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Multisymplectic structure of numerical methods derived using nonstandard finite difference schemes

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Abstract. In the present work we investigate a class of numerical techniques, that take advantage of discrete variational principles, for the numerical solution of multi-symplectic PDEs arising at various physical problems. The resulting integrators, which use the nonstandard finite difference framework, are also multisymplectic. For the derivation of those integrators, the necessary discrete Lagrangian is expressed at the appropriate discrete jet bundle using triangle and square discretization. The preliminary results obtained by the resulting numerical schemes show that for the case of the linear wave equation the discrete multisymplectic structure is preserved.

1. Introduction and motivation

In the present work we investigate the geometric structure for multisymplectic integrators using nonstandard finite difference schemes for variational partial differential equations (PDEs). The approach we consider is first to develop a Veselov type discretization for PDEs in variational form [1, 2] (see also [3]) and second to combine this approach with nonstandard finite difference schemes of [6, 7]. These resulting multisymplectic-momentum integrators have, under appropriate circumstances, very good energy performance in the sense of the conservation of a nearby Hamiltonian up to exponentially small error [5]. Furthermore, the nonstandard finite difference schemes was developed for compensating the weaknesses that may be caused by standard finite difference methods, for example, the numerical instabilities. Following the steps of the derivation of the Euler-Lagrange equations in the continuous formulation of Lagrangian dynamics, the discrete Euler-Lagrange equations can be derived [3]. Denoting the tangent bundle of the configuration manifold $Q$ by $TQ$, the continuous Lagrangian $L : TQ \rightarrow \mathbb{R}$ can be defined. In the discrete setting, considering approximate configurations $q_k \approx q(t_k)$ and $q_{k+1} \approx q(t_{k+1})$ at the time nodes $t_k, t_{k+1}$ with $h = t_{k+1} - t_k$ being the time step, a discrete Lagrangian $L_d : Q \times Q \rightarrow \mathbb{R}$ is defined to approximate the action integral along the curve segment between $q_k$ and $q_{k+1}$, i.e.

\begin{equation}
L_d(q_k, q_{k+1}) \approx \int_{t_k}^{t_{k+1}} L(q(t), \dot{q}(t))dt.
\end{equation}
Figure 1. Triangle discretization. a) Three ordered triple and b) the triangles which touch \((i,j)\).

Defining the discrete trajectory \(\gamma_d = (q_0, \ldots, q_N), N \in \mathbb{N}\) one can obtain the action sum

\[
S_d(\gamma_d) = \sum_{k=1}^{N-1} L_d(q_k, q_{k+1}).
\]  

(2)

Discrete Hamilton’s principle states that a motion \(\gamma_d\) of the discrete mechanical system extremizes the action sum, i.e. \(\delta S_d = 0\). By differentiation and rearrangement of the terms, holding the end points \(q_0\) and \(q_N\) fixed, the discrete Euler-Lagrange equations are obtained

\[
D_2 L_d(q_{k-1}, q_k) + D_1 L_d(q_k, q_{k+1}) = 0, \quad k = 1, \ldots, N-1
\]  

(3)

where the notation \(D_i L_d\) indicates the slot derivative with respect to the \(i\)-th argument of \(L_d\), see [3].

2. Triangle discretization

Just as the ODEs of classical mechanics can be described by a Lagrangian variational structure, PDEs theory can as well. For that, in order to express the discrete Lagrangian function, we need to define an appropriate generalization of the tangent bundle \(TQ\) and cotangent bundle \(T^*Q\) to fields over the higher-dimensional manifold \(X\). Following the work of [3] we consider fields over \(X\) as sections of some fiber bundle \(B \rightarrow X\), with fiber \(Y\), and then we consider the first jet bundle \(J^1B\) and its dual \((J^1B)^*\) as the appropriate analogs of the tangent and cotangent bundles.

We now generalize the Veselov discretization given [1, 2] to multisymplectic field theory, by discretizing the spacetime \(X\). For simplicity we restrict to the discrete analogue of \(\dim X = 2\). Thus, we take \(X = \mathbb{Z} \times \mathbb{Z} = (i,j)\) and the fiber bundle \(Y\) to be \(X \times F\) for some smooth manifold \(F\), see [3].

2.1. Triangle discretization

Assume that we have a uniform quadrangular mesh in the base space, with mesh lengths \(\Delta x\) and \(\Delta t\). The nodes in this mesh are denoted by \((i,j) \in \mathbb{Z} \times \mathbb{Z}\), corresponding to the points \((x_i, t_j) := (i\Delta x, j\Delta t) \in \mathbb{R}^2\). We denote the value of the field \(u\) at the node \((i,j)\) by \(u^i_j\). We label the triangle at \((i,j)\) with three ordered triple \((i,j), (i,j+1), (i+1,j+1)\) as \(\triangle_{ij}\), and we define \(X_\Delta\) to be the set of all such triangles, see Figure 1a.

