A Modified Equations Approach for Multi-Symplectic Integration Methods

Brian Edward Moore

Submitted for the degree of Doctor of Philosophy

Department of Mathematics and Statistics
School of Electronics and Physical Sciences
University of Surrey

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To my wife, Wendy,
who is coping with having a mathematician for a husband, remarkably well.
I would first like to thank my wife, Wendy, because I could not go without her patience, encouragement, and support. I am also thankful for the encouragement and support offered by my friends and family, especially my parents, in spite of our decision to pursue these endeavors thousands of miles away from home.

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Abstract

A useful method for understanding discretization error in the numerical solution of ODEs is to compare the system of ODEs with the modified equations, the equations solved by the numerical solution, which are obtained through backward error analysis. Using symplectic integration for Hamiltonian ODEs provides more insight into the modified equations. In this thesis, the ideas of symplectic integration are extended to Hamiltonian PDEs, such that the symplectic structure in both space and time is exactly preserved. This paves the way for the development of a local modified equation analysis solely as a useful diagnostic tool for the study of these types of discretizations.

In particular, the multi-symplectic Euler, explicit mid-point, and Preissman box schemes are considered for general multi-symplectic equations. It is shown that these methods exactly preserve a multi-symplectic conservation law, as well as semi-discrete conservation laws of energy and momentum, and in some specific cases other fully discrete conservation laws. For a full discretization, local conservation laws of energy and momentum are not, in general, preserved exactly, but using Taylor series expansions one obtains a modified multi-symplectic PDE. Then, the modified equations are used to derive modified conservation laws that are preserved to higher order along the numerical solution.

It is also shown that the modified equations for linear problems converge to the numerical scheme, and numerical dispersion relations are also derived, giving more insight into the behavior of each method. The idea of multi-symplectic integration and modified equations are also applied to Hamiltonian PDEs with added dissipation. It is shown that it is possible to numerically preserve dissipation properties of the PDE, making it clear that a key characteristic of multi-symplectic integrators is that there is no dissipation added by the discretization. Various model problems are considered throughout the thesis, including the Korteweg-de Vries and nonlinear wave equations.
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A wide class of problems in the study of dynamical systems, which are fundamental to understanding classical mechanics, are classified as Hamiltonian systems. The dynamics modeled by these problems are known to be conservative. In addition, the types of applications for these systems are numerous and cover many fields, including applications in celestial mechanics, particle dynamics, plasma physics, optics, and wave motion. In fact, as Whitham [56] put it, “almost any field of science or engineering involves some questions of wave motion,” and in many applications, such as ocean waves and atmospheric flow, a conservative model is accurate.

These are the types of problems considered throughout this thesis, and in particular we are concerned with numerical simulation for Hamiltonian partial differential equations (PDEs), which are essential to the theory of wave phenomena. Numerical computation of solutions for these problems is often very important for visualizing the behavior of a particular dynamical system. More importantly, exact solutions for applications are difficult to achieve due to the nonlinearity of these problems, and numerical approximations are often the best one can hope for.

Recent trends in the numerical computation of solutions for differential equations have changed, and this change can be attributed to seeing a numerical method as a dynamical system. One way to discern the accuracy and efficiency of a numerical method is to analyze particular trajectories, but this is clearly not the best way to make general conclusions concerning the overall behavior of a method. Hence, a more favorable viewpoint is to compare the behavior of a numerical scheme to that of the problem it is being used to solve.

This new viewpoint has led to a field of study all its own, known as geometric integration. The main idea behind geometric integration is to preserve the underlying structure or certain geometric properties of particular equations. For example, there are methods
that give approximations which lie on a manifold which is defined by the problem, such as Lie group methods. There are also methods which preserve first integrals of the equations and symmetric methods are known to preserve the reversibility of certain systems. Numerical structure preservation for differential equations has proven to be extremely useful for improving the qualitative behavior of numerical solutions and for yielding more accurate long-time integration.

Regarding structure preservation for Hamiltonian systems more specifically, it is important to preserve the symplectic structure of the system, and deriving such schemes for ordinary differential equations (ODEs) has become almost routine. These types of schemes are commonly used by the scientific community in many applications, including celestial mechanics and molecular dynamics. Our focus is the extension of symplectic integration to PDE applications with a concentrated study on the effects certain discretizations have on the intrinsic properties of Hamiltonian PDEs.

Concerning the behavior of symplectic integrators, it is essential to know how well a particular scheme approximates the exact solution of certain problems. The only completely accurate way to find the error in the numerical solution is to compare it with the exact solution, but obviously this is not always possible, and in this new framework, in which we consider the behavior of a numerical method, it becomes increasingly more difficult. Hence, it is necessary to creatively find other means for deriving error estimates and for showing that a numerical method yields the desired solution behavior. One method for understanding a numerical method is to consider the differential equation that is actually solved by the numerical solution through what is known as backward error analysis, and Hamiltonian systems clear the way for a useful interpretation of backward error analysis.

1.1 Hamiltonian ODEs

Before introducing Hamiltonian dynamics, it is important to understand its foundations in Lagrangian mechanics, because the connection will become significant as we make a transition to conservative PDEs. Based on Newton’s laws of motion, the positions of objects, denoted by the column vector \( q(t) = q = (q_1, q_2, \ldots, q_d)^T \), obey the system of differential equations, known as the Lagrange equations,

\[
\frac{d}{dt} L_q = L_{\dot{q}}, \quad \text{where} \quad L = T - V
\]

such that \( T = T(q, \dot{q}) \) denotes the kinetic energy and \( V = V(q) \) denotes the potential energy. Here and throughout, we define \( \dot{\eta} = d\eta/dt \), for any \( \eta = \eta(t) \) and let subscripts
INTRODUCTION AND BACKGROUND MATERIAL

Denote partial derivatives in the usual way unless stated otherwise, i.e. $L_{\eta} = \partial L/\partial \eta$ is a row vector of partial derivatives.

Based on this formulation, one can derive Hamilton's equations, which make the understanding of such systems more simple. This can be done by first defining the new variables $p = (p_1, p_2, \ldots, p_d)^T$ such that

$$p_j = L_{q_j}(q, \dot{q}) \quad \text{for} \quad j = 1, 2, \ldots, d,$$

(1.1)

are known as the conjugate momenta, and defining the function

$$H(p, q) = p^T \dot{q} - L(q, \dot{q}),$$

which is accomplished by stating $\dot{q}$ in terms of $p$ and $q$ using a Legendre transform (cf. [28, page 169]) in conjunction with (1.1). This immediately implies

$$H_q = p^T \frac{\partial \dot{q}}{\partial q} - \frac{\partial L}{\partial q} \frac{\partial L}{\partial \dot{q}} q = \frac{\partial L}{\partial \dot{q}} = -p^T$$

and

$$H_p = q^T - p^T \frac{\partial \dot{q}}{\partial p} - \frac{\partial L}{\partial \dot{q}} \frac{\partial \dot{q}}{\partial q} = q^T.$$

This implies Hamilton's equations

$$\dot{p} = -\nabla_q H(p, q), \quad \dot{q} = \nabla_p H(p, q),$$

(1.2)

where we introduce the gradient notation

$$H_q(p, q) = \nabla_q H(p, q), \quad H_p(p, q) = \nabla_p H(p, q),$$

and $H$ is known as the Hamiltonian, representing the total energy of the system.

From another point of view, Hamilton's equations can be derived from a Lagrangian formulation in a different way, which is more useful for the formulations used throughout this thesis. Consider the Lagrangian density

$$L(y, \dot{y}) = \frac{1}{2} y^T J \dot{y} - H(y),$$

where $H : \mathbb{R}^{2d} \to \mathbb{R}$ is a smooth function, and where we introduce the matrix

$$J = \begin{pmatrix} 0_d & I_d \\ -I_d & 0_d \end{pmatrix},$$

(1.3)

such that $I_d$ is the $d \times d$ identity matrix, and $0_d$ is the $d \times d$ matrix consisting of all zeros. In this case, the Lagrangian $L = L(y, \dot{y})$ is irregular or singular, meaning the relationship between the Lagrangian and the Hamiltonian are not firmly established by writing $\dot{y}$ in
terms of \( y \) using a Legendre transform. Nevertheless, the positions \( q \) and the momenta \( p \), obey an Euler-Lagrange equation (derived in Appendix A) of the form
\[
\frac{d}{dt} L_y = L_y,
\] (1.4)
where \((p^T, q^T)^T = y(t) \in \mathbb{R}^{2d}\). Throughout the remainder of the text, we use the notation \((\mu, \nu)^T\), where \(\mu\) and \(\nu\) are column vectors, to denote the column vector made up of \(\mu\) and \(\nu\), so that \(y\) takes the simpler form \(y = (p, q)^T\). This implies
\[
0 = \frac{d}{dt} L_y - L_y = \frac{d}{dt} \left( \frac{1}{2} y^T J \right) + \frac{1}{2} y^T J + H_y(y) = y^T J + H_y(y),
\]
and we obtain a Hamiltonian ODE in the general form
\[
J \dot{y} = \nabla_y H(y),
\] (1.5)
which is a compact form of (1.2).

