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MULTISYMPLECTIC AND VARIATIONAL INTEGRATORS

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Abstract: Recently multisymplectic discretizations are attracting much attention, because they are the vigorous component of the structure-preserving algorithms. In this paper, the new development in the field of multisymplectic discretizations is systematically described and some very interesting new results are given. Multisymplectic and variational integrators are studied from a comparative point of view. The composition method for constructing higher order multisymplectic integrators is presented. The equivalence of variational integrators to multisymplectic integrators is proved.

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1. Introduction

The introduction of symplectic integrators is a milestone in the development of numerical analysis (Feng [30], [31]). The consequence is the establishment of structure-preserving algorithms, a very promising subject. Due to its high accuracy, good stability and in particular the capability for long-term computation, the structure-preserving algorithms are very powerful in numerical simulations. The applications of structure-preserving algorithms can be found in diverse branches of physics such as celestial mechanics, quantum mechanics, fluid dynamics, geophysics, etc. (see [47], [49], [73]).

Symplectic algorithms for finite dimensional Hamiltonian systems are well established. They offer new insight into old methods and also lead to many powerful new numerical methods. The structure-preserving algorithms for infinite dimensional Hamiltionian systems are comparatively less explored (Qin [45], [51], [52]). The basic idea is to discretize appropriately the space variables so that the resulting semi-discrete system is a Hamiltonian system in time and then to apply symplectic methods. The obtained symplectic integrator preserves a symplectic form which is a sum over the discrete space variables. But the symplectic structure over the spatial domain is not reflected in such methods.

This problem is solved by introducing the concept of multisymplectic integrators (Bridges and Reich [5], [7]). In general, an infinite dimensional Hamiltonian system can be reformulated as a multisymplectic Hamiltonian system. Then in each time and space direction there exists a symplectic structure and a multisymplectic conservation law. The multisymplectic conservation law is local and reflects the symplecticity over the space domain. A multisymplectic integrator is a numerical scheme for the multisymplectic Hamiltonian system preserving a discrete multisymplectic conservation law characterizing the spatial change of the discrete symplectic structure. The multisymplectic integrator is the generalization of the symplectic integrator and has good performance in maintaining local conservation laws. A disadvantage is the introduction of many new variables which usually are not needed in numerical experiments. To solve this problem, one can eliminate the additional variables and obtain a series of new schemes. Using symplectic Runge-Kutta integrators in both directions leads to multisymplectic integrators (Reich [55]). In this paper, another approach, namely the composition method, will be presented.

The multisymplectic integrator is based on the Hamiltonian formalism. In the Lagrangian formalism a geometric-variational approach to continuous and discrete mechanics and field theories is known (Marsden, Patrik and Shkoller [48]). The multisymplectic form is obtained directly from the variational principle, staying entirely on the Lagrangian side. But the local energy and momentum conservation laws are not particularly addressed. By disretizing the Lagrangian and using a discrete variational principle, variational integrators are obtained, which satisfy a discrete multisymplectic form (see [48]). Taking the Sine-Gordon equation and the nonlinear Schrödinger equation as examples, it will be shown that some variational integrators are equivalent to multisymplectic integrators.

In addition to the standard multisymplectic and variational integrators, the more ambitious goal is to present generalizations including multisymplectic Fourier pseudospectral methods on real space, nonconservative multisymplectic Hamiltonian systems, constructions of multisymplectic integrators for modified equations and multisymplectic Birkhoffian systems (Su et al [60], [59]).

This paper is organized as follows. In the next Section, the basic theory of multisymplectic geometry and multisymplectic Hamiltonian systems will be presented. Section 3 is devoted to developing multisymplectic integrators. In Section 4, the variational integrators are discussed. In Section 5, some generalizations are given.

2. Multisymplectic Geometry and Hamiltonian System

In this section, the basic theory needed for multisymplectic and variational integrators is discussed including multisymplectic geometry and multisymplectic Hamiltonian systems. The theory is presented from the perspective of the total variation, always named *Lee variational integrator* (Lee [43], [44], Chen [10], Chen et al [23]).

2.1. Multisymplectic Geometry

Exclusively local coordinates are used and the notion of prolongation spaces instead of jet bundles (see [50], [15]) is employed, where the covariant configuration space is denoted by $X \times U$, X represents the space of independent variables with coordinates $x^\mu, \mu = 1, 2, \ldots, n, 0,$ and U the space of dependent variables with coordinates $u^A, A = 1, 2, \ldots, N$. The first order prolongation of $X \times U$ is defined to be

$$U^{(1)} = X \times U \times U_1, \tag{2.1}$$

where U_1 represents the space consisting of first order partial derivatives of u^A with respect to x^μ. Let $\phi : X \to U$ be a smooth function, then its first prolongation is denoted by

$$\mathrm{pr}^1\phi = (x_\mu, \phi^A, \phi^A_\mu).$$

A Lagrangian density $\mathcal{L}$ is defined as follows

$$\begin{aligned} &\mathcal{L} : U^{(1)} \to \Lambda^{n+1}(X), \\ &\mathcal{L}(\mathrm{pr}^1\phi) = L(x_\mu, \phi^A, \phi^A_\mu)d^{n+1}x, \end{aligned} \tag{2.2}$$

where $\Lambda^{n+1}(X)$ is the space of $n+1$ forms over X. Corresponding to the Lagrangian density (2.2), the action functional is defined by

$$\mathcal{S}(\phi) = \int_M L(x_\mu, \phi^A, \phi^A_\mu)d^{n+1}x, \tag{2.3}$$

where M is an open set in X. Let V be a vector field on $X \times U$ with the form

$$V = \xi^\mu(\boldsymbol{x})\frac{\partial}{\partial x^\mu} + \alpha_A(\boldsymbol{x}, \boldsymbol{u})\frac{\partial}{\partial u^A},$$

where $\boldsymbol{x} = (x^1, \ldots, x^n, x^0), \boldsymbol{u} = (u^1, \ldots, u^N)$ and the Einstein summation is used. The flow $\exp(\lambda V)$ of the vector field V is a one-parameter transformation group of $X \times U$ and transforms a map $\phi : M \to U$ to a family of maps $\tilde{\phi} : \tilde{M} \to U$ depending on the parameter λ. Now the variation of the action functional (2.3) is calculated. For simplicity let $n = 1, N = 1$ and $x^1 = x,\ x^0 = t,\ u^1 = u, \alpha_1 = \alpha$, then it follows

$$\delta\mathcal{S} = \frac{d}{d\lambda}\bigg|_{\lambda=0} \mathcal{S}(\tilde{\phi}) = \frac{d}{d\lambda}\bigg|_{\lambda=0} \int_{\tilde{M}} L(\tilde{x}, \tilde{t}, \tilde{\phi}, \tilde{\phi}_{\tilde{x}}, \tilde{\phi}_{\tilde{t}})d\tilde{x} \wedge d\tilde{t} = A + B,$$

where

$$\begin{aligned} A = \int_M \Bigg[&\left(\frac{\partial L}{\partial t} + D_t\left(\frac{\partial L}{\partial \phi_t}\phi_t - L\right) + D_x\left(\frac{\partial L}{\partial \phi_x}\phi_t\right)\right)\xi^0 \\ &+ \left(\frac{\partial L}{\partial x} + D_x\left(\frac{\partial L}{\partial \phi_x}\phi_x - L\right) + D_t\left(\frac{\partial L}{\partial \phi_t}\phi_x\right)\right)\xi^1 \\ &+ \left(\frac{\partial L}{\partial \phi} - D_x\frac{\partial L}{\partial \phi_x} - D_t\frac{\partial L}{\partial \phi_t}\right)\alpha \Bigg] dx \wedge dt \end{aligned} \tag{2.4}$$

and

$$\begin{aligned} B = \int_{\partial M} \Bigg[&\left(\left(\frac{\partial L}{\partial \phi_t}\phi_t - L\right)dx - \frac{\partial L}{\partial \phi_x}\phi_t dt\right)\xi^0 \\ &+ \left(\left(L - \frac{\partial L}{\partial \phi_x}\phi_x\right)dt + \frac{\partial L}{\partial \phi_t}\phi_x dx\right)\xi^1 + \left(\frac{\partial L}{\partial \phi_x}dt - \frac{\partial L}{\partial \phi_t}dx\right)\alpha\Bigg]. \end{aligned} \tag{2.5}$$

