Spectral variational integrators for semi-discrete Hamiltonian wave equations

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Abstract

In this paper, we present a highly accurate Hamiltonian structure-preserving numerical method for simulating Hamiltonian wave equations. This method is obtained by applying spectral variational integrators (SVI) to the system of Hamiltonian ODEs which are derived from the spatial semi-discretization of the Hamiltonian PDE. The spatial variable is discretized by using high-order symmetric finite-differences. An efficient implementation of SVI for high-dimensional systems of ODEs is presented.

Keywords: Hamiltonian PDEs, Spectral variational integrator, Semi-discrete, Symmetric difference

1. introduction

During the past decade, there have been many attempts to derive geometric structure-preserving numerical methods for Hamiltonian PDEs [4, 11, 19]. Researchers have tried to extend the ideas in the geometric integration of ODE systems to construct numerical schemes for some specific PDEs, so as to preserve as many invariants of the systems as possible. These approaches have mainly focused on multisymplectic variational integrators [16], multisymplectic reformulation of the Hamiltonian PDEs [5] or using some geometric structure-preserving ODE solvers, such as Gauss collocation, discrete gradients and the method of lines, applied to the invariant preserving semi-discrete ODEs [7], etc. Without lose of generality, we consider the Hamiltonian wave equations described in [16],

$$\frac{\partial^2 u}{\partial t^2} - \Delta u - V'(u) = 0, \quad u \in \Gamma(\pi_{XY}),$$

where $\pi_{XY} : Y \to X$ is a fiber bundle over the oriented space-time manifold $X$, $V$ is a real valued $C^\infty$ function, and $u : X \to Y$ is a section of $\pi_{XY}$, and $j^1(u)$ is its first jet extension. For a more in-depth discussion of multisymplectic geometry, the reader is referred to Gotay [9].

By drawing upon variational formulations of field theories and multisymplectic geometry, Marsden et al. [16] introduced the abstract multisymplectic formulation of Hamiltonian PDEs and constructed multisymplectic variational integrators based on triangles and rectangles (see Figure 1). The main
advantage for discretization of the covariant multisymplectic perspective of Hamiltonian PDEs is that it allows one to consider discretizations of the configuration bundle that are not simply global tensor products of spatial and temporal discretizations, which is what one would obtain otherwise by applying a symplectic integrator to the semi-discretization of the Hamiltonian PDE. This flexibility is exploited in Lew et al. [14] to obtain multisymplectic integrators in which the different spatial elements are time-marched using different time-steps.

\[
\begin{align*}
\text{(i-1,j-1)} & \quad \text{(i,j-1)} & \quad \text{(i-1,j)} & \quad \text{(i,j)} & \quad \text{(i+1,j)} \\
\text{(i-1,j)} & \quad \text{(i,j)} & \quad \text{(i+1,j)} & \quad \text{(i+1,j+1)} & \\
\text{(i-1,j-1)} & \quad \text{(i,j-1)} & \quad \text{(i+1,j-1)} & \quad \text{(i+1,j+1)} & \\
\text{(i-1,j)} & \quad \text{(i,j)} & \quad \text{(i+1,j)} & \quad \text{(i+1,j+1)} & \\
\end{align*}
\]

Figure 1: On the left, the method based on a regular triangular mesh; on the right, the method based on a regular rectangular mesh.

In analogy to variational integrators for ODEs, there are two main steps for constructing multi-symplectic variational integrators. One is to choose a finite-dimensional function space to approximate sections \( \phi : X \to Y \) of the configuration bundle \( Y \). The other is to choose a quadrature method to approximate the action integral \( S = \int_X L(j^1\phi) \).

An alternative approach to the construction of multisymplectic integrators was introduced by Bridges and Reich [6], and is based on a description of a Hamiltonian PDE in terms of multiple skew-symmetric matrices, which is the notion of multisymplectic geometry introduced in Bridges [5]. In this framework, the \((1 + 1)\)-dimensional nonlinear wave equation (1) can be expressed as

\[
v_t - w_x - V(u) = 0, \quad v = u_t, \ w = u_x,
\]

which can be written in multisymplectic form

\[
\begin{bmatrix}
0 & -1 & 0 \\
1 & 0 & 0 \\
0 & 0 & 0
\end{bmatrix}
\begin{bmatrix}
u_t \\
v_t \\
w_t
\end{bmatrix}
+ \begin{bmatrix}
0 & 0 & -1 \\
0 & 0 & 0 \\
1 & 0 & 0
\end{bmatrix}
\begin{bmatrix}
u_x \\
v_x \\
w_x
\end{bmatrix}
= \begin{bmatrix}
V(u) \\
v \\
-w
\end{bmatrix},
\]

or more compactly as

\[
MZ_t + KZ_x = \nabla Z H(Z).
\]

Many high-order multisymplectic integrators [8, 17] have been constructed and analyzed based on both semi-discretizations and full-discretizations using this formulation.