It is a well known fact that Hamiltonian systems of this form have two particularly important properties that determine the dynamics of the system. First of all, the total energy, denoted by the Hamiltonian \(H\), is constant for all time. This is easily seen by noting that
\[
\frac{d}{dt} H(y) = \left( \nabla_y H(y) \right)^T \dot{y} = -y^T J \dot{y} = 0,
\]
because \(J\) is skew-symmetric. Thus, \(H\) is constant along trajectories, and this implies conservation of total energy.

The second important property of these systems concerns their symplectic structure. By definition, a map \(\psi(y) : \mathbb{R}^{2d} \rightarrow \mathbb{R}^{2d}\) is symplectic if the Jacobian \(\partial_y \psi\) satisfies
\[
\left[ \partial_y \psi \right]^T J \left[ \partial_y \psi \right] = J.
\] (1.6)
Assuming \(\psi_t(y)\) is the time \(t\) flow map of (1.5), we get the variational equation
\[
\frac{d}{dt} \left[ \partial_y \psi_t \right] = J^{-1} H_{yy} \partial_y \psi_t,
\]
which implies
\[
\frac{d}{dt} \left( \left[ \partial_y \psi_t \right]^T J \left[ \partial_y \psi_t \right] \right) = \left[ \frac{d}{dt} \partial_y \psi_t \right]^T J \left[ \partial_y \psi_t \right] + \left[ \partial_y \psi_t \right]^T J J^{-1} H_{yy} \left[ \partial_y \psi_t \right]
= \left[ \partial_y \psi_t \right]^T H_{yy} \left[ \partial_y \psi_t \right] + \left[ \partial_y \psi_t \right]^T H_{yy} \left[ \partial_y \psi_t \right]
= 0,
\]
since the Hessian $H_{yy}$ is symmetric and $J^T = -J$. Now, since $\psi_0 = \text{id}$ implies $[\partial_y \psi_0]^T J [\partial_y \psi_0] = J$, we know that the flow map of any canonical Hamiltonian system is symplectic. In fact, a differential equation is locally Hamiltonian if and only if its flow map is symplectic (cf. [28, Theorem 2.6]). This conservation of symplecticity leads to certain implications regarding a set of initial conditions for the differential equation. Specifically, the volume defined by a set of points in phase space that are used as initial conditions for a Hamiltonian system is constant, and hence conserved, for all time.

Since the symplectic structure is so significant to the definition of a Hamiltonian system, it is desirable to have numerical methods that preserve this property. Such schemes are known as symplectic integrators, and they have proven to be both accurate and efficient in the long-time approximation of solutions to Hamiltonian ODEs [6, 18, 26, 50, 52]. This is due to the numerical reproduction of the qualitative solution behavior.

To demonstrate this fact, we use the Kepler problem with two degrees of freedom, given

![Figure 1.1: For a step size of .005 over ten periods, comparison of explicit (dashed) and symplectic (solid) Euler schemes for the Kepler problem, and a comparison of the modified (solid) and unmodified (dotted) Hamiltonians for the symplectic scheme (lower right).](image)
by the system of differential equations
\[
\dot{q}_j = -\frac{q_j}{(q_1^2 + q_2^2)^{3/2}}, \quad \dot{p}_j = p_j, \tag{1.7}
\]
for \( j = 1, 2 \). This is equivalent to the Hamiltonian system (1.5) with
\[
H(p, q) = \frac{1}{2} (p_1^2 + p_2^2) - \frac{1}{(q_1^2 + q_2^2)^{1/2}}, \tag{1.8}
\]
where \( p = (p_1, p_2)^T \) and \( q = (q_1, q_2)^T \). Figure 1.1 shows a vast difference in behavior between the explicit and symplectic Euler schemes applied to this problem. The orbits for the explicit scheme spiral away from the exact solution, but the orbits of the symplectic scheme remain close to the exact orbit. We also notice that the energy is not conserved exactly for either scheme, but the energy drift for the explicit scheme is significant, while the symplectic scheme shows no significant drift in energy, leading to good long-time approximations.

Numerically, one would like to preserve as many properties of the exact evolution equation as possible. However, it is often not possible to numerically conserve both energy and the symplectic structure. As a result, it is important to ask how well symplectic integrators preserve the energy conservation property. A useful method for answering this question is known as backward error analysis, in which a system of differential equations is compared with the modified equations that are satisfied by the numerical solution, and this is one of the best ways to analyze the effects of discretization error in a numerical solution.

Currently, there are many results concerning the backward error analysis of numerical methods for ODEs. In particular, the modified equations of a Hamiltonian system are also locally Hamiltonian if the integrator used is symplectic [6]. Since the modified equations are Hamiltonian and represent the numerical method, intuition says that the scheme preserves energy conservation as well. Yet, in practice, the modified equations cannot always be found exactly. In fact, they are found to high order by truncating an asymptotic series expansion, and we are not guaranteed that these expansions converge. But, it is true that the total energy is conserved up to an exponentially small term, and this ensures that long-time simulations remain accurate. For an in-depth discussion on these results refer to Hairer, Lubich, and Wanner [28], and references therein.

Though some of these remarks are made more precise in later sections, this can be demonstrated through the Kepler problem. In the lower right-hand corner of Figure 1.1 we plot the numerical solution along the modified (truncated after the first term) and unmodified Hamiltonians, showing that the numerical solution conserves energy remarkably well.
Similar numerical results have been obtained in the context of PDEs. However, the extension of symplectic integration to Hamiltonian PDEs was only introduced within the last ten years (cf. [38]), and the study of local properties of such schemes has only taken place within the last five years (cf. [15, 36]). Though many of the methods that fall under this category have been used in applications for quite some time, this new geometric approach has granted a better understanding of their behavior. Since this topic is still in its infancy, little is known or understood about such schemes, and it is our intent to extend our understanding of symplectic integration for ODEs to multi-symplectic integration for PDEs.

1.2 Extension to PDEs

Before discussing the ideas behind the extension of symplectic integration to Hamiltonian PDEs, we must first introduce the equations. Given a functional

$$H[z] = \int \mathcal{F}(z, z_x) dx,$$

where $z = z(x, t)$ is a vector of state variables, denote the Frechet derivative of $H$ by the row vector (of functions)

$$D_z H = \mathcal{F}_z - \partial_\eta \mathcal{F}_{z_\eta},$$

where we use $\partial_\eta$ as shorthand notation for a partial derivative with respect to $\eta$. The origin of this formulation can be found in Appendix A, where a brief introduction to the calculus of variations is presented, and where the relation between Hamiltonian and Lagrangian dynamics for systems of PDEs is made more clear. Then we can introduce an analog of the gradient such that

$$\frac{\delta H}{\delta z} = [D_z H]^T.$$

Using this notation, we consider the most common formulation for Hamiltonian PDEs as infinite dimensional systems defined by

$$J_z = \frac{\delta H}{\delta z}$$

similar to (1.5), where $H$ is known as the Hamiltonian.

This formulation for Hamiltonian PDEs can be obtained from a Lagrangian functional, given by

$$\mathcal{L}[z] = \int L \, dt dx,$$
where
\[ L = L(z, z_t, z_x) = \frac{1}{2} z^T J z_t - F(z, z_x), \]
is known as the Lagrangian density. This is done using the Euler-Lagrange equation
\[ L_z = \partial_t L_{z_t} + \partial_x L_{z_x}, \tag{1.12} \]
which yields equation (1.10).

The Lagrangian used in this derivation is irregular, but for problems in first order field theory, such as the nonlinear wave equation, Hamilton's equations can easily be found using a regular Lagrangian. In this case the relation between the Lagrangian and the Hamiltonian is made precise with a Legendre transform. However, the Legendre transform used in this derivation is only a partial Legendre transform, meaning the picture is not complete. Such equations have a symplectic structure in time, and this formulation has been useful for proving results, but it is possible to consider Hamiltonian PDEs that employ a symplectic structure in space as well, and such a formulation may become even more useful. This was first noted by Bridges [10], who used a full Legendre transform to obtain a Hamiltonian system with a multi-symplectic structure. These results are demonstrated in the following text for the nonlinear wave equation, but in our general derivations we continue to use an irregular Lagrangian to derive the same multi-symplectic equations, making the extension to higher order field theories straightforward.