If $\xi^1(x)$, $\xi^0(x)$, and $\alpha(x, t, \phi(x, t))$ have compact support on M, then $B = 0$. In this case, with the requirement of $\delta\mathcal{S} = 0$ and from (2.4) the variation ξ^0

yields the local energy evolution equation

$$\frac{\partial L}{\partial t} + D_t\left(\frac{\partial L}{\partial \phi_t}\phi_t - L\right) + D_x\left(\frac{\partial L}{\partial \phi_x}\phi_t\right) = 0 \tag{2.6}$$

and the variation ξ^1 the local momentum evolution equation

$$\frac{\partial L}{\partial x} + D_x\left(\frac{\partial L}{\partial \phi_x}\phi_x - L\right) + D_t\left(\frac{\partial L}{\partial \phi_t}\phi_x\right) = 0. \tag{2.7}$$

For a conservative L, i.e., it does not depend on x, t explicitly, (2.6) and (2.7) become the local energy conservation law and the local momentum conservation law respectively. The variation α yields the Euler-Lagrange equation

$$\frac{\partial L}{\partial \phi} - D_x\frac{\partial L}{\partial \phi_x} - D_t\frac{\partial L}{\partial \phi_t} = 0. \tag{2.8}$$

If the condition that $\xi^1(x,t)$, $\xi^0(x,t)$, $\alpha(x,t,\phi(x,t))$ have compact support on M is not imposed, then from the boundary integral B one can define the Cartan form

$$\Theta_{\mathcal{L}} = \frac{\partial L}{\partial \phi_x}d\phi \wedge dt - \frac{\partial L}{\partial \phi_t}d\phi \wedge dx + \left(L - \frac{\partial L}{\partial \phi_x}\phi_x - \frac{\partial L}{\partial \phi_t}\phi_t\right) dx \wedge dt. \tag{2.9}$$

Using the interior product $\lrcorner$ and the pull back mapping $()^*$ it follows

$$B = \int_{\partial M} (\mathrm{pr}^1\phi)^*(\mathrm{pr}^1 V \lrcorner\, \Theta_{\mathcal{L}}). \tag{2.10}$$

The multisymplectic form is defined to be $\Omega_{\mathcal{L}} = d\Theta_{\mathcal{L}}$.

Theorem 2.1. (see [48], [32]) *Suppose ϕ is the solution of* (2.8), *and let η^λ and ζ^λ be two one-parameter symmetry groups of equation* (2.8), *and V_1 and V_2 are the corresponding infinitesimal symmetries, then it follows the multisymplectic form*

$$\int_{\partial M} (\mathrm{pr}^1\phi)^*(\mathrm{pr}^1 V_1 \lrcorner\, \mathrm{pr}^1 V_2 \lrcorner\, \Omega_{\mathcal{L}}) = 0. \tag{2.11}$$

2.2. Multisymplectic Hamiltonian Systems

A large class of partial differential equations can be represented as (see [3], [4])

$$M\boldsymbol{z}_t + K\boldsymbol{z}_x = \bigtriangledown_{\boldsymbol{z}} S(\boldsymbol{z}), \tag{2.12}$$

where $\boldsymbol{z} \in \mathbf{R}^n$, M and K are antisymmetric matrices in $\mathbf{R}^{n\times n}, n \geq 3$ and $S : \mathbf{R}^n \to \mathbf{R}$ is a smooth function. Here for simplicity, only one space dimension is considered. The system (2.12) is called a multisymplectic Hamiltonian system, since it possesses a multisymplectic conservation law

$$D_t\omega + D_x\kappa = 0, \tag{2.13}$$

where $D_t = \frac{d}{dt}$, $D_x = \frac{d}{dx}$ and ω and κ are the pre-symplectic forms

$$\omega = \frac{1}{2} d\boldsymbol{z} \wedge M d\boldsymbol{z}, \qquad \kappa = \frac{1}{2} d\boldsymbol{z} \wedge K d\boldsymbol{z}$$

associated to the time and space direction, respectively. (2.12) satisfies a local energy conservation law

$$D_t E + D_x F = 0, \tag{2.14}$$

where E is the energy density and F the energy flux

$$E = S(\boldsymbol{z}) - \frac{1}{2}\boldsymbol{z}^T K \boldsymbol{z}_x, \quad F = \frac{1}{2}\boldsymbol{z}^T K \boldsymbol{z}_t.$$

(2.12) also satisfies a local momentum conservation law

$$D_t I + D_x G = 0, \tag{2.15}$$

where I is the momentum density and G the momentum flux

$$I = \frac{1}{2}\boldsymbol{z}^T M \boldsymbol{z}_x \quad G = S(\boldsymbol{z}) - \frac{1}{2}\boldsymbol{z}^T M \boldsymbol{z}_t.$$

The multisymplectic Hamiltonian system can be obtained from the Lagrangian density and the covariant Legendre transform, or the Legendre-Hodge transformation (see [4]). The relationship between the Lagrangian and the Hamiltonian formalisms is explained in the following diagram, where in each line the corresponding equations are given (see [15], [10], [46]):

$$L = L(\phi, \phi_x, \phi_t) \quad \Longleftrightarrow \quad H = L - \frac{\partial L}{\partial \phi_x}\phi_x - \frac{\partial L}{\partial \phi_t}\phi_t\,,$$

$$\frac{\partial L}{\partial \phi} - D_x \frac{\partial L}{\partial \phi_x} - D_t \frac{\partial L}{\partial \phi_t} = 0 \quad \Longleftrightarrow \quad M\boldsymbol{z}_t + K\boldsymbol{z}_x = \bigtriangledown_{\boldsymbol{z}} S(\boldsymbol{z})\,,$$

$$\int_{\partial M} (\mathrm{pr}^1\phi)^* (\mathrm{pr}^1 V_1 \rfloor \, \mathrm{pr}^1 V_2 \rfloor \, \Omega_{\mathcal{L}}) = 0 \quad \Longleftrightarrow \quad D_t \omega + D_x \kappa = 0\,,$$

$$D_t \left(\frac{\partial L}{\partial \phi_t}\phi_t - L \right) + D_x \left(\frac{\partial L}{\partial \phi_x}\phi_t \right) = 0 \quad \Longleftrightarrow \quad D_t E + D_x F = 0\,,$$

$$D_x \left(\frac{\partial L}{\partial \phi_x}\phi_x - L \right) + D_t \left(\frac{\partial L}{\partial \phi_t}\phi_x \right) = 0 \quad \Longleftrightarrow \quad D_t I + D_x G = 0\,.$$

3. Multisymplectic Integrators and Composition Methods

The concept of multisymplectic integrators for the system (2.12) is introduced by Bridges and Reich [5]. A multisymplectic integrator is a numerical scheme preserving a discrete multisymplectic conservation law. The multisymplectic integrator is the generalization of the symplectic integrator and shows good performance in maintaining local conservation laws. Using symplectic Runge-Kutta integrators in both directions leads to multisymplectic integrators (see [55]).