**Remark 1.1.** **Multisymplectic field theories expressed in terms of a multisymplectic \((n+2)\)-differential form in the sense proposed by Marsden reduce to the Bridges’ formulation of multisymplectic field theories for a suitable choice of skew-symmetric matrices for each of the spatial and temporal components.**

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However, the converse is not true. This is because the skew-symmetric matrices in the Bridges formulation have to satisfy an integrability condition for them to be expressible as a single multisymplectic \((n+2)\)-differential form. This is analogous to the fact that every \(n\)-order differential equation can be expressed as a system of \(n\) first-order differential equations, but not every system of \(n\) first-order differential equations can be expressed as a single \(n\)-order differential equation.

In this paper, we focus on solving the large system of Hamiltonian ODEs obtained by semi-discretization of the Hamiltonian PDE using spectral variational integrators (SVI), which fall within the framework of generalized Galerkin variational integrators that have been discussed in [10, 12, 13, 15]. Hall and Leok [10] provide a systematic introduction to spectral variational integrators. In addition to the spectral accuracy, the SVI is symplectic, momentum preserving and exhibits excellent energy behavior. We will also see that the stability and computational efficiency of spectral variational integrators are both favorable when compared with some symplectic Runge-Kutta methods, which makes SVIs an excellent choice to deal with the semi-discrete Hamiltonian ODEs. As to the Hamiltonian preserving semi-discretization of the spatial variables, one may choose symmetric finite-difference [3], spectral discretizations or the rescaled Fourier discretization [20]. No matter which discretization we choose, the basic goal is to conserve discrete counterparts of the continuous invariants.

The outline of this paper is as follows. In Section 2, we introduce the Hamiltonian preserving semi-discretization of the given Hamiltonian PDE. In Section 3, we briefly review the construction of SVIs and give an efficient implementation of SVIs for high-dimensional systems of ODEs. In Section 4, a simple error estimate is given. Numerical examples are then presented in Section 5. Here, we consider the linear wave equation and the breather solution of sine-Gordon equations. In the last section, we draw some conclusions and provide possible future directions.

2. Semi-discretization of the Hamiltonian wave equation

The basic idea of our approach is that we first discretize the spatial dimensions in a highly accurate way, so that the resulting semi-discrete problem is a Hamiltonian system of ODEs to which Galerkin variational integrators can be applied directly. Without loss of generality, we consider the one-dimensional wave equation with periodic boundary conditions which are given as,

\[
\begin{aligned}
\frac{\partial^2 u(x,t)}{\partial t^2} &= \frac{\partial^2 u(x,t)}{\partial x^2} + V'(u(x,t)), \quad (x,t) \in (-R,R) \times (0,\infty), \\
u(x,0) &= \phi_0(x), \quad u_t(x,0) = \phi_1(x), \\
u(-R,t) &= u(R,t).
\end{aligned}
\]  

(2)

2.1. Symmetric finite-difference approach

There are several ways we can use to approximate the second-order spatial derivative, such as, finite-differences, finite elements, or Fourier–Galerkin, all of which yield a set of Hamiltonian ODEs of the following form,

\[
\frac{d^2 \mathbf{u}}{dt^2} = D \mathbf{u} + F(t, \mathbf{u}), \quad 0 < t \leq \infty,
\]

(3)

where

\[
\mathbf{u}(t) = (u_1(t), \ldots, u_N(t))^T \quad \text{with} \quad u_i(t) \approx u(x_i,t),
\]

\[
F(t, \mathbf{u}) = (V'(u_1), \ldots, V'(u_N))^T.
\]
A semi-discretization on the spatial variable by using second-order symmetric differences is given by,

\[
\frac{d^2 u_i}{dt^2} = \frac{u_{i+1} - 2u_i + u_{i-1}}{\Delta x^2} + V'(u_i), \quad 0 < t \leq \infty,
\]

which lead to a system of ODEs of the form (3) with differentiation matrix

\[
D = \frac{1}{\Delta x^2} \begin{pmatrix}
-2 & 1 & & \\
1 & -2 & 1 & \\
& \ddots & \ddots & \ddots \\
& & 1 & -2 & 1 \\
& & & 1 & -2
\end{pmatrix}_{N \times N},
\]

For higher-order symmetric differences methods

\[
\frac{\partial^2 u(x_i, t)}{\partial x^2} \approx \frac{1}{\Delta x^2} \sum_{j=-k}^{k} \alpha_{i+j} u_{i+j},
\]

which are even-order generalizations of the central difference scheme, we can refer to Table 1. It should be mentioned that for the use of \( p = 2k \) order schemes for boundary-value problems we need \( k \) initial conditions. For a more systematic introduction of high-order finite-difference scheme, readers may refer to [2, 3].