Consider the Lagrangian formulation (1.11) such that
\[ L = \frac{1}{2} (z^T K z_t + z^T L z_x) - S(z), \tag{1.13} \]
where \( S : \mathbb{R}^d \to \mathbb{R} \) is a smooth function, \( z \) is the \( d \)-dimensional vector of state variables, and \( K, L \in \mathbb{R}^{d \times d} \) are constant skew-symmetric matrices that can be singular. Now using the Euler-Lagrange equation (1.12) implies
\[ -\frac{1}{2} (\partial_t (K z_t) + \partial_x (L z_x) + K z_t + L z_x) + \nabla_x S(z) = 0. \]
Hence,
\[ K z_t + L z_x = \nabla_x S(z), \tag{1.14} \]
and this is a natural generalization of the Hamiltonian system (1.10) on a multi-symplectic structure. In fact, several Hamiltonian PDEs can be formulated in this way, including nonlinear Schrödinger, Boussinesq, Korteweg-de Vries, Zakharov-Kuznetsov, and nonlinear wave equations. For examples of PDEs that have been formulated this way refer to [9, 10, 11, 13, 14, 16].
To demonstrate this for a particular problem, we use the nonlinear wave equation as an example. Assuming the spatial domain \([0, l]\) and the time domain \([0, t^*]\), consider the Lagrangian functional

\[
L = \int_0^{t^*} \int_0^l L \, dx \, dt
\]  

(1.15)

with the Lagrangian density

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

where \(\sigma\) and \(f\) are smooth functions and \(u = u(x, t)\) for \(x, t \in \mathbb{R}\). Then, using the variational principle, we derive the nonlinear wave equation

\[
\frac{\partial}{\partial t} \sigma'(u_x) - f'(u),
\]

(1.16)

from the Euler-Lagrange equation

\[
\partial_t L_{u_t} + \partial_x L_{u_x} - L_u = 0.
\]

To put this in Hamiltonian form, one merely uses the Legendre transform \(v = L_{u_t} = u_t\), implying the first order in time system of equations

\[
\frac{\partial}{\partial t} \sigma'(u_x) - f'(u), \quad u_t = v.
\]

Then it becomes clear that this system is just (1.10) with \(z = (v, u)^T\),

\[
J = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \quad \text{and} \quad H(u, v) = \int_0^l \left( \frac{v^2}{2} + \sigma(u_x) + f(u) \right) \, dx.
\]

On the other hand, setting \(\sigma(w) = w^2/2\) gives the semi-linear wave equation

\[
\frac{\partial}{\partial t} \sigma'(u_x) - f'(u),
\]

(1.17)

which is a well known nonlinear generalization of Klein-Gordon equation. Then, using a Legendre transform such that \(w = L_{u_x} = u_x\) implies this equation is equivalent to

\[
w_x = u_t + f'(u), \quad u_x = w.
\]

This is a Hamiltonian system in space for

\[
H(u, w) = \int_0^{t^*} \left( \frac{1}{2} (w^2 + (u_t)^2) - f(u) \right) \, dt
\]

with an associated symplectic structure in space.
Combining these two formulations, equation (1.16) can also be stated as a system of first-order equations such that

\[-v_t - p_x = f'(u), \quad u_t = v, \quad 0 = p + \sigma'(w), \quad u_x = w.\]  

(1.18)

This is equivalent to a multi-symplectic PDE (1.14) where we have taken

\[
K = \begin{pmatrix}
0 & -1 & 0 & 0 \\
1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0
\end{pmatrix} \quad \text{and} \quad L = \begin{pmatrix}
0 & 0 & 0 & -1 \\
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 \\
1 & 0 & 0 & 0
\end{pmatrix},
\]

and

\[
z = (u, v, w, p)^T,
\]

with

\[
S(z) = \frac{v^2}{2} + pw + \sigma(w) + f(u).
\]

The move to a multi-symplectic formulation for Hamiltonian PDEs has made the theory behind such systems more transparent in many respects. This has become obvious through the simple analysis of local properties of such systems [9, 10] and through the study of stability for traveling wave solutions [11, 12, 13, 14]. It has also become very useful for the study of discretizations for such systems by making the extension from symplectic integration to multi-symplectic integration simple [15, 51].

Multi-symplectic integration has been presented by Marsden, Patrick, and Shkoller [36], who use the multi-symplectic structure of wave equations. Their approach derives a numerical scheme from the Lagrangian formulation in first-order field theory using a discrete variational principle. Our approach to multi-symplectic integration, which was suggested by Bridges and Reich [15], is based on the multi-symplectic structure of the equations. This approach uses the application of a symplectic method to each independent variable, and defines multi-symplectic integrators as methods that preserve a discrete version of a multi-symplectic conservation law.

Numerical results show that these schemes are superior to other numerical methods in many ways (cf. [3, 31, 58]). There is also numerical evidence that these schemes locally conserve energy and momentum remarkably well, though not exactly (cf. [51]). Note that local conservation of these properties is a much stronger result than the global conservation achieved in past results (cf. [38]).

The purpose of this thesis is to extend the ideas of symplectic integration for ODEs to PDEs by way of a multi-symplectic formulation with the aim of showing why some methods that are already commonly used work well for such problems. This is done in part
through the development of a modified equations approach for these types of problems as a means of understanding the effects of the discretization on certain properties of the equation, which are local conservation laws [44, 45]. As a result, one receives a better understanding of the behavior of the method. In effect, the development of this approach is the main result.

There are few results concerning backward error analysis in relation to PDEs, compared to the results that have been achieved for ODEs. However, we must note that the idea of a modified PDE is not new. It has been presented by Warming and Hyett [55] as a means of determining the accuracy and stability of numerical integrators for PDEs in a different context, and Matthies [37] has performed a rigorous backward error analysis of a particular scheme for parabolic PDEs.

The outline is as follows. We begin with an explanation of the geometric properties associated with multi-symplectic PDEs, demonstrating how multi-symplectic, energy, momentum and other conservation laws can be derived directly from the multi-symplectic equation (1.14). Then the general space-time versions of the symplectic Euler, implicit midpoint, and explicit midpoint schemes are introduced along with their structure preserving properties. This is followed by a thorough study of the application of these methods to linear equations, where it is possible to derive numerical dispersion relations that fully describe the numerical method and to show that the numerical solution is the exact solution of the fully modified equation. Since similar rigorous results for nonlinear equations are difficult to achieve, we use backward error analysis to understand the behavior of each numerical scheme. This is done first by considering lattice differential equations, which are a large system of ODEs representing the PDE, usually by way of a spatial discretization. This enables one to use what is currently known concerning backward error analysis for ODEs. Then a new modified equations approach is introduced, which describes the behavior of the numerical scheme applied to the PDE. This is followed by an application of multi-symplectic schemes to Hamiltonian PDEs with linear dissipation. Several model problems are used throughout the text, and the thesis is concluded with numerical results demonstrating the analysis.
Before we can understand geometric integration for multi-symplectic PDEs, we must first understand the geometric properties of these types of equations. Specifically we need to understand what is meant by 'multi-symplectic structure'. It is also important to understand other conservation laws inherited from the equations in order to know how well a numerical scheme behaves in relation to the problem being solved, because these properties play a major role in defining the dynamics of the systems. After these properties are understood, we discuss three numerical schemes, and show what properties they preserve exactly.

To begin, we introduce the conservation laws of symplecticity, energy, and momentum, that are discussed throughout this text. Each of these conservation laws can be derived from the equation (1.14), and in the following chapter we discuss these laws in light of multi-symplectic integration.

### 2.1 Symplecticity

For \(a, b : \mathbb{R}^d \to \mathbb{R}^m\), let \(da\) and \(db\) denote \(m\)-dimensional vectors of differentials. Then, we define the wedge product such that

\[
\sum_{j=1}^{m} da_j \wedge db_j = da \wedge db,
\]

with the following properties. First, it is skew-symmetric, i.e.

\[
da \wedge db = -db \wedge da.
\]

Second, it is bilinear, i.e.

\[
da \wedge (\alpha db + \beta dc) = \alpha da \wedge db + \beta da \wedge dc,
\]

for any \(\alpha, \beta \in \mathbb{R}\). Based on this definition, we arrive at the following important result.
Corollary 2.1 The identity

\[ da \wedge A db = A^T da \wedge db \]

is satisfied by the wedge product for any real, \( m \times m \) matrix \( A \).

Proof Suppose \( da = (a_1, a_2, \ldots, a_m)^T \), \( db = (b_1, b_2, \ldots, b_m)^T \), and \( A = \{ A_{ij} \} \). Then

\[
\begin{align*}
    da \wedge A db &= da_1 \wedge (A_{11} db_1 + A_{12} db_2 + \ldots + A_{1m} db_m) + \ldots \\
    &+ da_m \wedge (A_{m1} db_1 + A_{m2} db_2 + \ldots + A_{mm} db_m) \\
    &= A_{11} da_1 \wedge db_1 + A_{12} da_1 \wedge db_2 + \ldots + A_{1m} da_1 \wedge db_m + \ldots \\
    &+ A_{m1} da_m \wedge db_1 + A_{m2} da_m \wedge db_2 + \ldots + A_{mm} da_m \wedge db_m \\
    &= (A_{11} da_1 + A_{12} da_2 + \ldots + A_{mm} da_m) \wedge db_1 + \ldots \\
    &+ (A_{11} da_1 + A_{12} da_2 + \ldots + A_{mm} da_m) \wedge db_m \\
    &= A^T da \wedge db,
\end{align*}
\]

and this completes the proof. \( \Box \)

This immediately implies the identities

\[ da \wedge J db = db \wedge J da \tag{2.1} \]

for \( J \) skew-symmetric, and

\[ da \wedge A db = -db \wedge A da \]

for \( A \) symmetric. These identities are used repeatedly throughout the thesis in relation to symplecticity.