Very popular is the multisymplectic Preissman integrator which is obtained by using the midpoint method in both directions. Discretizing (2.12) by the midpoint method with the step-size Δt and Δx yields

$$M\frac{\boldsymbol{z}_{i+\frac{1}{2}}^{j+1}-\boldsymbol{z}_{i+\frac{1}{2}}^{j}}{\Delta t}+K\frac{\boldsymbol{z}_{i+1}^{j+\frac{1}{2}}-\boldsymbol{z}_{i}^{j+\frac{1}{2}}}{\Delta x}=\bigtriangledown_{\boldsymbol{z}}S(\boldsymbol{z}_{i+\frac{1}{2}}^{j+\frac{1}{2}}), \tag{3.1}$$

where z_i^j approximates $z(i\Delta x, j\Delta t)$ and

$$\boldsymbol{z}_{i+\frac{1}{2}}^{j+1}=\frac{1}{2}(\boldsymbol{z}_i^{j+1}+\boldsymbol{z}_{i+1}^{j+1}),\quad \boldsymbol{z}_{i+\frac{1}{2}}^{j+\frac{1}{2}}=\frac{1}{4}(\boldsymbol{z}_i^{j}+\boldsymbol{z}_{i+1}^{j}+\boldsymbol{z}_i^{j+1}+\boldsymbol{z}_{i+1}^{j+1}),\quad \text{etc.}$$

The scheme (3.1) satisfies the discrete multisymplectic conservation law

$$\frac{\omega_{i+\frac{1}{2}}^{j+1}-\omega_{i+\frac{1}{2}}^{j}}{\Delta t}+\frac{\kappa_{i+1}^{j+\frac{1}{2}}-\kappa_{i}^{j+\frac{1}{2}}}{\Delta x}=0 \tag{3.2}$$

to be proved by direct calculations.

Example 1. Consider the *Sine-Gordon equation* (see [18], [71])

$$u_{tt}-u_{xx}+\sin u=0. \tag{3.3}$$

Introducing the new variables $v=u_t$ and $w=u_x$, equation (3.3) is equivalent to

$$-v_t+w_x=\sin u,\quad u_t=v,\quad -u_x=-w \tag{3.4}$$

which can be represented as

$$M_1\boldsymbol{z}_t+K_1\boldsymbol{z}_x=\bigtriangledown_{\boldsymbol{z}}\mathcal{S}_1(\boldsymbol{z}), \tag{3.5}$$

where

$$\boldsymbol{z}=(u,v,w)^T,\quad \mathcal{S}_1(\boldsymbol{z})=\frac{1}{2}(v^2-w^2)-\cos(u)$$

and

$$M_1=\begin{pmatrix}0&-1&0\\1&0&0\\0&0&0\end{pmatrix},\quad K_1=\begin{pmatrix}0&0&1\\0&0&0\\-1&0&0\end{pmatrix}.$$

The multisymplectic integrator (3.1) applied to (3.3) yields

$$\begin{aligned} -\frac{v_{i+\frac{1}{2}}^{j+1}-v_{i+\frac{1}{2}}^{j}}{\Delta t}+\frac{w_{i+1}^{j+\frac{1}{2}}-w_{i}^{j+\frac{1}{2}}}{\Delta x} &= \sin u_{i+\frac{1}{2}}^{j+\frac{1}{2}}, \\ \frac{u_{i+\frac{1}{2}}^{j+1}-u_{i+\frac{1}{2}}^{j}}{\Delta t} &= v_{i+\frac{1}{2}}^{j+\frac{1}{2}}, \\ -\frac{u_{i+1}^{j+\frac{1}{2}}-u_{i}^{j+\frac{1}{2}}}{\Delta x} &= -w_{i+\frac{1}{2}}^{j+\frac{1}{2}}. \end{aligned} \tag{3.6}$$

Eliminating v and w from (3.6), a nine-point integrator for u is derived

$$\frac{u_{(i)}^{j+1}-2u_{(i)}^{j}+u_{(i)}^{j-1}}{\Delta t^2}-\frac{u_{i+1}^{(j)}-2u_{i}^{(j)}+u_{i-1}^{(j)}}{\Delta x^2}+\overline{\sin}(\bar{u}_i^j)=0, \tag{3.7}$$

where

$$\begin{aligned} &u_{(i)}^{l}=\frac{u_{i-1}^{l}+2u_{i}^{l}+u_{i+1}^{l}}{4}, \quad l=j-1,j,j+1, \\ &u_{m}^{(j)}=\frac{u_{m}^{j-1}+2u_{m}^{j}+u_{m}^{j+1}}{4}, \quad m=i-1,i,i+1, \\ &\overline{\sin}(\bar{u}_i^j)=\frac{1}{4}\left(\sin(\bar{u}_i^j)+\sin(\bar{u}_{i-1}^j)+\sin(\bar{u}_{i-1j-1})+\sin(\bar{u}_{ij-1})\right), \\ &\bar{u}_i^j=\frac{1}{4}\left(u_i^j+u_{i+1}^j+u_{i+1}^{j+1}+u_i^{j+1}\right),\ \bar{u}_{i-1}^j=\frac{1}{4}\left(u_{i-1}^j+u_i^j+u_i^{j+1}+u_{i-1}^{j+1}\right), \\ &\bar{u}_{i-1}^{j-1}=\frac{1}{4}\left(u_{i-1}^{j-1}+u_i^{j-1}+u_i^j+u_{i-1}^j\right),\ \bar{u}_i^{j-1}=\frac{1}{4}\left(u_i^{j-1}+u_{i+1}^{j-1}+u_{i+1}^j+u_i^j\right). \end{aligned}$$

Example 2. Consider the *nonlinear Schrödinger equation* (c.f. [14], [17], [18], [26], [28], [62], [63], [67]) written in the form (with $i=\sqrt{-1}$)

$$i\psi_t+\psi_{xx}+V'\left(|\psi|^2\right)\psi=0. \tag{3.8}$$

Using $\psi=p+iq$ and introducing a pair of conjugate momenta $v=p_x, w=q_x$, equation (3.8) can be represented as a multisymplectic Hamiltonian system

$$M_2 z_t+K_2 z_x=\nabla_{\boldsymbol{z}}\mathcal{S}_2(z), \tag{3.9}$$

where

$$\boldsymbol{z}=(p,q,v,w)^T, \quad \mathcal{S}_2(z)=\frac{1}{2}\left(v^2+w^2+V(p^2+q^2)\right)$$

and

$$M_2 = \begin{pmatrix} 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad K_2 = \begin{pmatrix} 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}.$$

From the multisymplectic Preissman integrator (3.1), a six-point integrator for (3.8) is deduced

$$i\,\frac{\psi_{[i]}^{j+1} - \psi_{[i]}^{j}}{\Delta t} + \frac{\psi_{i+1}^{j+\frac{1}{2}} - 2\psi_{i}^{j+\frac{1}{2}} + \psi_{i-1}^{j+\frac{1}{2}}}{\Delta x^2} + \frac{1}{2}G_{i,j} = 0, \tag{3.10}$$

where

$$\psi_{[i]}^{r} = \frac{1}{4}\left(\psi_{i-1,r} + 2\psi_{i,r} + \psi_{i+1,r}\right), \quad r = j, j+1,$$
$$G_{i,j} = V'(|\psi_{i-\frac{1}{2}}^{j+\frac{1}{2}}|^2)\psi_{i-\frac{1}{2}}^{j+\frac{1}{2}} + V'(|\psi_{i+\frac{1}{2}}^{j+\frac{1}{2}}|^2)\psi_{i+\frac{1}{2}}^{j+\frac{1}{2}}.$$