**Remark 2.1.** Since the eigenvalue \( \lambda \) of (5) is between \(-\frac{4}{\Delta x^2}\) and 0, the semi-discrete system (3) becomes extremely stiff when we choose a small \( \Delta x \). But numerically we will see that the spectral variational integrators are still effective for this high-dimensional system of ODEs. Refer to Figure 2 for the eigenvalues of \( D \) which we will use later in the numerical simulations.

<table>
<thead>
<tr>
<th>Order</th>
<th>( \alpha_{i-4} )</th>
<th>( \alpha_{i-3} )</th>
<th>( \alpha_{i-2} )</th>
<th>( \alpha_{i-1} )</th>
<th>( \alpha_i )</th>
<th>( \alpha_{i+1} )</th>
<th>( \alpha_{i+2} )</th>
<th>( \alpha_{i+3} )</th>
<th>( \alpha_{i+4} )</th>
</tr>
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<td>-2</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>4</td>
<td>-1/12</td>
<td>4/3</td>
<td>-5/2</td>
<td>4/3</td>
<td>-1/12</td>
<td>4/3</td>
<td>-5/2</td>
<td>4/3</td>
<td>-1/12</td>
</tr>
<tr>
<td>8</td>
<td>-1/560</td>
<td>8/315</td>
<td>-1/5</td>
<td>8/315</td>
<td>-205/72</td>
<td>8/5</td>
<td>-1/5</td>
<td>8/315</td>
<td>-1/560</td>
</tr>
</tbody>
</table>

Table 1: Coefficients of symmetric differences for the approximation of the second-order spatial derivative
**Theorem 2.1.** Suppose $V$ is continuously differentiable and $u(t) = (u_1(t), ..., u_N(t))^T$ is the solution of (3), then the Hamiltonian of (3) is given by

$$H(u, \dot{u}) = \Delta x \left[ \frac{1}{2} \dot{u}^T \dot{u} + \frac{1}{2} u^T D u + \sum_{i=1}^{N} V(u_i) \right]. \quad (7)$$

**Proof.** It is easy to verify that $\frac{dH(t)}{dt} = 0$ by using the fact that $D$ is symmetric. \qedsymbol

A more natural way to convert the infinite-dimensional nonlinear wave equation to finite-dimensional Hamiltonian systems is to discretize the continuous Lagrangian of the wave equation directly. We will see that this implementation can give us systems of Hamiltonian ODEs with arbitrarily high accuracy. As a simple example, we can replace the Lagrangian of (2)

$$L(t, x, u, u_t, u_x) = \frac{1}{2} \left[ \left( \frac{\partial u}{\partial t} \right)^2 - \left( \frac{\partial u}{\partial x} \right)^2 \right] + V(u), \quad (8)$$

by the following semi-discrete analogue,

$$L(t, u, u_t) = \sum_{i=0}^{M-1} \left\{ \frac{1}{2} \left[ \left( \frac{\partial u_i}{\partial t} \right)^2 - \left( \frac{u_{i+1} - u_i}{h} \right)^2 \right] + V(u_i) \right\}.$$ 

Then, the Euler–Lagrange equations

$$\frac{d}{dt} \frac{\partial L}{\partial \dot{u}_i} - \frac{\partial L}{\partial u_i} = 0,$$

lead to the second-order finite-difference scheme,

$$\ddot{u}_i - \frac{1}{h^2} (u_{i-1} - 2u_i + u_{i+1}) + V'(u_i) = 0,$$

which is the same as (4). The Hamilton’s canonical equations can also be obtained by discretizing the spatial variables of the continuous Hamiltonian,

$$H(t, u, u_t) = \sum_{i=0}^{M-1} \left\{ \frac{1}{2} \left[ \left( \frac{\partial u_i}{\partial t} \right)^2 + \left( \frac{u_{i+1} - u_i}{h} \right)^2 \right] + V(u_i) \right\}.$$ 