Using these properties for wedge product notation, Hamiltonian ODEs can be shown to be symplectic in such a way that the condition (1.6) is stated

\[ \partial_y \psi_t(y) dy \wedge J \partial_y \psi_t(y) dy = dy \wedge J dy, \]

which is equivalent to

\[ \partial_t \omega = 0 \quad \text{for} \quad \omega = \frac{1}{2} (dy \wedge J dy). \tag{2.2} \]

Taking differentials of both sides of (1.5) yields the variational equation

\[ J dy = H_{yy}(y) dy, \]
and we can take the wedge product of $dy$ with this equation to get

$$dy \wedge Jd\dot{y} = dy \wedge H_{yy}(y)dy = 0,$$

because the Hessian $H_{yy}$ is symmetric. Since

$$dy \wedge Jd\dot{y} = d\dot{y} \wedge Jdy,$$

this implies (2.2), and we refer to this property as conservation of symplecticity.

Now, consider the multi-symplectic equation (1.14). We derive the multi-symplectic conservation law following Bridges [9, 10]. The variational equation associated with (1.14) is

$$Kdz_t + Ldz_a = S_{zz}(z)dz,$$  \hfill (2.3)

such that $S_{zz}(z)$ denotes the Hessian of $S(z)$, and $dz$ denotes the vector of differentials. After taking the wedge product of (2.3) and $dz$, we obtain

$$dz \wedge Kdz_t + dz \wedge Ldz_a = dz \wedge S_{zz}(z)dz = 0,$$

because the Hessian is symmetric. Then, using (2.1), we get the identities

$$dz \wedge Kdz_t = dz_t \wedge Kdz \quad \text{and} \quad dz \wedge Ldz_a = dz_a \wedge Ldz,$$  \hfill (2.4)

which imply the conservation law of multi-symplecticity

$$\partial_t \omega + \partial_a \kappa = 0,$$  \hfill (2.5)

where

$$\omega = \frac{1}{2} (dz \wedge Kdz) \quad \text{and} \quad \kappa = \frac{1}{2} (dz \wedge Ldz).$$

One can restrict this conservation law to the space of solutions by applying the pull-back

$$dz = z_t dt + z_a dx,$$

which implies

$$\omega = \frac{1}{2} ((z_t dt + z_a dx) \wedge K (z_t dt + z_a dx))$$

$$= \frac{1}{2} (z_t dt \wedge K z_a dx + z_a dx \wedge K z_t dt)$$

$$= (z_t dt \wedge K z_a dx)$$

$$= (z_t, K z_a)(dt \wedge dx)$$
and
\[ \kappa = \langle z_t, L z_a \rangle (dt \wedge dx), \]
where we denote the standard inner product on \( \mathbb{R}^d \) by \( \langle \cdot, \cdot \rangle \). Hence,
\[ \partial_t \langle (z_t, K z_a) (dt \wedge dx) \rangle + \partial_a \langle (z_t, L z_a) (dt \wedge dx) \rangle = 0, \]
and this yields the conservation law
\[ \partial_t \langle z_t, K z_a \rangle + \partial_a \langle z_t, L z_a \rangle = 0. \] (2.6)

The conservation law (2.5) can be simplified by taking a (non-unique) splitting of the matrices \( K \) and \( L \) such that
\[ K = K_+ + K_- \quad \text{and} \quad L = L_+ + L_, \] (2.7)
with
\[ K_+^T = -K_- \quad \text{and} \quad L_+^T = -L_. \] (2.8)

For first order field theories, such a splitting is naturally given by the Legendre transform. A splitting of this form immediately implies
\[ dz \wedge K_+ dz = dz \wedge K_- dz \quad \text{and} \quad dz \wedge L_+ dz = dz \wedge L_+ dz, \]
hence, (2.5) holds with
\[ \omega = dz \wedge K_+ dz \quad \text{and} \quad \kappa = dz \wedge L_+ dz. \]

This splitting also becomes helpful as we study multi-symplectic discretizations of (1.14), and this will become evident in the next chapter.

### 2.2 Energy and Momentum

Following the analysis of Bridges [9, 10], we can derive the conservation laws of energy and momentum. Using the time invariance of (1.14), an energy conservation law can easily be derived by taking the inner product of (1.14) with \( z_t \). Then
\[ \langle z_t, L z_a \rangle = \langle z_t, \nabla_S(x) \rangle, \] (2.9)
since the skew-symmetry of \( K \) implies \( \langle z_t, K z_a \rangle = 0 \). Noting that
\[ \langle z_t, L z_a \rangle = \frac{1}{2} \partial_t \langle z_t, L z_a \rangle + \frac{1}{2} \partial_a \langle z_t, L z \rangle, \]
and
\[ \langle z_t, \nabla_z S(z) \rangle = \partial_z S(z), \]
we obtain the energy conservation law
\[ \partial_t E + \partial_z F = 0, \quad (2.10) \]
where
\[ E = S(z) + \frac{1}{2} \langle z_t, L_z \rangle \quad \text{and} \quad F = \frac{1}{2} \langle z_t, L_z t \rangle \quad (2.11) \]
are known respectively as the energy density and the energy flux. Similarly, the spatial invariance of (1.14) can be used to take the inner product of (1.14) and \( z_\phi \) to get
\[ \langle z_\phi, K z_t \rangle = \langle z_\phi, \nabla_z S(z) \rangle = \partial_\phi S(z). \]
Since
\[ \langle z_\phi, K z_t \rangle = \frac{1}{2} \partial_\phi \langle z_t, K z \rangle + \frac{1}{2} \partial_t \langle z_\phi, K z \rangle, \]
we have the momentum conservation law
\[ \partial_\phi G + \partial_t I = 0, \quad (2.12) \]
for
\[ G = S(z) + \frac{1}{2} \langle z_t, K z \rangle \quad \text{and} \quad I = \frac{1}{2} \langle z_t, K z_\phi \rangle. \]

We can also simplify the conservation laws of energy and momentum. Using the splitting (2.7)-(2.8) implies
\[ \langle z_t, L z_\phi \rangle = (x_t, L_+ z_\phi) + (x_t, L_- z_\phi) = (x_t, L_+ z_\phi) - (x_t, L_- z_\phi) = \partial_\phi (z_\phi, L_+ z) - \partial_t (z_\phi, L_- z), \]
and substituting this into (2.9) we obtain the energy conservation law (2.10), where the energy density and energy flux are given by
\[ E = S(z) + \langle x_\phi, L_+ x \rangle \quad \text{and} \quad F = -\langle x_t, L_+ x \rangle. \quad (2.13) \]
Similarly, the momentum conservation law can be simplified by noting that
\[ \partial_\phi S(z) = \langle z_\phi, K z_t \rangle = \partial_t \langle z_\phi, K_+ x \rangle - \partial_\phi \langle z_t, K_+ x \rangle. \]
Thus, the momentum conservation law is given by (2.12), where
\[ G = S(z) + \langle x_t, K_+ x \rangle \quad \text{and} \quad I = -\langle x_\phi, K_+ x \rangle. \]
It is interesting to note that the conservation law (2.6) is equivalent to the one obtained from differentiation of the energy and momentum conservation laws such that

$$\partial_\pi (\partial_t E + \partial_\omega F) - \partial_t (\partial_\pi G + \partial_\omega I) = 0.$$ 

Notice that the momentum conservation law is achieved by reversing the roles of space and time (the inner product is taken with $z_\pi$ rather than $z_t$), and using the same steps used to get the energy conservation law. Thus, it is not necessary to derive each conservation law separately, and in order to avoid this redundancy in the remainder of the text, we shall consider only the energy conservation law in the general derivations with the understanding that the same holds for momentum, while both will be considered for specific case of the nonlinear wave equation.