Example 3. Consider the *KdV (Korteweg-de Vries) equation* (see [2], [75])

$$u_t + 3(u^2)_x + u_{xxx} = 0. \tag{3.11}$$

Introducing the new variables ϕ, v and w, equation (3.11) leads to

$$M_3\boldsymbol{z}_t + K_3\boldsymbol{z}_x = \bigtriangledown_{\boldsymbol{z}}\mathcal{S}_3(\boldsymbol{z}), \tag{3.12}$$

where

$$\boldsymbol{z} = (\phi, u, v, w)^T, \quad \mathcal{S}_3(\boldsymbol{z}) = \frac{1}{2}v^2 + u^2 - uw$$

and

$$M_3 = \begin{pmatrix} 0 & \frac{1}{2} & 0 & 0 \\ -\frac{1}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad K_3 = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & 0 \\ 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix}.$$

From the multisymplectic Preissman integrator (3.1), an eight-point integrator is deduced

$$\frac{u_{(i)}^{j+1} - u_{(i)}^{j}}{\Delta t} + 3\frac{\bar{u}_{i+1}^2 - \bar{u}_{i-1}^2}{2\Delta x} + \frac{u_{i+1}^{j+\frac{1}{2}} - 3u_{i}^{j+\frac{1}{2}} + 3u_{i-1}^{j+\frac{1}{2}} - u_{i-2}^{j+\frac{1}{2}}}{\Delta x^3} = 0, \tag{3.13}$$

where

$$u_{(i)}^{\ell} = \frac{1}{8}\left(u_{i-2}^{\ell} + 3u_{i-1}^{\ell} + 3u_{i}^{\ell} + u_{i+1}^{\ell}\right), \quad \ell = j, j+1,$$

$$\bar{u}_m^2 = \frac{1}{2}((u_{m+1}^{j+\frac{1}{2}})^2 + (u_m^{j+\frac{1}{2}})^2), \quad m = i-1, i+1.$$

A twelve-point integrator for the KdV equation is known (see [2], [75]), which can be reduced to the eight-point integrator (3.13). Numerical experiments with the integrators mentioned above are known (see [28], [72], [75]). For other soliton equations such as the Zakharov-Kuznetsov equation and the Kadomtsev-Petriashvil equation similar results are obtained (see [11], [46]).

Example 4. Consider the *coupled Klein-Gordon-Schrödinger (KGS) equation* (see [42])

$$\begin{aligned} i\psi_t + \frac{1}{2}\psi_{xx} + \psi\varphi = 0, \\ \varphi_{tt} - \varphi_{xx} + \varphi - |\psi|^2 = 0, \end{aligned} \tag{3.14}$$

which describes interaction between conservative complex neutron field and neutral meson Yukawa in quantum field theory. Using the initial boundary value conditions

$$\begin{aligned} &\psi(0,x) = \psi_0(x),\ \varphi(0,x) = \varphi_0(x),\ \varphi_t(0,x) = \varphi_1(x), \\ &\psi(t,x_L) = \psi(t,x_R) = \varphi(t,x_L) = \varphi(t,x_R) = 0, \end{aligned} \tag{3.15}$$

where $\psi_0(x), \varphi_0(x)$ and $\varphi_1(x)$ are given functions, the problem has the conservative quantity

$$\|\psi\|^2 = \int_{x_L}^{x_R} \psi\bar{\psi}\mathrm{d}x = 1.$$

Setting $\psi = p + i\ q,\ \psi_x = p_x + i\ q_x = f + i\ g,\ p_t = v,\ \varphi_x = w,\ z = (p,q,f,\varphi,v,w)^{\mathrm{T}}$, the multisymplectic form of the KGS system (3.14) reads

$$\begin{aligned} q_t + \frac{1}{2}\ f_x &= -\varphi p, \\ p_t + \frac{1}{2}\ g_x &= -\varphi q, \\ -\frac{1}{2}\ p_x &= \frac{1}{2}\ f, \\ -\frac{1}{2}\ q_x &= -\frac{1}{2}\ g, \\ -\frac{1}{2}\ v_t + \frac{1}{2}w_x &= \frac{1}{2}\varphi - \frac{1}{2}\ (p^2+q^2), \\ \frac{1}{2}\ \varphi_t &= \frac{1}{2}\ v, \\ -\frac{1}{2}\ \varphi_x &= -\frac{1}{2}\ w. \end{aligned} \tag{3.16}$$

System (3.16) can be written in the standard Bridge form

$$M\frac{\partial z}{\partial t}+K\frac{\partial z}{\partial x}=\nabla S, \tag{3.17}$$

where M and K are

$$M=\frac{1}{2}\begin{bmatrix}0&-2&0&0&0&0&0\\2&0&0&0&0&0&0\\0&0&0&0&0&0&0\\0&0&0&0&0&0&0\\0&0&0&0&0&-1&0\\0&0&0&0&1&0&0\\0&0&0&0&0&0&0\end{bmatrix},\quad K=\frac{1}{2}\begin{bmatrix}0&0&1&0&0&0&0\\0&0&0&1&0&0&0\\-1&0&0&0&0&0&0\\0&-1&0&0&0&0&0\\0&0&0&0&0&0&1\\0&0&0&0&0&0&0\\0&0&0&0&-1&0&0\end{bmatrix}$$

and the Hamiltonian function reads

$$S(z)=-\frac{1}{2}\varphi(p^2+q^2)+\frac{1}{4}(\varphi^2+v^2-w^2-f^2-g^2).$$

For the three local conservation laws corresponding to (3.16), (3.17) it follows

$$\begin{aligned}\omega(z)&=-2\mathrm{d}p\wedge\mathrm{d}q-\mathrm{d}\varphi\wedge\mathrm{d}v,\\ \kappa(z)&=\mathrm{d}p\wedge\mathrm{d}f+\mathrm{d}q\wedge\mathrm{d}q+\mathrm{d}\varphi\wedge\mathrm{d}w,\\ E(z)&=-\frac{1}{2}\ \varphi(p^2+q^2)+\frac{1}{4}\ (\varphi^2+v^2-pf_x-qg_x-\varphi w_x),\\ F(z)&=\frac{1}{4}\ (pf_t+qg_t+\varphi w_t-fp_t-gq_t-rw),\\ I(z)&=-\frac{1}{2}\ \varphi(p^2+q^2)+\frac{1}{4}\ (\varphi^2-w^2-f^2-g^2+\varphi v_t)+\frac{1}{2}\ (pq_t-qp_t),\\ G(z)&=\frac{1}{4}\ (-2pg+2qf-qv_x+vw).\end{aligned} \tag{3.18}$$

Recently many mathematical equations in physics can be solved by multisymlectic methods such as Gross-Pitaevskii equation (see [69], [70]), Maxwell's equations (see [8], [56], [58], [59]), Camassa-Holm equation (see [29]), Kadomtsev-Petviashvili equation (see [41]), seismic wave equation (see [13], [14], [20], [21], [22]), Dirac equation (see [35]) and nonlinear "good" Boussinesq equation (see [16], [39]), etc.