Then, Hamilton’s canonical equations are given as,

$$\ddot{u}_i = -\frac{\partial H}{\partial \dot{u}_i}, \quad \dot{u}_i = \frac{\partial H}{\partial \dot{u}_i},$$

or more compactly as

$$\frac{dZ}{dt} = J^{-1} \Delta H(Z),$$

where $Z = (u, \dot{u})$ and $J$ is the symplectic matrix,

$$J = \begin{pmatrix} 0_M & I_M \\ -I_M & 0_M \end{pmatrix}.$$
2.2. Spectral collocation approach

We can also use a spectral collocation method to discretize the spatial derivative which led to Hamiltonian ODEs with higher-order spatial approximation. Combined with the SVI for solving the resultant system of Hamiltonian ODEs, the numerical methods can obtain overall (space-time) spectral accuracy.

We discretize (8) in space by using the spectral collocation method, which led to the following discrete Lagrangian

\[
L(t, u, u_t) = \sum_{i=0}^{M-1} \left\{ \frac{1}{2} \left[ \left( \frac{\partial u_i}{\partial t} \right)^2 - \left( \sum_{k=0}^{M} D_{ik}^{(1)} u_k \right)^2 \right] + V(u_i) \right\},
\]

where \( D_{ik}^{(p)} \) is the \( p \)-th order differentiation matrix in the spatial domain \([-R, R] \). Then the Euler–Lagrange equations led to the corresponding ODEs,

\[
\ddot{u} = Au + V'(u),
\]

where

\[
A = \begin{pmatrix}
(c_1, c_1) & (c_1, c_2) & \ldots & (c_1, c_{M+1}) \\
(c_2, c_1) & (c_2, c_2) & \ldots & (c_2, c_{M+1}) \\
\vdots & \vdots & \ddots & \vdots \\
(c_{M+1}, c_1) & (c_{M+1}, c_2) & \ldots & (c_{M+1}, c_{M+1})
\end{pmatrix}
\]

and \((c_i, c_j)\) is the inner product of the \(i\)-th and \(j\)-th column of the matrix \(D^{(1)}\). We can see that matrix \(A\) is automatically symmetric. The derivative of \(u\) respect to \(x\) may be approximated by any appropriate differentiation matrix, such as Legendre, Hermite and sinc differentiation matrix [20]. We can also use a Fourier–Galerkin approximation [1, 7]. It should be pointed out that the spectral variational integrators may not be stable for every system of Hamiltonian ODEs constructed in this way, but we will see from the numerical experiments that SVIs are effective for many of the resulting stiff systems which cannot otherwise be solved by many conventional ODE solvers.

3. Galerkin variational integrators from spectral-collocation methods

Now we briefly recall the construction of spectral variational integrators which falls within the framework of generalized Galerkin variational integrators that were discussed in [10, 12, 15, 18]. Here we will introduce an efficient implementation for high-dimensional Hamiltonian systems, which are suitable for semi-discrete systems of Hamiltonian ODEs (9).

**Approximation of the exact discrete Lagrangian.** To approximate the exact discrete Lagrangian, we should first approximate the variables \(u : [0, T] \to U\). We divide the total time interval \([0, T]\) into \(M\) subintervals of equal length \(h\),

\[
[0, T] = \bigcup_{k=0}^{M-1} [kh, (k+1)h], \quad M = T/h,
\]
and then approximate the exact discrete Lagrangian $L_d^E(u_k, u_{k+1})$ with a highly-accurate and numerically computable discrete Lagrangian $L_d(u_k, u_{k+1})$. To be specific, for a given Lagrangian functional $L : TU \to \mathbb{R}$, we approximate the infinite-dimensional function space,

$$\mathcal{C}([kh, (k+1)h], U) = \{ u \in C^2([kh, (k+1)h], U) \mid u(kh) = u_k, u((k+1)h) = u_{k+1} \},$$

with a finite-dimensional function subspace,

$$\mathcal{C}^s([kh, (k+1)h], U) = \{ u \in \mathcal{C}([kh, (k+1)h], U) \mid u \text{ is a polynomial of degree } s \}.$$

![Figure 3: The red dots represent the quadrature points, which may or may not be the same as the interpolation points which represented by black dots.](image)