Then the discrete jet bundle is defined as follows [3]
\[ J^1_{\Delta Y} := \{(u_i^j, u_i^{j+1}, u_{i+1}^{j+1}) \in \mathbb{R}^3 : ((i, j), (i, j + 1), (i + 1, j + 1)) \in X_\Delta \} \] (4)

which is equal to \( X_\Delta \times \mathbb{R}^3 \). The field \( u \) can be now defined by averaging the fields over all vertices of the triangle (see Figure 1a)

\[ u \to \frac{u_i^j + u_i^{j+1} + u_{i+1}^{j+1}}{3} \] (5)

while the derivatives can be expressed using nonstandard finite differences

\[ \frac{du}{dt} \to \frac{u_i^{j+1} - u_i^j}{\phi(\Delta t)}, \quad \frac{du}{dx} \to \frac{u_{i+1}^{j+1} - u_i^{j+1}}{\psi(\Delta x)} \] (6)

with

\[ \phi(\Delta t) = \frac{1}{2} \sin \left( \frac{\Delta t}{2} \right), \quad \psi(\Delta x) = \frac{1}{2} \sin \left( \frac{\Delta x}{2} \right). \] (7)

For a more comprehensive study on the above expressions see [6, 7]. Using the above expressions, we can obtain the discrete Lagrangian at any triangle, that depends on the edges of the triangle, i.e.

\[ L_d(u_i^j, u_i^{j+1}, u_{i+1}^{j+1}) = \frac{1}{2} \Delta t \Delta x \left( \frac{1}{2} \left( \frac{u_i^{j+1} - u_i^j}{\phi(\Delta t)} \right)^2 - \frac{1}{2} \left( \frac{u_{i+1}^{j+1} - u_i^{j+1}}{\psi(\Delta x)} \right)^2 \right) \] (11)

For the special case that \( c = -1 \), the corresponding Lagrangian is

\[ L(u, u_t, u_x) = \frac{1}{2} u_t^2 - \frac{1}{2} u_x^2 \] (10)

where \( \partial u/\partial t = u_t \) and \( \partial u/\partial x = u_x \). The triangle discretization of Section 2.1 leads to the discrete Lagrangian

\[ L_d(u_i^j, u_i^{j+1}, u_{i+1}^{j+1}) = \frac{1}{2} \Delta t \Delta x \left( \frac{1}{2} \left( \frac{u_i^{j+1} - u_i^j}{\phi(\Delta t)} \right)^2 - \frac{1}{2} \left( \frac{u_{i+1}^{j+1} - u_i^{j+1}}{\psi(\Delta x)} \right)^2 \right) \] (11)

where \( \Delta t \) and \( \Delta x \) are the mesh lengths for time and space respectively. Applying the above discrete Lagrangian to the discrete Euler-Lagrange field equations (8) we get

\[ \frac{u_i^{j+1} - 2u_i^j + u_i^{j-1}}{(\phi(\Delta t))^2} - \frac{u_{i+1}^{j+1} - 2u_i^j + u_{i-1}^j}{(\psi(\Delta x))^2} = 0 \] (12)

which is the expression of the variational integrator for the linear wave equation (9) using nonstandard finite difference schemes.
Figure 2. The waveforms of linear wave equation (9).

In Figure 2 the solution of the above equation is presented. On that we have considered initial conditions $0 < x < 1$, $u(x, 0) = 0.5[1 - \cos(2\pi x)]$, $u_t(x, 0) = 0.1$ and periodic boundary conditions $u(0, t) = u(1, t)$, $u_x(0, t) = u_x(1, t)$. The grid discretization has been considered to be $\Delta t = 0.01$ and $\Delta x = 0.01$. Figure 2 shows that the time evolution of the solution is continuous and the periodicity is also preserved.

Furthermore in Figure 3 the evolution of the discrete energy, both temporal and spatial,

\[
e_j = \frac{1}{2} \sum_{i=0}^{N-1} \left( \frac{u_{i+1}^{j+1} - u_i^{j+1}}{\phi(\Delta t)} \right)^2 + \left( \frac{u_{i+1}^{j+1} - u_i^{j+1}}{\psi(\Delta x)} \right)^2 \Delta x, \tag{13}
\]

\[
e_i = \frac{1}{2} \sum_{j=0}^{M-1} \left( \frac{u_{j+1}^{i+1} - u_j^{i+1}}{\phi(\Delta t)} \right)^2 + \left( \frac{u_{j+1}^{i+1} - u_j^{i+1}}{\psi(\Delta x)} \right)^2 \Delta t, \tag{14}
\]

is presented. Figure 3 shows clearly that during the numerical simulation no energy loss or blow-up appears.

4. Summary and conclusions
The derivation of multisymplectic numerical methods derived from nonstandard finite difference schemes is investigated. Even though the results are preliminary, the numerical examples which have been already tested (e.g. the linear wave equation) show that these numerical schemes have good energy behavior and preserve the discrete multisymplectic structure. Thus, applying these schemes in the field of incompressible fluid dynamics, see e.g. [11] and [12], would be interesting. Furthermore, in complex geometries which appear in real world problems, it is necessary to extend this methodology to non-uniform grids.
Figure 3. a) The temporal evolution of the discrete energy (13) and b) the spatial evolution of the discrete energy of (14).

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