3.1. Constructing Higher Order Integrators

Now the composition method for constructing high order multisymplectic integrators is discussed (see [15], [27]). First, recall the definition of a composition method for ODEs (see [53], [68], [74]): Suppose there are n integrators with corresponding operators $s_1(\tau)$, $s_2(\tau)$, $\ldots$, $s_n(\tau)$ of corresponding order $p_1, p_2, \ldots, p_n$, respectively, having maximal order $\mu = \max_i(p_i)$. If there exist constants $c_1, c_2, \ldots, c_n$ such that the order of the integrator whose operator is the composition $s_1(c_1\tau)s_2(c_2\tau)\cdots s_n(c_n\tau)$ is $m > \mu$, then the new integrator is called composition integrator of the original n integrators. This construction of higher order integrators from the lower order ones is called the composition method. Constructing higher order integrators, the main task is to determine constants $c_1, c_2, \ldots, c_n$ such that the scheme with the corresponding operator

$$G_m(\tau) = s_1(c_1\tau)s_2(c_2\tau)\cdots s_n(c_n\tau)$$

has order $m > \mu$. Now the basic formula for determining the constants c_i ($i = 1, \ldots, n$) is deduced. For this purpose, consider the symmetrization operator S

$$S(x^p z^q) = \frac{p!q!}{(p+q)!} \sum_{P_m} P_m(x^p z^q),$$

where x, z are arbitrary noncommutable operators and P_m denotes the summation of all the operators obtained in all possible ways of permutation (see [68]). Further, consider a time-ordering operator P defined as

$$P(x_i x_j) = \begin{cases} x_i x_j, & \text{if } i < j, \\ x_j x_i & \text{if } j < i, \end{cases}$$

where x_i, x_j are noncommutable operators (see [68]). Set

$$G_m(\tau) = s_1(c_1\tau)\cdots s_n(c_n\tau).$$

The condition on which G_m has order m reads

$$PS(x_1^{n_1} x_2^{n_2} x_3^{n_3} \cdots) = 0, \qquad \sum_{i=1}^{n} c_i = 1, \tag{3.19}$$

where $n_1 + 2n_2 + 3n_3 + \cdots \le m$, excluding $n_2 = n_3 = \cdots = 0$. Given a multisymplectic integrator for (2.12) with accuracy of order $\mathcal{O}(\tau^p + \hat{\tau}^q)$

$$M(s(\tau)z_{i,j}) + K(\hat{s}(\hat{\tau})z_{i,j}) = \bigtriangledown_z(\tilde{z}_{i,j}), \tag{3.20}$$

where $s(\tau)$ and $\hat{s}(\hat{\tau})$ are discrete operators in t-direction and x-direction, respectively, and τ and $\hat{\tau}$ are time step and space step, respectively, and $\tilde{z}_{i,j} = f_{s,\hat{s}}(z_{i,j})$ is a function of $z_{i,j}$ corresponding to the operators $s(\tau)$ and $\hat{s}(\hat{\tau})$. Suppose $G_m(\tau)$ is the composition operator of $s(\tau)$ with accuracy of order $\mathcal{O}(\tau^m)$, and

$\hat{G}_n(\hat{\tau})$ is the composition operator of $\hat{s}(\hat{\tau})$ with accuracy of order $\mathcal{O}(\hat{\tau}^n)$. Then the multi-symplectic integrator

$$M(G_m(\tau)z_{i,j}) + K(\hat{G}_n(\hat{\tau})z_{i,j}) = \bigtriangledown_z S(\tilde{z}_{i,j}) \tag{3.21}$$

has accuracy of order $\mathcal{O}(\tau^m + \hat{\tau}^n)$.

4. Variational Integrators

In this section, variational integrators are discussed. First, the Veselov-type dicretizations of one order multisymplectic field theory is presented (see [48]). For simplicity, let $n = 1$, $N = 1$, $X = (x, t)$, $U = (u)$, and take $\widehat{\mathbb{X}} = (x_i, t_j)$ and $\mathbb{U} = (u_{ij})$ as the discrete versions of X and U. It is more suitable to use only the indices of the grid and set $\mathbb{X} = (i, j)$. A rectangle $\square$ of $\mathbb{X}$ is an ordered quadruple of the form

$$\square = ((i, j), (i + 1, j), (i + 1, j + 1), (i, j + 1)). \tag{4.1}$$

The i-th component of $\square$ is the i-th vertex of the rectangle, denoted $\square^i$. A point $(i, j) \in \mathbb{X}$ is touched by a rectangle, if it is a vertex of that rectangle. If $\mathbb{M} \subseteq \mathbb{X}$, then (i, j) is an interior point of $\mathbb{M}$, if $\mathbb{M}$ contains all four rectangles that touch (i, j). $\overline{\mathbb{M}}$ denotes the union of all rectangles touching interior points of $\mathbb{M}$. A boundary point of $\mathbb{M}$ is a point in $\overline{\mathbb{M}}$ which is not an interior point. If $\mathbb{M} = \overline{\mathbb{M}}$, then $\mathbb{M}$ is called regular. $int\,\mathbb{M}$ is the set of the interior points of $\mathbb{M}$, and $\partial\mathbb{M}$ is the set of boundary points. The discrete first order prolongation of $\mathbb{X} \times \mathbb{U}$ is defined by

$$\mathbb{U}^{(1)} \equiv (\square;\, u_{ij}, u_{i+1j}, u_{i+1j+1}, u_{ij+1}),$$

and the first order prolongation of the discrete map $\varphi : \mathbb{X} \to \mathbb{U}$, $\varphi(i, j) := \varphi_{i,j}$ by

$$\mathrm{pr}^1\varphi \equiv (\square;\, \varphi_{ij}, \varphi_{i+1j}, \varphi_{i+1j+1}, \varphi_{ij+1}). \tag{4.2}$$

Corresponding to a discrete Lagrangian $\mathbb{L} : \mathbb{U}^{(1)} \to R$, the discrete functional

$$\mathbb{S}(\varphi) = \sum_{\square\subset\mathbb{M}} \mathbb{L}(\mathrm{pr}^1\varphi)\Delta x\Delta t = \sum_{\square\subset\mathbb{M}} \mathbb{L}(\square, \varphi_{ij}, \varphi_{i+1j}, \varphi_{i+1j+1}, \varphi_{ij+1})\Delta x\Delta t \tag{4.3}$$

is used, where Δx and Δt are the grid sizes in direction x and t, and $\mathbb{M}$ is a subset of $\mathbb{X}$. In this paper, only an equally spaced grid is considered. Now for abbreviation of notations, let $\mathcal{M} = [a, b] \times [c, d]$ be a rectangular domain and consider a uniform rectangular subdivision

$$\begin{aligned} &a = x_0 < x_1 < \cdots < x_{M-1} < x_M = b, \\ &c = t_0 < t_1 < \cdots < t_{N-1} < t_N = d, \\ &x_i = a + i\Delta x, t_j = c + j\Delta t, \\ &i = 0, 1, \ldots, M, \;\; j = 0, 1, \ldots, N, \\ &M\Delta x = b - a, \;\; N\Delta t = d - c. \end{aligned} \tag{4.4}$$

For autonomous Lagrangian and uniform rectangular subdivisions, the discrete action functional takes the form

$$\mathbb{S}(\varphi) = \sum_{i=0}^{M-1} \sum_{j=0}^{N-1} \mathbb{L}(\varphi_{ij}, \varphi_{i+1j}, \varphi_{i+1j+1}, \varphi_{ij+1}) \Delta x \Delta t. \tag{4.5}$$