As illustrated in Figure 3, we approximate the exact discrete Lagrangian by a $s$-degree polynomial generated by Lagrangian interpolating polynomials based on the Chebyshev points $c_j = \frac{(2k+1)h}{2} + \frac{h}{2} \sin \left( \frac{(s-2j)\pi}{2s} \right)$, where $c_j$ are the Chebyshev points, $x_j = \sin \left( \frac{(s-2j)\pi}{2s} \right)$, $0 \leq j \leq s$, rescaled and shifted from $[-1, 1]$ to $[kh, (k+1)h]$. Then, for any chosen numerical quadrature formula $(w_i, \tau_i)_{i=1}^m$, where $w_i$ are the quadrature weights and $\tau_i \in [-1, 1]$ are the quadrature points, we obtain,

$$u(d_i; u^v_k, h) = \sum_{v=0}^s u^v_k \hat{l}_{v,s}(\tau(d_i)),$$

$$\dot{u}(d_i; u^v_k, h) = \sum_{v=0}^s \frac{u^v_k \hat{l}_{v,s}(\tau(d_i))}{h} \frac{d\tau}{dt} = \frac{2}{h} \sum_{v=0}^s u^v_k \hat{l}_{v,s}(\tau(d_i)),$$

where $\tau(t) = \frac{2}{h}(t - t_k) - 1 \in [-1, 1]$, $d_i$ are the quadrature points in the interval $[t_k, t_{k+1}]$, and $l_{v,s}(\tau)$ are the Lagrange basis polynomials of degree $s$, $l_{v,s}(\tau) : [-1, 1] \to \mathbb{R}$, that are given by

$$l_{v,s}(\tau) = \prod_{0 \leq j \leq s, j \neq v} \frac{\tau - x_j}{x_v - x_j}.$$

1Since $u$ is a vector, we mean that each component of $u$ is a polynomial of degree $s$.

2We change the conventional Chebyshev points $x_j = \cos(\frac{j\pi}{2s})$ to this form by using the identity $\cos(\theta) = \sin(\frac{\pi}{2} - \theta)$. In floating-point arithmetic, Chebyshev points that are computed using this formula are more symmetric about the origin than the conventional one [20].
Then, we can approximate the discrete Lagrangian as follows

\[ L_d(u_k = u_k^0, u_k^1, \ldots, u_k^s = u_{k+1}; h) \]

\[ = \text{ext}_{u \in C^s((kh,(k+1)h),Q)} \frac{h}{2} \sum_{i=1}^{m} w_i L(u(d_i; u_k^i, h), \dot{u}(d_i; u_k^i, h)) \]

\[ = \text{ext}_{u^0, u^1, \ldots, u^s} \frac{h}{2} \sum_{i=1}^{m} w_i L \left( \sum_{v=0}^{s} u_k^{i,v} l_{v,s}(\tau_i), \frac{2}{h} \sum_{v=0}^{s} u_k^{i,v} i_{v,s}(\tau_i) \right). \] (10)

### Implementation of spectral variational integrators for multi-dimensional Hamiltonian ODEs.

From (10), we know that \( u_k^v, v = 1, \ldots, s - 1 \) are the stationary points which provides \( (N-1) \times (s-1) \) equations:

\[ D_i L_d(u_k^0, u_k^1, \ldots, u_k^s; h) = 0, \quad i = 1, \ldots, s - 1, \]

which when combined with the discrete Euler–Lagrange equations,

\[ D_{s+1} L_d(u_k = u_k^0, u_k^1, \ldots, u_k^s = u_{k+1}; h) + D_1 L_d(u_{k+1} = u_k^0, u_{k+1}^1, \ldots, u_k^s = u_{k+2}; h) = 0, \]

yields the following set of nonlinear equations:

\[ p_k = -\sum_{n=1}^{m} w_n \left[ \frac{h}{2} l_{0,s}(\tau_n) \frac{\partial L}{\partial u} \left( \sum_{v=0}^{s} u_k^{v} l_{v,s}(\tau_n), \frac{2}{h} \sum_{v=0}^{s} u_k^{v} i_{v,s}(\tau_n) \right) + \dot{l}_{0,s}(\tau_n) \frac{\partial L}{\partial u} \left( \sum_{v=0}^{s} u_k^{v} l_{v,s}(\tau_n), \frac{2}{h} \sum_{v=0}^{s} u_k^{v} i_{v,s}(\tau_n) \right) \right] \] (11)

\[ 0 = -\sum_{n=1}^{m} w_n \left[ \frac{h}{2} l_{r,s}(\tau_n) \frac{\partial L}{\partial u} \left( \sum_{v=0}^{s} u_k^{v} l_{v,s}(\tau_n), \frac{2}{h} \sum_{v=0}^{s} u_k^{v} i_{v,s}(\tau_n) \right) + \dot{l}_{r,s}(\tau_n) \frac{\partial L}{\partial u} \left( \sum_{v=0}^{s} u_k^{v} l_{v,s}(\tau_n), \frac{2}{h} \sum_{v=0}^{s} u_k^{v} i_{v,s}(\tau_n) \right) \right] \] (12)