### 2.3 Linear Symmetries

According to Bridges [10], there may also be additional conservation laws for (1.14) related to linear symmetries. Essentially, this follows from Noether theory and derivation of the multi-symplectic PDE (1.14) from a Lagrangian formulation (1.11)-(1.13). More specifically, take a linear one-parameter family of linear coordinate transformations [48] given by the group action

$$g_\epsilon (z) = e^{\epsilon B} z, \quad (2.14)$$

which is chosen in such a way that it is symplectic with respect to both $\omega$ and $\kappa$. Symplecticity is equivalent to

$$B^T K + KB = 0, \quad B^T L + LB = 0. \quad (2.15)$$

Using these identities, the invariance of a Lagrangian under such a change of variables leads to

$$0 = \lim_{\epsilon \to 0} \left( \frac{1}{\epsilon} (\mathcal{L} [e^{\epsilon B} z] - \mathcal{L}[z]) \right)$$

$$= \lim_{\epsilon \to 0} \frac{1}{\epsilon} \int \left( \frac{1}{2} (\langle e^{\epsilon B} z, K e^{\epsilon B} z \rangle + \langle e^{\epsilon B} z, L e^{\epsilon B} z \rangle) - S(e^{\epsilon B} z) \right.$$

$$\left. - \frac{1}{2} (\langle z, K z \rangle + \langle z, L z \rangle) + S(z) \right) \, dt \, dz.$$

Then, using the identity

$$e^{\epsilon B} = I + \epsilon B + \mathcal{O}(\epsilon^2)$$
implies
\[ 0 = \frac{1}{2} \int \left( \langle B_z, K z_t \rangle + \langle z, K B z_t \rangle + \langle B_z, L z_x \rangle + \langle z, L B z_x \rangle - 2 \langle B_z, \nabla_z S(z) \rangle \right) \, dt \, dx \]
\[ = \int \langle B_z, \nabla_z S(z) \rangle \, dt \, dx \]
and we obtain the invariance condition
\[ \langle B_z, \nabla_z S(z) \rangle = 0. \tag{2.16} \]

Direct application of (2.16) to the multi-symplectic PDE formulation (1.14) yields
\[ \langle B_z, K z_t \rangle + \langle B_z, L z_x \rangle = \langle B_z, \nabla_z S(z) \rangle = 0, \]
and using (2.15), this can be written as a conservation law
\[ \partial_t \langle z, K B z \rangle + \partial_x \langle z, L B z \rangle = 0. \tag{2.17} \]

The Nonlinear Schrödinger Equation

To demonstrate this through an example, consider the NLS equation (cf. \cite{20, 31})
\[ i \psi_t + \psi_{xx} + V'(|\psi|^2)\psi = 0, \]
where \( \psi \) is complex-valued. Letting \( \psi = u + iw \), we can rewrite this as the system of equations
\[ u_t = -w_{xx} - wV'(v^2 + w^2) \]
\[ w_t = v_{xx} + vV'(v^2 + w^2), \]
which is a Hamiltonian system for
\[ H = \frac{1}{2} \int \left( v_x^2 + w_x^2 - V(v^2 + w^2) \right) \, dx. \]

Defining \( \psi_z = \sigma + i \phi \), this system of equations can also be written as the multi-symplectic PDE (1.14) where \( z = (v, w, \sigma, \phi) \),
\[ K = \begin{pmatrix} J & 0_2 \\ 0_2 & 0_2 \end{pmatrix}, \quad L = \begin{pmatrix} 0_2 & -I_2 \\ I_2 & 0_2 \end{pmatrix}, \]
where \( J \) is given in (1.3) with \( d = 1 \) and
\[ S(z) = \frac{1}{2} \left( \sigma^2 + \phi^2 + V(v^2 + w^2) \right). \]
This system is invariant under the action of the one-parameter group of rotations $SO(2)$ [12], given by $G_\theta(z) = R_\theta z$, for

$$R_\theta = \begin{pmatrix}
\cos \theta & -\sin \theta & 0 & 0 \\
\sin \theta & \cos \theta & 0 & 0 \\
0 & 0 & \cos \theta & -\sin \theta \\
0 & 0 & \sin \theta & \cos \theta
\end{pmatrix}.$$ 

Now, define the matrix $B$ such that

$$Bz = \left. \frac{d}{d\theta} G_\theta(z) \right|_{\theta=0} = (-w, v, -\phi, \sigma)^T.$$ 

Then

$$\langle z, KBz \rangle = w^2 + v^2 \quad \text{and} \quad \langle z, LBz \rangle = 2(w\phi - w\sigma),$$

satisfies the conservation law (2.17).

Each of the conservation laws discussed in this section is preserved locally, and these formulations are made possible by the multi-symplectic structure of the PDE. This is in contrast to a Hamiltonian formulation which yields global conservation of densities and neglects the fluxes. We make the distinction here because the preservation of a local conservation law numerically is a stronger result than the global conservation that has been achieved in the past, and these are the issues discussed as we consider a numerical method.
In the current literature there are two approaches for defining symplectic one-step methods for ODEs. The first approach takes a Hamiltonian viewpoint and defines a symplectic method to be one in which the one-step map for the method is symplectic. The second approach takes the Lagrangian viewpoint and uses a discrete variational principle (cf. [28, Chapter 6] and references therein). Essentially, these two approaches are linked by the idea of generating functions. Now, as we work to extend the ideas of symplectic integration for ODEs to that of PDEs, we can use similar approaches to define a multi-symplectic integrator.

The approach first used for defining a multi-symplectic integrator, was presented by Marsden, Patrick, and Shkoller [36] and is based on the variational approach. Originally, it was limited by the fact that it could only be used for first order field theories, though it has since been extended to second order field theories. We use a different approach, which is not affected by this limitation and is superior with regard to simplicity. This approach was first used by Bridges and Reich [15], and defines a multi-symplectic integrator as a numerical method that satisfies a discrete multi-symplectic conservation law. Though our approach is different from the variational approach, some of the methods obtained from each are the same, and since there is no analog of generating functions for PDEs, except for first order field theories, there is currently no natural connection between these two approaches.

Here and throughout the remainder of the thesis, we use the notation \( z_{n,i} \) to denote a numerical approximation of \( z(x_n, t_i) \), for \( n = 0, 1, 2, \ldots, J \) and \( i = 0, 1, 2, \ldots, N_t, \) where \( J \) is the number of grid points and \( N_t \) is the number of time steps. We also define \( t/J = \Delta x = x_n - x_{n-1} \) and \( (t^F - t^B)/N_t = \Delta t = t_i - t_{i-1}. \) We only consider discretizations on a uniform mesh, and this requirement is essential for our analysis.

Using both forward and backward differences, we define discrete approximations to \( z_x \).
by
\[ \delta^+_t z^{n,i} := \frac{z^{n+1,i} - z^{n,i}}{\Delta t} \quad \text{and} \quad \delta^-_t z^{n,i} := \frac{z^{n,i} - z^{n-1,i}}{\Delta t}, \]
and discrete approximations to \( z_t \) by
\[ \delta^+_t z^{n,i} := \frac{z^{n,i+1} - z^{n,i}}{\Delta t} \quad \text{and} \quad \delta^-_t z^{n,i} := \frac{z^{n,i} - z^{n,i-1}}{\Delta t}, \]
where \( \delta^\pm \) has been introduced for the sake of compact notation. Furthermore, we define the central difference approximation for second order derivatives with respect to \( x \) and \( t \) by
\[ \delta^+_x z^{n,i} := \frac{z^{n,i+1} - 2z^{n,i} + z^{n,i-1}}{\Delta x^2} = \delta^+_x \delta^-_x z^{n,i}, \]
and
\[ \delta^+_t z^{n,i} := \frac{z^{n,i+1} - 2z^{n,i} + z^{n,i-1}}{\Delta t^2} = \delta^+_t \delta^-_t z^{n,i}, \]
respectively.

3.1 The Euler Box Scheme

It was briefly discussed in the introduction that a multi-symplectic PDE, given by (1.14), exploits the symplectic structure for each independent variable \( x \) and \( t \). Now, as we consider a discretization of (1.14), we use a similar idea and apply a symplectic Euler discretization to each independent variable. This yields a first-order explicit one-step numerical method that we refer to as the Euler box scheme, and this method is given by
\[ K_+ \delta^+_t z^{n,i} + K_- \delta^-_t z^{n,i} + L_+ \delta^+_x z^{n,i} + L_- \delta^-_x z^{n,i} = \nabla_z S(z^{n,i}). \quad (3.1) \]

3.1.1 Conservation Properties

We call this scheme a multi-symplectic numerical method because it satisfies a discrete version of the multi-symplectic conservation law, and this is shown in the proof of the following proposition.