Using the discrete variational principle, the discrete Euler-Lagrange equation (variational integrator) follows

$$\mathcal{D}_1 \mathbb{L}^{ij} + \mathcal{D}_2 \mathbb{L}^{i-1j} + \mathcal{D}_3 \mathbb{L}^{i-1j-1} + \mathcal{D}_4 \mathbb{L}^{ij-1} = 0, \tag{4.6}$$

which satisfies the discrete multisymplectic form formula

$$\sum_{\square; \square \cap \partial \mathbb{M} \neq \emptyset} \left(\sum_{l; \square^l \in \partial \mathbb{M}} (\mathrm{pr}^1 \varphi)^* (\mathrm{pr}^1 \mathbb{V}_1 \rfloor \mathrm{pr}^1 \mathbb{V}_2 \rfloor \Omega^l_{\mathbb{L}}) \right) = 0, \tag{4.7}$$

where $\Omega^l_{\mathbb{L}} = d\Theta^l_{\mathbb{L}}$, $l = 1, \ldots, 4$ and $\mathbb{V}_1$ and $\mathbb{V}_2$ are solutions of the linearized equation of (4.6). Now the discretizations of an autonomous Lagrangian $L(\varphi, \varphi_x, \varphi_t)$ is considered

$$\begin{aligned} &\mathbb{L}(\varphi_{ij}, \varphi_{i+1,j}, \varphi_{i+1,j+1}, \varphi_{i,j+1}) \\ &\qquad = L\left(\bar{\varphi}_{ij}, \frac{\varphi_{i+1,j+\frac{1}{2}} - \varphi_{ij+\frac{1}{2}}}{\Delta x}, \frac{\varphi_{i+\frac{1}{2}j+1} - \varphi_{i+\frac{1}{2}j}}{\Delta t} \right), \end{aligned} \tag{4.8}$$

where

$$\bar{\varphi}_{ij} = \frac{1}{4} \left(\varphi_{ij} + \varphi_{i+1,j} + \varphi_{i+1,j+1} + \varphi_{i,j+1} \right),$$

$$\varphi_{ij+\frac{1}{2}} = \frac{1}{2} \left(\varphi_{ij} + \varphi_{i,j+1} \right), \quad \varphi_{i+\frac{1}{2}j+1} = \frac{1}{2} \left(\varphi_{i,j+1} + \varphi_{i+1,j+1} \right), \quad \text{etc.}$$

For the discrete Lagrangian, the discrete Euler-Lagrange equation (4.6) is a nine-point variational integrator.

The following results demonstrate the equivalence of variational integrators and multisymplectic integrators. Consider the Sine-Gordon equation (3.3), then the Lagrangian is given by

$$L(u, u_x, u_t) = \frac{1}{2}u_x^2 - \frac{1}{2}u_t^2 - \cos(u). \tag{4.9}$$

The discrete Euler-Lagrange equation (4.6) corresponding to (4.9) is just the nine-point integrator (3.7). Consider the nonlinear Schrödinger equation (3.8), then the Lagrangian for (3.8) is given by

$$L(p, q, p_x, q_x, p_t, q_t) = \frac{1}{2}[p_x^2 + q_x^2 + pq_t - qp_t - V(p^2 + q^2)]. \tag{4.10}$$

The discrete Euler-Lagrange equation (4.6) corresponding to (4.10) reads

$$\begin{aligned} i\,\frac{\psi_{[i]}^{j+1} - \psi_{[i]}^{j-1}}{2\Delta t} &+ \frac{\psi_{i+1}^{j+\frac{1}{2}} + \psi_{i+1}^{j-\frac{1}{2}} - 2\psi_i^{j+\frac{1}{2}} - 2\psi_i^{j-\frac{1}{2}} + \psi_{i-1}^{j+\frac{1}{2}} + \psi_{i-1}^{j-\frac{1}{2}}}{\Delta x^2} \\ &+ \frac{1}{4}G_{i,j} + \frac{1}{4}G_{i,j-1} = 0. \end{aligned} \tag{4.11}$$

The integrator (4.11) is equivalent to the integrator (3.10), since replacing j by $j-1$ in (3.10) and adding the resulting equation to (3.10) leads to (4.11) (see [26]).

5. Some Generalizations

In this section, some generalizations based on the multisymplectic geometry and multisymplectic Hamiltonian systems are presented.

5.1. Multisymplectic Fourier Pseudospectral Methods

On Fourier space, multisymplectic Fourier pseudospectral methods are considered (see [6]). Now these methods are discussed on real space (see [25]) and the nonlinear Schrödinger equation is taken as an example. Applying the Fourier pseudospectral method to the multisymplectic system (3.9) and using the notations

$$\begin{aligned} \mathbf{p} &= (p_0, \cdots, p_{N-1})^T,\ \mathbf{q} = (q_0, \cdots .q_{N-1})^T, \\ \mathbf{v} &= (v_0, \cdots, v_{N-1})^T,\ \mathbf{w} = (w_0, \cdots .w_{N-1})^T, \end{aligned}$$

it follows

$$\begin{aligned} \frac{dq_j}{dt} - (D_1\mathbf{v})_j &= 2(p_j^2 + q_j^2)p_j, \\ -\frac{dp_j}{dt} - (D_1\mathbf{w})_j &= 2(p_j^2 + q_j^2)q_j, \\ (D_1\mathbf{p})_j = v_j, &\quad (D_1\mathbf{q})_j = w_j, \end{aligned} \tag{5.1}$$

where $j = 0, 1, \cdots, N-1$ and D_1 is the first order spectral differentiation matrix. The Fourier pseudospectral semidiscretization (5.1) has N semidiscrete multisymplectic conservation laws

$$\frac{d}{dt}\omega_j + \sum_{k=0}^{N-1} (D_1)_{j,k}\kappa_{jk} = 0, \quad j = 0, 1, \cdots, N-1, \tag{5.2}$$

where

$$\omega_j = \frac{1}{2}(dz_j \wedge M dz_j),\ \kappa_{jk} = dz_j \wedge K dz_k,\ z_j = (p_j, q_j, v_j, w_j)^T, j = 0, 1, \ldots, N-1.$$

5.2. Nonconservative Multisymplectic Hamiltonian Systems

Nonconservative multisymplectic Hamiltonian systems refer to those depending on the independent variables explicitly. Such an example is the Schrödinger equation with variable coefficients (see [38]). Another example is the three-dimensional scalar seismic wave equation (see [13], [14], [19], [20], [22])

$$\bigtriangledown^2 u - \frac{1}{c(x,y,z)e^2} u_{tt} = 0, \tag{5.3}$$

where $\bigtriangledown^2 u = u_{xx} + u_{yy} + u_{zz}$ and $c(x, y, z)$ is the wave velocity. Introducing the new variables

$$v = \frac{1}{c(x,y,z)} u_t, \quad w = u_x, \quad p = u_y, \quad q = u_z,$$

equation (5.3) can be rewritten as

$$M(x, y, z)\mathcal{Z}_t + K\mathcal{Z}_x + L\mathcal{Z}_y + N\mathcal{Z}_z = \bigtriangledown_{\mathcal{Z}}\mathcal{S}(\mathcal{Z}), \tag{5.4}$$

where $\mathcal{Z} = (u, v, w, p, q)^T$, $\mathcal{S}(\mathcal{Z}) = \frac{1}{2}\left(v^2 - w^2 - p^2 - q^2\right)$ and

$$M(x,y,z) = \begin{pmatrix} 0 & -\frac{1}{c(x,y,z)} & 0 & 0 & 0 \\ \frac{1}{c(x,y,z)} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix}, \quad K = \begin{pmatrix} 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix},$$

$$L = \begin{pmatrix} 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix}, \qquad N = \begin{pmatrix} 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 & 0 \end{pmatrix}.$$

The corresponding four pre-symplectic forms associated to the time direction and to the three space directions are

$$\begin{aligned} \omega &= \frac{1}{2} d\mathcal{Z} \wedge M(x,y,z) d\mathcal{Z}, \qquad & \kappa_x &= \frac{1}{2} d\mathcal{Z} \wedge K d\mathcal{Z}, \\ \kappa_y &= \frac{1}{2} d\mathcal{Z} \wedge L d\mathcal{Z}, & \kappa_z &= \frac{1}{2} d\mathcal{Z} \wedge N d\mathcal{Z}. \end{aligned} \tag{5.5}$$

Note that the time direction pre-symplectic form ω depends on the space variables (x, y, z). The corresponding multisymplectic integrators are obtained (see [19]).