\[ p_{k+1} = \sum_{i=n}^{m} w_n \left[ \frac{h}{2} l_{s,s}(\tau_n) \frac{\partial L}{\partial u} \left( \sum_{v=0}^{s} u_k^{v} l_{v,s}(\tau_n), \frac{2}{h} \sum_{v=0}^{s} u_k^{v} i_{v,s}(\tau_n) \right) + \dot{l}_{s,s}(\tau_n) \frac{\partial L}{\partial u} \left( \sum_{v=0}^{s} u_k^{v} l_{v,s}(\tau_n), \frac{2}{h} \sum_{v=0}^{s} u_k^{v} i_{v,s}(\tau_n) \right) \right] \] (13)

where \( r = 1, \ldots, s - 1 \). The multi-interval algorithm for solving (11), (12), (13) can be obtained by cycling through the following diagram,

\[ (u_k, p_k) \xrightarrow{(11),(12)} (u_k^1, u_k^2, \ldots, u_k^s) \xrightarrow{(13)} (u_{k+1}, p_{k+1}) \]

\[ \xrightarrow{k \leftarrow k + 1} \]

\[ ^3\text{Here, } N \text{ denotes the dimension of the Hamiltonian system, specifically, we semi-discretize (2) with } N + 1 \text{ points, the resultant system of semi-discrete ODEs are of dimension } N - 1, \text{ since the boundary conditions are given.} \]
To implement the algorithm efficiently for the semi-discrete equation (9), we give the matrix form of (11), (12), (13) for (9),

\[ \tilde{A}_k \tilde{U}_k = F_k, \tag{14} \]

where \( \tilde{A}_k \) is a \( s \times (s+1) \) matrix and the entries are given by

\[ \tilde{A}_{k}^{i,j} = \frac{2}{h} \sum_{n=1}^{m} w_n \dot{l}_{i-1,s}(\tau_n) l_{j-1,s}(\tau_n), \tag{15} \]

\( \tilde{U}_k \) is a \( (s+1) \times (N-1) \)-dimensional matrix,

\[ \tilde{U}_k = [u^0_k, u^1_k, \ldots, u^s_k]^T, \quad u_k^i = [u^i_1(x_1,t), \ldots, u^i_N(x_{N-1},t)]. \]

\( F_k \) is a \( s \times (N-1) \)-dimensional matrix,

\[ F_k = [f^0_k, f^1_k, \ldots, f^{s-1}_k]^T \]

\[ = \frac{h}{2} \sum_{n=1}^{m} w_n l_{0,s}(\tau_n) \cdot \frac{\partial L}{\partial u}, \quad \frac{h}{2} \sum_{n=1}^{m} w_n l_{1,s}(\tau_n) \cdot \frac{\partial L}{\partial u}, \ldots, \frac{h}{2} \sum_{n=1}^{m} w_n l_{s-1,s}(\tau_n) \cdot \frac{\partial L}{\partial u}]^T, \]

where \( \frac{\partial L}{\partial u} = [\frac{\partial L}{\partial u_N(x_1,t)}, \ldots, \frac{\partial L}{\partial u_N(x_{N-1},t)}] \). By using the partitions \( \tilde{A}_k = [A^1_k, A_k] \) and \( \tilde{U}_k = [u^0_k, U_k]^T \) where \( A^1_k \) is the first column of the matrix \( \tilde{A}_k \), we can rewrite (14) as

\[ A_k \otimes I_{N-1} \text{vec}(U_k) + A^1_k \otimes (u^0_k)^T + \text{vec}(F_k) = [-p_k, 0_{(N-1)(s-1)}]^T. \tag{16} \]

4. Error estimation

The error of our numerical approach mainly comes from two parts. One is the approximation of derivative of \( u \) with respect to \( x \). The other comes from the chosen spectral variational integrator. Now we recall the geometric convergence of spectral variational integrators,

**Theorem 4.1.** (Theorem 3.7 of [10]) For a canonical Lagrangian and a sufficiently small time-step \( h \), a Galerkin variational integrator constructed from a basis \( \{ \phi_i \}_{i=0}^n \) of polynomials of degree at most \( n \) and a quadrature rule of at least order \( 2n+1 \) will have error at most \( O(K^n) \) for some \( K \) independent of \( n \) and less than 1. The internal stage Euler–Lagrange equations needed to construct the Galerkin variational integrator will also have a unique solution.