Proposition 3.1 The Euler box scheme given by (3.1) satisfies a discrete multi-symplectic conservation law
\[ \delta^+_t \omega^{n,i} + \delta^+_x \kappa^{n,i} = 0 \quad (3.2) \]
where
\[ \omega^{n,i} = dz^{n,i-1} \wedge K_+ dz^{n,i} \quad \text{and} \quad \kappa^{n,i} = dz^{n-1,i} \wedge L_+ dz^{n,i}. \]
Proof

Consider the discrete variational equation

\[ K_+ \delta^+_t \, dx^{n,i} + K_- \delta^-_t \, dx^{n,i} + L_+ \delta^+_z \, dz^{n,i} + L_- \delta^-_z \, dz^{n,i} = S_{z^i}(z^{n,i}) \, dz^{n,i}. \]

Now take the wedge product of this equation with \( dz^{n,i} \), and notice that we have

\[ dx^{n,i} \wedge S_{z^i}(z^{n,i}) \, dz^{n,i} = 0, \]

because \( S_{z^i} \) is symmetric. Then, for the terms containing \( \delta^+_t \), we get

\[ dx^{n,i} \wedge K_+ \delta^+_t \, dx^{n,i} + dz^{n,i} \wedge K_+ \delta^+_z \, dz^{n,i} = \delta^+_t \, (dz^{n,i} \wedge K_+ \, dz^{n,i}), \]

Doing the same for the terms containing \( \delta^+_z \) yields

\[ dx^{n,i} \wedge L_+ \delta^+_z \, dx^{n,i} + dz^{n,i} \wedge L_+ \delta^+_z \, dz^{n,i} = \delta^+_z \, (dz^{n,i} \wedge L_+ \, dz^{n,i}), \]

which implies (3.2). □

This method can also be derived from a Lagrangian formulation using a discrete variational principle. We approximate the Lagrangian functional (1.11) with

\[ L \approx \sum_{n,i} L^{n,i} \]

(3.3)

for the discrete Lagrangian 'density'

\[ L^{n,i} = \frac{1}{2} \langle z^{n,i}, (K_+ \delta^+_x z^{n,i} + K_- \delta^-_x z^{n,i} + L_+ \delta^+_z z^{n,i} + L_- \delta^-_z z^{n,i}) \rangle - S(z^{n,i}). \]

We have neglected the \( \Delta t \Delta x \) dependency in (3.3), because it is not necessary when considering variations, and as a result we use this notation for all functional approximations.

Now, rewriting \( L^{n,i} \) in the form

\[ L^{n,i} = \frac{1}{2\Delta t} \langle z^{n,i}, (K_+ z^{n,i+1} - K_- z^{n,i} + K_+ z^{n,i} - K_- z^{n,i-1}) \rangle + \frac{1}{2\Delta x} \langle z^{n,i}, (L_+ z^{n+1,i} - L_- z^{n,i} + L_+ z^{n,i} - L_- z^{n-1,i}) \rangle - S(z^{n,i}), \]

we can use the discrete variational principle

\[ \frac{\partial}{\partial z^{n,i}} L = 0, \]

to get

\[ \nabla z S(z^{n,i}) = \frac{1}{2\Delta t} \langle K_+ (z^{n,i+1} - 2z^{n,i}) + K_- (2z^{n,i} - z^{n,i-1}) \rangle + \frac{1}{2\Delta x} \langle L_+ (z^{n+1,i} - 2z^{n,i}) + L_- (2z^{n,i} - z^{n-1,i}) \rangle + \frac{1}{2\Delta t} \langle K_+ z^{n,i+1} - K_- z^{n,i-1} \rangle + \frac{1}{2\Delta x} \langle L_+ z^{n+1,i} - L_- z^{n-1,i} \rangle. \]
Then, after rearranging terms, we notice that this is just the Euler box scheme (3.1). More on this variational approach can be found in Appendix A. We note the similarity to the analysis of Marsden, Patrick and Shkoller [36], in that the method can be obtained using the variational approach. However, we must also note the difference between these approaches due to the fact that, the Lagrangian used here is not regular.

We also note here that there are three other versions of the Euler box scheme different from the formulation in (3.1). These other versions correspond to the adjoint method as it relates to the Euler method for ODEs. For example, one could write the Euler box scheme

\[ K_+ \delta_t z^{n+1} + K_- \delta_t z^{n-1} + L_+ \delta_u z^{n+1} + L_- \delta_u z^{n-1} = \nabla z S(z^{n+1}), \]

where we have exchanged the forward and backward differences in (3.1). Clearly, this scheme has the same properties as (3.1). Now this raises an interesting question concerning composition methods. For ODEs, a method can be composed with the adjoint method to yield a higher order scheme while preserving the properties of the original scheme, and a similar result may apply for PDEs, but this is still an open problem.

Now it is important to understand how well this method preserves the other conservation laws associated with the PDE, namely the energy and momentum conservation laws. There may be special cases where these conservation laws are exactly conserved by the Euler box scheme, but in general this is not so. However, there are semi-discrete conservation laws that are preserved exactly, and this will become useful for error analysis.

**Proposition 3.2** Applying a symplectic Euler discretization in space to (1.14) yields an exact semi-discrete energy conservation law

\[ \partial_t E^n + \partial_u F^n = 0, \quad (3.4) \]

with

\[ E^n = S(z^n) + (\delta_u z^n, L_+ z^n), \quad \text{and} \quad F^n = -(z_{n+1} - z_n, L_+ z^n). \quad (3.5) \]

A (formal) symplectic Euler discretization in time yields an exact semi-discrete momentum conservation law

\[ \partial_u G^i + \partial_t I^i = 0, \quad (3.6) \]

with

\[ G^i = S(z^i) + (\delta_t z^i, K_+ z^i), \quad \text{and} \quad I^i = -(z_{i+1} - z_i, K_+ z^i), \]

which is only achieved formally due to the CLF stability condition.
Proof  First apply a symplectic Euler discretization to (1.14) in space to get the semi-discrete equation

\[ \mathbf{K} \mathbf{z}^n + \mathbf{L}_+ \delta^+ \mathbf{z}^n + \mathbf{L}_- \delta^- \mathbf{z}^n = \nabla_z S(\mathbf{z}^n). \]

Taking the inner product with \( \mathbf{z}^n \) and noting that

\[ \langle \mathbf{z}^n, \nabla_z S(\mathbf{z}^n) \rangle = \partial_t S(\mathbf{z}^n), \]

yields

\[
\partial_t S(\mathbf{z}^n) = \langle \mathbf{z}^n, \mathbf{L}_+ \delta^+ \mathbf{z}^n \rangle + \langle \mathbf{z}^n, \mathbf{L}_- \delta^- \mathbf{z}^n \rangle \\
= \langle \mathbf{z}^n, \mathbf{L}_+ \delta^+ \mathbf{z}^n \rangle - \langle \delta^- \mathbf{z}^n, \mathbf{L}_+ \mathbf{z}^n \rangle \\
= -\partial_t (\delta^- \mathbf{z}^n, \mathbf{L}_+ \mathbf{z}^n) + \langle \delta^+ \mathbf{z}^n, \mathbf{L}_+ \mathbf{z}^n \rangle + \langle \delta^- \mathbf{z}^n, \mathbf{L}_+ \mathbf{z}^n \rangle \\
= -\partial_t (\delta^- \mathbf{z}^n, \mathbf{L}_+ \mathbf{z}^n) + \delta^+ (\mathbf{z}^{n-1}, \mathbf{L}_+ \mathbf{z}^n). 
\]

Thus, we have proved (3.4). To continue our formal analysis and find a semi-discrete momentum conservation law, simply discretize (1.14) in time (leaving space continuous and disregarding stability issues) with a symplectic Euler scheme, then take the inner product with \( \mathbf{z}^n \) to get (3.6). □

In order to make the conservation properties of the Euler box scheme more clear, we consider a model problem.

### 3.1.2 The Nonlinear Wave Equation

For the system (1.18), take a splitting of the matrices \( \mathbf{K} \) and \( \mathbf{L} \) defined by

\[
\mathbf{K}_+ = \begin{pmatrix}
0 & -1 & 0 & 0 \\
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0
\end{pmatrix} \quad \text{and} \quad \mathbf{L}_+ = \begin{pmatrix}
0 & 0 & 0 & -1 \\
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0
\end{pmatrix},
\]

and define \( \mathbf{K}_- \) and \( \mathbf{L}_- \) such that (2.8) is satisfied. Using this splitting, the conservation law of symplecticity automatically becomes (2.5) for

\[ \omega = du \wedge dv \quad \text{and} \quad \kappa = du \wedge dp. \]

This is easily observed by noting that

\[ du \wedge dv + du \wedge dp_x = 0, \quad dv \wedge du = 0, \]

and

\[ dw \wedge dp = 0 \quad \text{implies} \quad dp \wedge du_x = 0. \]
It is also easy to show that the energy conservation law (2.10) is satisfied with

\[ E = \frac{1}{2} v^2 + \sigma(w) + f(u) = \frac{1}{2} u_x^2 + \sigma(u_x) + f(u) \]

and

\[ F = v p = -u_x \sigma'(u_x), \]

because

\[ \frac{\partial}{\partial t} E = vv_t + \sigma'(w)w_t + f'(u)u_t \]
\[ = -v (p_w + f'(u)) + \sigma'(w)w_t + f'(u)v \]
\[ = \nu \sigma'(w) w_x + \sigma'(w) u_x \]
\[ = \partial_u (\nu \sigma'(u)) \]

where we have used the first order system of equations (1.18). Similarly, the momentum conservation law (2.12) holds for

\[ G = \sigma(w) + pw - \frac{1}{2} v^2 + f(u) = \sigma(u_x) - \sigma'(u_x) u_x - \frac{1}{2} u_x^2 + f(u) \]

and

\[ I = uv = u_x u_t, \]

because

\[ \partial_u G = \sigma'(w) u_x + p_w w + pw_x - vv_x + f'(u) u_x \]
\[ = -w (u_t + f'(u)) - vv_t + f'(u) u_x \]
\[ = \partial_u (uv). \]

Discretizing the system of equations (1.18) first in space gives

\[ -v^n_t - \delta^n_x p^n = f'(u^n), \quad u^n_t = v^n, \quad p^n = -\sigma'(u^n), \quad \delta^- u^n = w^n, \]

which is equivalent to

\[ v^n_t = \delta^n_x \sigma'(\delta^- u^n) - f'(u^n), \quad u^n_t = v^n, \quad (3.7) \]

after eliminating \( p \) and \( w \). Notice that, for \( \Delta x = 1, \sigma(w) = w^2/2 + w^3/3, \) and \( f'(u) = 0, \) these equations become the Fermi-Pasta-Ulam problem (cf. [22, 29]). Under periodic boundary conditions, the system of equations (3.7) is also a Hamiltonian system (a large Hamiltonian system of ODEs) given by

\[ \dot{v}^n = -\frac{\delta}{\delta u^n} H(u^n, v^n), \quad \dot{u}^n = \frac{\delta}{\delta v^n} H(u^n, v^n) \quad (3.8) \]
with

\[ H = \sum_{n=1}^{J} E^n, \quad \text{where} \quad E^n = \frac{1}{2}(u^n)^2 + \sigma(\delta_x u^n) + f(u^n), \quad (3.9) \]

is the approximated energy density.