5.3. Construction of Multisymplectic Integrators for Modified Equations

Consider the linear wave equation

$$u_{tt} = u_{xx}. \tag{5.6}$$

Based on the two Hamiltonian formulations of (5.6) and using the hyperbolic functions, various symplectic integrators are constructed in [54]. By deriving the corresponding Lagrangians and their discrete counterparts, these symplectic integrators are proved to be multisymplectic integrators for the modified versions of (5.6) (see [65]). Consider an example. Using hyperbolic function $\tanh x$, a symplectic integrator for (5.6) of accuracy $\mathcal{O}(\Delta t^{2s} + \Delta x^{2m})$ is given by

$$\begin{aligned} &u_i^{j+1} - 2u_i^j + u_i^{j-1} \\ &\qquad = \tanh\left(2s, \frac{\Delta t}{2}\right) \tanh\left(2s, \frac{\Delta t}{2}\Delta(2m)\right) (u_i^{j+1} - 2u_i^j + u_i^{j-1}), \end{aligned} \tag{5.7}$$

where

$\Delta(2m)$

$$= \nabla_+ \nabla_- \sum_{j=0}^{m-1} (-1)^j \beta_j \left(\frac{\Delta x^2 \nabla_+ \nabla_-}{4} \right)^j, \ \beta_j = [(j!)^2 2^{2j}]/[(2j+1)!(j+1)]$$

and ∇_+ and ∇_- are forward and backward difference operators, respectively. For $m = 2$ and $s = 2$, the integrator (5.7) is a multisymplectic integrator of the modified equation

$$u_{tt} = u_{xx} - \frac{\Delta t^2}{12} u_{xx} + \left(1 - \frac{\Delta t^2}{12}\right) \frac{\Delta t^2}{12} u_{xxxxxx}. \tag{5.8}$$

For other hyperbolic functions, similar results can be obtained.

5.4. Multisymplectic Birkhoffian Systems

The multisymplectic Hamiltonian system can be generalized to include dissipation terms. This generalization leads to the following multisymplectic Birkhoffian system

$$M(t, x, \boldsymbol{z})\boldsymbol{z}_t + K(t, x, \boldsymbol{z})\boldsymbol{z}_x = \nabla_{\boldsymbol{z}} B(t, x, \boldsymbol{z}) + \frac{\partial F}{\partial t} + \frac{\partial G}{\partial x}, \tag{5.9}$$

where $\boldsymbol{z} = (z_1, \ldots, z_n)^T$, $F = (f_1, \ldots, f_n)^T$, $G = (g_1, \ldots, g_n)^T$ and $M = (m_{ij})$ and $K = (k_{ij})$ are two antisymmetric matrices with entries respectively:

$$m_{ij} = \frac{\partial f_j}{\partial z_i} - \frac{\partial f_i}{\partial z_j}, \quad k_{ij} = \frac{\partial g_j}{\partial z_i} - \frac{\partial g_i}{\partial z_j}.$$

The system (5.9) satisfies the multisymplectic dissipation law

$$\frac{d}{dt}\left(\frac{1}{2} d\boldsymbol{z} \wedge M d\boldsymbol{z}\right) + \frac{d}{dx}\left(\frac{1}{2} d\boldsymbol{z} \wedge K d\boldsymbol{z}\right) = 0. \tag{5.10}$$

Consider as an example the equation describing the linear damped string (see [60])

$$u_{tt} - u_{xx} + u + \alpha u_t + \beta u_x = 0. \tag{5.11}$$

Introducing new variables $p = u_t$ and $q = u_x$, the equation (5.11) can be transformed to the type of (5.9) with

$$M = \begin{pmatrix} 0 & e^{\alpha t - \beta x} & 0 \\ -e^{\alpha t - \beta x} & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad K = \begin{pmatrix} 0 & 0 & -e^{\alpha t - \beta x} \\ 0 & 0 & 0 \\ e^{\alpha t - \beta x} & 0 & 0 \end{pmatrix},$$

and

$$\boldsymbol{z} = (u, p, q)^T, \quad B = -\frac{1}{2}e^{\alpha t - \beta x}(u^2 + p^2 - q^2 + \alpha up + \beta uq),$$
$$F = \left(-\frac{1}{2}e^{\alpha t - \beta x}p, \frac{1}{2}e^{\alpha t - \beta x}u, 0\right)^T, \quad G = \left(\frac{1}{2}e^{\alpha t - \beta x}q, 0, -\frac{1}{2}e^{\alpha t - \beta x}\right)^T.$$

Similarly, multisymplectic dissipation integrators for the system (5.9) can be deduced which preserve a discrete version of the multisymplectic dissipation law (5.10).

6. Discrete Mechanics Based on Finite Element Methods

In this section, discrete mechanics based on finite element methods are considered (see [23], [24]). Remember the variation problem of the action factional (2.3) in case of ordinary equation

$$\mathcal{S}(q^i(t)) = \int_a^b L(t, q^i(t), \dot{q}^i(t))dt, \tag{6.1}$$

where $q^i(t)$ is a $\mathcal{C}^2$ curve in Q. The finite element method is an approximation method for solving the variation problem. Instead of solving the variation problem in the space $\mathcal{C}^2([a,b])$, the finite element method solves the problem in a subspace of $\mathcal{C}^2([a,b])$. Consider the subspace $V_{h^m}([a,b])$ consisting of piecewise m-degree polynomials interpolating the curves $q(t) \in \mathcal{C}^2([a,b])$. First, repeat the piecewise linear interpolation. Given a partition of $[a,b]$

$$a = t_0 < t_1 < \cdots < t_k < \cdots < t_{N-1} < t_N = b, \tag{6.2}$$

the intervals $I_k = [t_k, t_{k+1}]$ are called elements. $h_k = t_{k+1} - t_k$. $V_h([a,b])$ consists of piecewise linear function interpolating $q(t)$ at $(t_k, q_k), k = 0, 1, \cdots, N$. Now the expressions of $q_h(r_t) \in V_h([a,b])$ are derived. First, the basis functions $\varphi_k(t)$ are constructed, which are piecewise linear function on $[a,b]$ satisfying $\varphi_k(t_i) = \delta_k^i,\ i, k = 0, 1, \ldots, n$:

$$\varphi_0(t) = \begin{cases} 1 - \dfrac{t - t_0}{h_0}, & t_0 \le t \le t_1, \\ 0, & \text{otherwise}, \end{cases} \qquad \varphi_N(t) = \begin{cases} 1 - \dfrac{t - t_N}{h_{N-1}}, & t_{N-1} \le t \le t_N, \\ 0, & \text{otherwise}, \end{cases} \tag{6.3}$$

and for $k = 1, 2, \ldots, N-1$,

$$\varphi_k(t) = \begin{cases} 1 - \dfrac{t - t_k}{h_{k-1}}, & t_{k-1} \le t \le t_k, \\ 1 - \dfrac{t - t_k}{h_k}, & t_k \le t \le t_{k+1}, \\ 0, & \text{otherwise.} \end{cases} \tag{6.4}$$

