions. Most of the theoretic results rely neither on this space-plus-time splitting nor on $X$ being a subset of an Euclidean space. Thus $X$ can be replaced by a differentiable manifold, in which case the results are valid locally in a coordinate chart. Points on $F$ are denoted by $\mathrm{y} = (\mathrm{y}^a)$ with $1 \le a \le m$ and $m = \dim F$ being the number of field components. We make use of the Einstein summation convention on repeated indices, both for coordinates and fields.

The configuration of a field $u$ is geometrically represented by its graph

$$\mathrm{graph}(u) = \big\{(\mathrm{x}, \mathrm{y}) \;\big|\; \mathrm{y} = u(\mathrm{x})\big\},$$

which is a subset of the Cartesian product

$$Y = X \times F = \big\{(\mathrm{x}, \mathrm{y}) \;\big|\; \mathrm{x} \in X,\ \mathrm{y} \in F\big\}.$$

With the projection onto the first factor,

$$\begin{array}{rccc} \pi & : & Y & \to & X, \\ & & (\mathrm{x}, \mathrm{y}) & \mapsto & \mathrm{x}, \end{array}$$

we can define a geometrical structure $(Y, X, \pi)$ called (trivial) fibre bundle. Here, $X$ is called the base space, $Y$ the configuration space, and $F$ the fibre. Local coordinates on $Y$ are given by

$$(\mathrm{x}^\mu, \mathrm{y}^a) \quad \text{with } 0 \le \mu \le n,\ 1 \le a \le m.$$

A field $u$ can be identified with a section of the bundle, i.e., a map $\varphi : X \to Y$, satisfying the condition

$$\pi \circ \varphi = \mathrm{id}_X,$$