Applying a symplectic Euler discretization in time, (3.7) becomes

\[ \delta^+_t u^{n,i} = \delta^+_x \sigma'(\delta_x u^{n,i}) - f'(u^{n,i}), \quad \delta^-_t u^{n,i} = v^{n,i}. \quad (3.10) \]

Setting

\[ dp^{n,i} = -\sigma''(w^{n,i}) dw^{n,i} = -\sigma''(w^{n,i}) \delta_x du^{n,i}, \]

this discretization implies

\[ du^{n,i} \wedge \delta^-_t du^{n,i} = 0, \quad dp^{n,i} \wedge \delta^-_x du^{n,i} = 0, \]

and

\[ du^{n,i} \wedge \delta^+_t du^{n,i} + du^{n,i} \wedge \delta^+_x dp^{n,i} = 0. \]

Then using

\[
\begin{align*}
\delta^+_t (du^{n,i-1} \wedge du^{n,i}) &= \frac{1}{\Delta t} (du^{n,i} \wedge du^{n,i+1} - du^{n,i} \wedge du^{n,i} + du^{n,i} \wedge du^{n,i} - du^{n,i-1} \wedge du^{n,i}) \\
&= du^{n,i} \wedge \delta^+_t du^{n,i} + \delta^-_t du^{n,i} \wedge du^{n,i},
\end{align*}
\]

and a similar identity for terms containing discrete space derivatives, we find that a discrete multi-symplectic conservation law (3.2) is satisfied with

\[ \omega^{n,i} = du^{n,i-1} \wedge du^{n,i}, \quad \text{and} \quad \kappa^{n,i} = du^{n-1,i} \wedge dp^{n,i}. \]

Alternatively, to use the approach based on the Lagrangian formulation, we approximate the Lagrangian functional (1.15) with (3.3) for the discrete Lagrangian density

\[ L^{n,i} = L(\delta^-_t u^{n,i}, \delta^-_x u^{n,i}, \nu^{n,i}) \]

\[ = \frac{1}{2} (\delta^-_t u^{n,i})^2 - \sigma (\delta^-_x u^{n,i}) - f(u^{n,i}). \]

Now, using the associated discrete form of the variational principle, we derive a discrete form of the Euler-Lagrange equation given by

\[ \delta^+_t L_{\delta^-_t u^{n,i}} + \delta^+_x L_{\delta^-_x u^{n,i}} - L_{\nu^{n,i}} = 0. \]

(See Appendix A for details.) This yields the discretization

\[ \delta^2_t u^{n,i} = \delta^+_x \sigma'(\delta^-_x u^{n,i}) - f'(u^{n,i}). \]
which is the symplectic Euler discretization of the system (3.7), after eliminating the variable \(v\). Notice that this discretization is also just the standard leap-frog discretization for the nonlinear wave equation.

### 3.1.3 The Korteweg-de Vries Equation

For a demonstration of these results with an example in second order field theory, we consider the KdV equation [5, 17]

\[
\frac{u_t}{u} + uu_x + u_{xxx} = 0.  \tag{3.11}
\]

In order to derive this equation from a Lagrangian formulation using a variational principle, one must introduce a velocity potential \(\phi\) such that \(\phi_x = u\). This implies

\[
\phi_{xt} + \phi_x \phi_{xx} + \phi_{xxx} = 0, \tag{3.12}
\]

which is derived from the Lagrangian density

\[
L = L(\phi_t, \phi_x, \phi_{xx}) = \frac{1}{2} \left( -\phi_t \phi_x - \frac{1}{3} \phi_x^3 + \phi_{xx}^2 \right)
\]

using the Euler-Lagrange equation

\[
\partial_t L_{\phi_t} + \partial_x L_{\phi_x} - \partial_{xx}^2 L_{\phi_{xx}} = 0.
\]

This equation can also be written as the first order system of equations [11]

\[
u_t + w_x = 0, \quad -\phi_t - v_x = -w + u^2, \quad u_x = \frac{1}{2} v, \quad -\phi_x = -u,
\]

and this is the multi-symplectic equation (1.14) with \(z = (\phi, u, v, w)\),

\[
S(z) = \frac{1}{4} v^2 - u w + \frac{1}{3} u^3
\]

and

\[
K = \begin{pmatrix}
0 & 1 & 0 & 0 \\
-1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0
\end{pmatrix}
\quad \text{and} \quad
L = \begin{pmatrix}
0 & 0 & 0 & 1 \\
0 & 0 & -1 & 0 \\
0 & 1 & 0 & 0 \\
-1 & 0 & 0 & 0
\end{pmatrix} \tag{3.13}
\]

Using the Euler box scheme to discretize gives

\[
\begin{align*}
\delta^+_x u^{n,i} + \delta^+_x w^{n,i} &= 0, \\
-\delta^-_t \phi^{n,i} - \delta^-_x \phi^{n,i} &= -w^{n,i} + (u^{n,i})^2, \\
\delta^+_x u^{n,i} &= \frac{1}{2} v^{n,i}, \\
-\delta^-_x \phi^{n,i} &= -u^{n,i},
\end{align*}
\]
and after a few simple manipulations we can eliminate variables to get

\[ \delta_t^+ \delta_x^i \phi^{n,i} + \delta_t^- \delta_x^i \phi^{n,i} + 2 \delta_x^2 \delta_t^i \phi^{n,i} + \delta_x^2 (\delta_t^i \phi^{n,i})^2 = 0, \tag{3.14} \]

which is an equivalent scheme for (3.12). Now, for the discrete Lagrangian

\[ L^{n,i} = \frac{1}{2} \left( -\delta_t^- \phi^{n,i} \delta_x^i \phi^{n,i} - \frac{1}{3} (\delta_x^2 \phi^{n,i})^3 + (\delta_x^2 \phi^{n,i})^2 \right), \]

we can use a discrete variational principle (see Appendix A) to get

\[ \delta_t^+ L_{\delta_t^i \phi^{n,i}} + \delta_x^i L_{\delta_x^i \phi^{n,i}} - \delta_x^2 L_{\delta_x^2 \phi^{n,i}} = 0, \]

which implies (3.14).

### 3.2 The Preissman Box Scheme

We now present a centered scheme that we refer to as the Preissman box scheme [49], also known as the Keller box scheme [34], which is the space-time version of the implicit midpoint rule for ODEs [28, 52]. This method has been discussed in the context of multisymplectic discretizations in [5, 15, 45, 51], and it is commonly used for applications in hydraulics [1, 2]. The idea is to use the implicit midpoint scheme to discretize the multisymplectic PDE (1.14) in space and time separately. Hence, we write the Preissman box scheme in the form

\[ \mathbf{K} \delta_t^+ z^{n+1/2,i} + \mathbf{L} \delta_x^+ z^{n,i+1/2} = \nabla_z S(z^{n+1/2,i+1/2}), \tag{3.15} \]

where we define the midpoints

\[ z^{n+1/2,i} = \frac{1}{2} (z^{n+1,i} + z^n,i), \quad z^{n,i+1/2} = \frac{1}{2} (z^{n,i+1} + z^n,i), \]

and

\[ z^{n+1/2,i+1/2} = \frac{1}{4} (z^{n+1,i+1} + z^{n+1,i} + z^{n,i+1} + z^n,i). \]

#### 3.2.1 Conservation Properties

Though this method is implicit, it has many properties that make it desirable. There are in fact many properties of the original PDE that this scheme preserves exactly, and we start with the discrete multi-symplectic conservation law.
Proposition 3.3 The Preissman box scheme (3.15) preserves exactly a multi-symplectic conservation law

\[ \delta_t^+ \omega^{n+1/2,i} + \delta_x^+ \pi^{n,i+1/2} = 0 \]

for

\[ \omega^{n+1/2,i} = dz^{n+1/2,i} \wedge Kdz^{n+1/2,i} \quad (3.16) \]

and

\[ \pi^{n,i+1/2} = dz^{n,i+1/2} \wedge Ldz^{n,i+1/2} . \quad (3.17) \]

Proof of this result is due to Bridges and Reich [15], and can be stated as follows.