Using these basis functions, the representation of $q_h \in V_h([a,b])$ follows

$$q_h(t) = \sum_{k=0}^{N} q_k \varphi_k(t). \tag{6.5}$$

In the space $V_h([a,b])$, the action functional (2.3) has the form

$$\begin{aligned} S((t, q_h(t))) &= \int_a^b L(t, q_h(t), \dot{q}_h(t)) \mathrm{d}t \\ &= \sum_{k=0}^{N} \int_{t_k}^{t_{k+1}} L\Big(t, \sum_{i=0}^{N} (q_i \varphi_i(t), \frac{\mathrm{d}}{\mathrm{d}t} \sum_{i=0}^{N} (q_i \varphi_i(t))\Big) \mathrm{d}t \\ &= \sum_{k=0}^{N} \mathbb{L}(t_k, q_k, t_{k+1}, q_{k+1})(t_{k+1} - t_k), \end{aligned} \tag{6.6}$$

where

$$\begin{aligned} \mathbb{L}(t_k, q_k, t_{k+1}, q_{k+1}) &= \frac{1}{t_{k+1} - t_k} \int_{t_k}^{t_{k+1}} L\Big(t, \sum_{i=0}^{N} (q_i \varphi_i(t)), \frac{\mathrm{d}}{\mathrm{d}t} \sum_{i=0}^{N} (q_i \varphi_i(t))\Big) \mathrm{d}t \\ &= \frac{1}{t_{k+1} - t_k} \int_{t_k}^{t_{k+1}} L\Big(t, \sum_{i=k}^{k+1} (q_i \varphi_i(t)), \frac{\mathrm{d}}{\mathrm{d}t} \sum_{i=k}^{k+1} (q_i \varphi_i(t))\Big) \mathrm{d}t. \end{aligned} \tag{6.7}$$

Therefore, restricting to the subspace $V_h([a,b])$ of $\mathcal{C}^2)[a,b])$, the original variational problem reduces to the extremum problem of the function (6.6) in $q_k, k = 0, 1, \ldots, N$. Notice that (6.6) is just one of the discrete sections. And the only task is to perform the same calculations on (6.7). The discrete Euler-Lagrange equation preserving the discrete Lagrange two form can be obtained. Hence, discrete mechanics based on finite element methods consists of two steps. First, use finite element methods to obtain a kind of discrete Lagrangian. Second, use the methods of Veselov's mechanics to get the variational integrators.

Consider the previous example again. Instead of the classical Lagrangian choose the discrete Lagrangian $\mathbb{L}(t_k, q_k, t_{k+1}, q_{k+1})$ as

$$
\begin{aligned}
&\mathbb{L}(t_k, q_k, t_{k+1}, q_{k+1})\\
&\quad= \frac{1}{t_{k+1}-t_k}\int_{t_k}^{t_{k+1}} \Big(\frac{1}{2}\Big(\frac{\mathrm{d}}{\mathrm{d}t}\sum_{i=0}^{N}(q_i\varphi_i(t))\Big)^2 - V\Big(\sum_{i=0}^{N}(q_i\varphi_i(t))\Big)\Big)\mathrm{d}t\\
&= \frac{1}{t_{k+1}-t_k}\int_{t_k}^{t_{k+1}} \Big(\frac{1}{2}\Big(\frac{q_{k+1}-q_k}{t_{k+1}-t_k}\Big)^2 - V\Big(\frac{t_{k+1}-t}{t_{k+1}-t_k}q_k + \frac{t-t_k}{t_{k+1}-t_k}q_{k+1}\Big)\Big)\mathrm{d}t\\
&\qquad\qquad= \frac{1}{2}\Big(\frac{q_{k+1}-q_k}{t_{k+1}-t_k}\Big)^2 - F(q_k, q_{k+1}), \qquad (6.8)
\end{aligned}
$$

where

$$
F(q_k, q_{k+1}) = \frac{1}{t_{k+1}-t_k}\int_{t_k}^{t_{k+1}} V\Big(\frac{t_{k+1}-t}{t_{k+1}-t_k}q_k + \frac{t-t_k}{t_{k+1}-t_k}q_{k+1}\Big)\mathrm{d}t. \qquad (6.9)
$$

The discrete Euler-Lagrange equation reads

$$
\begin{aligned}
\Big(\frac{q_{k+1}-q_k}{t_{k+1}-t_k} - \frac{q_k-q_{k-1}}{t_k-t_{k-1}}\Big) + \frac{\partial F(q_k, q_{k+1})}{\partial q_k}(t_{k+1}-t_k) + \frac{\partial F(q_{k-1}, q_k)}{\partial q_k}(t_k-t_{k-1})&\\
= 0, \qquad (6.10)&
\end{aligned}
$$

which preserves the Lagrange two form

$$
\Big(\frac{1}{t_{k+1}-t_k} + (t_{k+1}-t_k)\frac{\partial^2 F(q_k, q_{k+1})}{\partial q_k \partial q_{k+1}}\Big)\mathrm{d}q_{k+1}\wedge \mathrm{d}q_k. \qquad (6.11)
$$

If fixed time steps $t_{k+1}-t_k = t_k - t_{k-1} = h$ are used, then (6.10) reads

$$
\frac{q_{k+1}-2q_k+q_{k-1}}{h^2} + \frac{\partial F(q_k, q_{k+1})}{\partial q_k} + \frac{\partial F(q_{k-1}, q_k)}{\partial q_k} = 0, \qquad (6.12)
$$

which preserves the Lagrange two form

$$
\Big(\frac{1}{h} + h\frac{\partial^2 F(q_k, q_{k+1})}{\partial q_k \partial q_{k+1}}\Big)\mathrm{d}q_{k+1}\wedge \mathrm{d}q_k.
$$

Suppose q_k is the solution of (6.10) and $q(t)$ is the solution of

$$
\frac{\mathrm{d}^2 q}{\mathrm{d}t^2} + \frac{\partial V(q)}{\partial q} = 0, \qquad (6.13)
$$

then from the convergence theory of finite element methods it follows

$$\|q(t) - q_h(t)\| \leq Ch^2, \tag{6.14}$$

where $\|\cdot\|$ is the L^2 norm, $q_h(t) = \sum_{k=0}^{N} q_k,\ h = \max_k\{h_k\}$ and C is a constant independent of h. Using the mid-point integration formula in (6.9), it follows

$$F(q_k, q_{k+1}) = \frac{1}{t_{k+1} - t_k} \int_{t_k}^{t_{k+1}} V\Big(\frac{t_{k+1} - t}{t_{k+1} - t_k} q_k + \frac{t - t_k}{t_{k+1} - t_k} q_{k+1}\Big) \mathrm{d}t \tag{6.15}$$

which is approximately

$$V\Big(\frac{q_k + q_{k+1}}{2}\Big). \tag{6.16}$$

Using the trapezoidal formula or Simpson's formula for the numerical integration of (6.9), then other kinds of discrete Lagrangian are obtained.

6.1. Differential Complex Methods and Multisymplectic Structures

Recently, differential complexes play an increasingly important role in numerical analysis. In particular, discrete differential complexes are crucial in designing stable finite element schemes (see [1], [40]). With regard to discrete differential forms, a generic Hodge operator is introduced (see [34]). It is shown that most finite element schemes emerge as its specializations. The connection between Veselov's discrete mechanics and finite element methods is first discussed in [48]. Symplectic and multisymplectic structures in simple finite element methods are explored in [33]. It will be of particular significance to study the multisymplectic structure for the finite element methods by using discrete differential complexes and in particular discrete Hodge operators. This topic will be continued in a forthcoming paper.

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