One might argue that spatial semi-discretization using symmetric finite-difference methods renders the use of spectrally accurate in time methods pointless, as one only achieves finite-order spatial accuracy, whereas the SVI is spectral accurate in time. But, we will see in practice that the numerical method can reach near machine precision with the given high-order symmetric difference and a relative small spatial-step.

**Theorem 4.2.** Suppose \( u \) is the solution of (2) and \( \dot{u} \) is the solution of the semi-discrete equation (3) with the \( p \)-th order symmetric difference matrix \( D \) solved by spectral variational integrators with a fixed time-step \( h \) and \( n \)-dimensional approximation space. Then, we have

\[ \|u - \dot{u}\| \leq C_0(\Delta x)^p + C_1 K^n, \quad \text{for } t \geq 0, \]

for some positive constants \( C_0, C_1, K, \Delta x < 1 \).
Proof. For any $x_i$ in the space-time grid, suppose $u_i(t)$ is the analytic solution of the semi-discrete Hamiltonian ODEs (3), then we have

$$|u(x_i, t) - \hat{u}_i(t)| = |u(x_i, t) - u_i(t) + u_i(t) - \hat{u}_i(t)|$$
$$\leq |u(x_i, t) - u_i(t)| + |u_i(t) - \hat{u}_i(t)|$$
$$\leq C_0(\Delta x)^p + |u_i(t) - \hat{u}_i(t)|.$$

From Theorem 4.1, we know there exists positive constants $C_1, K$, such that

$$|u_i(t) - \hat{u}_i(t)| \leq C_1 K^n.$$

So we can get,

$$\|u - \hat{u}\| \leq C_0(\Delta x)^p + C_1 K^n.$$

5. Numerical examples

In this section, we will introduce two numerical examples to verify the numerical schemes described above. The first example is the one-dimensional linear wave equation with an initial Gaussian pulse. The Gaussian pulse will eventually decay into two waves with smaller amplitude, with equal but opposite velocities (see Figure 4).

![Figure 4: Evolution of Gaussian wave](image)

For the second example, we consider the solitonic breather solution of the sine-Gordon equation. The sine-Gordon equation describes nonlinear waves in elastic media which can be solved analytically for some initial conditions, since it is completely integrable. The form of the breather solution is shown in Figure 5.
5.1. The Gaussian wave

We consider the linear wave equation,
\[ \frac{\partial^2 u}{\partial t^2} - \frac{\partial^2 u}{\partial x^2} = 0, \]
with an initial Gaussian pulse,
\[ \begin{cases} u(x, 0) = \exp(-x^2), \\ u_t(x, 0) = 0. \end{cases} \]

The analytic solution of the linear wave equation is,
\[ u(x, t) = \frac{1}{2} \left( \exp\left[ - (x + t)^2 \right] + \exp\left[ - (x - t)^2 \right] \right). \]

We first use the numerical scheme (5.8) in [16], and plot the solution and error (Figure 6) and the discrete energy error (Figure 7) of the linear wave equation. The discrete energy we calculated is given by:
\[ \sum_{i=1}^{N} \left( \frac{1}{2} \left( \frac{y_{i+1,j} - y_{ij}}{h} \right)^2 + \frac{1}{2} \left( \frac{y_{i+1,j} - y_{ij}}{2k} \right)^2 \right). \]

Figure 8 and 9 show the numerical solution, error and energy error of the second-order semi-discrete wave equation solved by SVI with 5 Chebyshev points and fixed time-step \( t = 1 \). The energy we calculated here was given in (7) and the energy error is the plot of \( H(u, \dot{u}) - H(u_0, \dot{u}_0) \). Figure 10 and 11 gives the numerical solution, error and energy error of the 4th-order symmetric-difference semi-discrete wave equation solved by SVI with 7 Chebyshev points in every time-step, and Figure 12 and 13 are for the 8th-order symmetric-difference with 11 Chebyshev points in every time-step.

Figure 14 shows the \( L^\infty \) error of \( u \) (left) and energy error (right) of the 8th-order semi-discrete equation with three different spatial-steps \( \Delta x = 0.5, \Delta x = 0.2, \Delta x = 0.1 \), solved by SVI with various Chebyshev points. It is clear that for an extreme accurate SVI, the order of the spatial semi-discretization is the limiting factor in the overall numerical accuracy, just as we discussed in the last
section. But we can still achieve very high accuracy with higher-order semi-discretizations. The discrete energy error mainly depends on the number of Chebyshev points we choose, since it is an exact integral of motion of the semi-discrete equations.

Figure 6: Solution(left) and error(right) for the linear wave equation using Marsden’s method [16] on a space-time grid with $\Delta t = 0.1$ and $\Delta x = 0.2$

Figure 7: Energy error for the linear wave equation using Marsden’s method [16] on a space-time grid with $\Delta t = 0.1$ and $\Delta x = 0.2$
Figure 8: Solution(left) and error(right) for the linear wave equation using SVI for the second-order semi-discrete ODEs on a space-time grid with $\Delta t = 1$, $\Delta x = 0.2$ and 5 Chebyshev points in every time-step.

Figure 9: Energy error for the linear wave equation using SVI for the second-order semi-discrete ODEs on a space-time grid with $\Delta t = 1$, $\Delta x = 0.2$ and 5 Chebyshev points in every time-step.

Figure 10: Solution(left) and error(right) for the linear wave equation using SVI for the 4th-order semi-discrete ODEs on a space-time grid with $\Delta t = 1$, $\Delta x = 0.2$ and 7 Chebyshev points in every time-step.
Figure 11: Energy error for the linear wave equation using SVI for the 4th-order semi-discrete ODEs on a space-time grid with $\Delta t = 1$, $\Delta x = 0.2$ and 7 Chebyshev points in every time-step.

Figure 12: Solution(left) and error(right) for the linear wave equation using SVI for the 8th-order semi-discrete ODEs on a space-time grid with $\Delta t = 1$, $\Delta x = 0.2$ and 11 Chebyshev points in every time-step.

Figure 13: Energy error for the linear wave equation using SVI for the 8th-order semi-discrete ODEs on a space-time grid with $\Delta t = 1$, $\Delta x = 0.2$ and 11 Chebyshev points in every time-step.
5.2. The sine-Gordon equation

Now we consider the sine-Gordon equation, which is in the form,

$$\frac{\partial^2 u}{\partial t^2} = \frac{\partial^2 u}{\partial x^2} - \sin(u(x,t)), \quad x \in [-30, 30], t \leq 0. \quad (17)$$

Here, we consider the so-called breather solutions with the initial conditions,

$$u(x,0) = 4 \tan^{-1}\left(\frac{\sqrt{1 - w^2}}{w} \frac{1}{\cosh(x\sqrt{1 - w^2})}\right), \quad u_t = 0,$$

and Dirichlet boundary conditions which can be obtained from the given exact solution,

$$u(x, t) = 4 \tan^{-1}\left(\frac{\sqrt{1 - w^2}}{w} \frac{\cos(w t)}{\cosh(x\sqrt{1 - w^2})}\right).$$

Figure 15, 16, 17 give the solution, absolute error and energy error of the 4th-order semi-discrete sine-Gordon equation when solved by SVI with 5 Chebyshev point in every uniform time-step $\Delta t = 1.$
Figure 15: Solution of the Sin-Gordon equation using SVI for the 4th-order semi-discrete ODEs on a space-time grid with \( \Delta t = 1 \), \( \Delta x = 0.2 \) and 5 Chebyshev points in every time-step.

Figure 16: Absolute error of \( u \) for the Sin-Gordon equation using SVI for the 4th-order semi-discrete ODEs on a space-time grid with \( \Delta t = 1 \), \( \Delta x = 0.2 \) and 5 Chebyshev points in every time-step.
Figure 17: Energy error for the Sin-Gordon equation using SVI for the 4th-order semi-discrete ODEs on a space-time grid with $\Delta t = 1$, $\Delta x = 0.2$ and 5 Chebyshev points in every time-step.

Figure 18 shows the $L^\infty$ error of $u$ for the 8th-order semi-discrete sine-Gordon equation with four different spatial-steps $\Delta x = 0.5$, $\Delta x = 0.2$, $\Delta x = 0.05$, $\Delta x = 0.02$, solved by SVI as the number of Chebyshev points is allowed to vary. Combined with the high-order semi-discretization and a relative small spatial-step, SVI can achieve very high accuracy for the Hamiltonian PDEs.

6. Conclusion

We have demonstrated that the combination of spectral variational integrators with high-order symmetric finite-differences can be successfully applied to simulate Hamiltonian PDEs with very high accu-
racy. With the given efficient implementation of spectral variational integrators for large-dimensional ODEs, we not only obtained a high accurate and energy preserving algorithm for Hamiltonian wave equations, but also verified the stability of SVI for the resulting stiff system of semi-discrete equations. In the future, we will construct overall (space-time) spectrally accurate invariant-preserving numerical methods and extend these methods to solve more complicate equations, such as Maxwell’s equations with gauge symmetry and higher-dimensional Schrödinger equations.

References