Proof Consider the variational equation

\[ K\delta_t^+ dz^{n+1/2,i} + L\delta_x^+ dz^{n,i+1/2} = S_x \left( z^{n+1/2,i+1/2} \right) dz^{n+1/2,i+1/2}, \]

and take the wedge product of \( dz^{n+1/2,i+1/2} \) with this equation to get

\[ dz^{n+1/2,i+1/2} \wedge K\delta_t^+ dz^{n+1/2,i} + dz^{n+1/2,i+1/2} \wedge L\delta_x^+ dz^{n,i+1/2} = 0. \]

The first term here can be written

\[
\begin{align*}
    & dz^{n+1/2,i+1/2} \wedge K\delta_t^+ dz^{n+1/2,i} \\
    & = \frac{1}{2\Delta t} \left( dz^{n+1/2,i+1} + dz^{n+1/2,i} \right) \wedge K \left( dz^{n+1/2,i+1} - dz^{n+1/2,i} \right) \\
    & = \frac{1}{2\Delta t} \left( dz^{n+1/2,i+1} \right) \wedge K \left( dz^{n+1/2,i+1} - dz^{n+1/2,i} \right) \\
    & = \frac{1}{2\Delta t} \left( dz^{n+1/2,i+1} \right) \wedge K \left( dz^{n+1/2,i+1} \right),
\end{align*}
\]

and similarly for the second term we have

\[ dz^{n+1/2,i+1/2} \wedge L\delta_x^+ dz^{n,i+1/2} = \frac{1}{2\Delta t} \left( dz^{n,i+1/2} \wedge Ldz^{n,i+1/2} \right), \]

where we have used the identities of (2.4), and this completes the proof. \( \Box \)

From the variational point of view, the numerical method (3.15) can also be derived from a discrete irregular Lagrangian (3.3) for

\[ L^{n,i} = \frac{1}{2} \left( z^{n+1/2,i+1/2} , \left( K\delta_t^+ z^{n+1/2,i} + L\delta_x^+ z^{n,i+1/2} \right) \right) - S \left( z^{n+1/2,i+1/2} \right). \]
Using a discrete variational principle, we obtain

\[ 0 = \frac{1}{\Delta t} K \left( z^{n+1/2,i+1} - z^{n+1/2,i-1} + z^{n-1/2,i+1} - z^{n-1/2,i-1} \right) \]
\[ + \frac{1}{\Delta x} L \left( z^{n+1,i+1/2} - z^{n-1,i+1/2} + z^{n+1,i-1/2} - z^{n-1,i-1/2} \right) \]
\[ - \nabla S \left( z^{n+1/2,i+1/2} \right) - \nabla S \left( z^{n+1/2,i-1/2} \right) \]
\[ - \nabla S \left( z^{n-1/2,i+1/2} \right) - \nabla S \left( z^{n-1/2,i-1/2} \right). \]

This is equivalent to

\[ 0 = K \delta^+_t z^{n+1/2,i} + L \delta^+_x z^{n,i+1/2} - \nabla_z S \left( z^{n+1/2,i+1/2} \right) \]
\[ + K \delta^+_t z^{n+1/2,i} + L \delta^+_x z^{n,i-1/2} - \nabla_z S \left( z^{n+1/2,i-1/2} \right) \]
\[ + K \delta^+_t z^{n-1/2,i} + L \delta^-_x z^{n,i+1/2} - \nabla_z S \left( z^{n-1/2,i+1/2} \right) \]
\[ + K \delta^+_t z^{n-1/2,i} + L \delta^-_x z^{n,i-1/2} - \nabla_z S \left( z^{n-1/2,i-1/2} \right) \]

where we use

\[ \frac{1}{\Delta t} (z^{n,i+1} - z^{n,i-1}) = \delta^+_t z^{n,i} + \delta^-_t z^{n,i} \]

and similar identities. Hence, we obtain four shifted versions of the Preissman box scheme.

It is well known that the implicit midpoint rule exactly preserves quadratic invariants for ODEs. Hence, we would like to show that a similar property holds for the Preissman box scheme, and we find that it does. For example, a discrete version of the conservation law (2.17) holds and this is the subject of the following proposition.

**Proposition 3.4** If the PDE (1.14) is invariant under an appropriate linear symmetry such that the conservation law (2.17) is satisfied, then the scheme (3.15) satisfies the discrete conservation law

\[ \delta^+_t \left( z^{n+1/2,i}, KB z^{n+1/2,i} \right) + \delta^+_x \left( z^{n,i+1/2}, LB z^{n,i+1/2} \right) = 0. \]

**Proof** To make this clear, take the inner product of (3.15) with \( B z^{n+1/2,i+1/2} \) to get

\[ \left( z^{n+1/2,i+1/2}, KB \delta^+_t z^{n+1/2,i} \right) + \left( z^{n+1/2,i+1/2}, LB \delta^+_x z^{n,i+1/2} \right) = 0, \]

where we make use of the symplectic and invariance conditions (2.15)-(2.16). Then, similar to the proof of Proposition 3.3 we have

\[ \left( z^{n+1/2,i+1/2}, KB \delta^+_t z^{n+1/2,i} \right) = \frac{1}{2} \delta^+_t \left( z^{n+1/2,i}, KB z^{n+1/2,i} \right), \]

...
and
\[
\langle z^{n+1/2,i+1/2}, \mathbf{L} \delta_z^+ z^{n,i+1/2} \rangle = \frac{1}{2} \delta_t^+ \langle z^{n,i+1/2}, \mathbf{L} \delta_z^+ z^{n,i+1/2} \rangle,
\]
which yields the desired result.

We note the similarity of this result to the discrete version of Noether's theorem for first order field theories, which was presented by Marsden, Patrick and Shkoller [36].

Likewise, the Preissman box scheme also preserves energy and momentum conservation laws exactly for linear PDEs, which is shown in the following proposition, and this result was first presented by Bridges and Reich [15].

**Proposition 3.5** The scheme (3.15) with \( S(z) = \frac{1}{2} \langle z, A z \rangle \) for \( A \) symmetric, satisfies a fully discrete energy conservation law
\[
\delta_t^+ E^{n+1/2,i} + \delta_z^+ E^{n,i+1/2} = 0
\]
for
\[
E^{n+1/2,i} = \langle z^{n+1/2,i}, A z^{n+1/2,i} \rangle - \langle z^{n+1/2,i}, \mathbf{L} \delta_z^+ z^{n,i} \rangle
\]
and
\[
E^{n,i+1/2} = \langle z^{n,i+1/2}, \mathbf{L} \delta_z^+ z^{n,i} \rangle,
\]
and a fully discrete momentum conservation law
\[
\delta_t^+ G^{n,i+1/2} + \delta_z^+ I^{n+1/2,i} = 0
\]
for
\[
G^{n,i+1/2} = \langle z^{n,i+1/2}, A z^{n,i+1/2} \rangle - \langle z^{n,i+1/2}, K \delta_z^+ z^{n,i} \rangle
\]
and
\[
I^{n+1/2,i} = \langle z^{n+1/2,i}, K \delta_z^+ z^{n,i} \rangle,
\]
exactly.

**Proof** To derive a discrete energy conservation law, take the inner product of \( \delta_t^+ z^{n+1/2,i} \) with the Preissman discretization
\[
K \delta_t^+ z^{n+1/2,i} + \mathbf{L} \delta_z^+ z^{n,i+1/2} = A z^{n+1/2,i+1/2},
\]
to get
\[
\langle \delta_t^+ z^{n+1/2,i}, \mathbf{L} \delta_z^+ z^{n,i+1/2} \rangle = \langle \delta_t^+ z^{n+1/2,i}, A z^{n+1/2,i+1/2} \rangle.
\]
The right hand side of this equation can be written
\[
\langle \delta_t^+ z^{n+1/2,i}, A z^{n+1/2,i+1/2} \rangle
\]
\[
= \frac{1}{2\Delta t} \left\langle \left( z^{n+1/2,i+1} - z^{n+1/2,i} \right), A \left( z^{n+1/2,i+1} + z^{n+1/2,i} \right) \right\rangle
\]
\[
= \frac{1}{2} \delta_t^+ \left\langle z^{n+1/2,i}, A z^{n+1/2,i} \right\rangle.
\]

Then, defining
\[
\delta = \frac{1}{4\Delta t \Delta x}
\]
for cleaner notation, the left hand side of (3.20) can be written
\[
\langle \delta_t^+ z^{n+1/2,i}, L \delta_x^+ z_{n,i+1/2} \rangle
= 4\delta \left( \left\langle z^{n+1/2,i+1}, L z^{n+1,i+1/2} \right\rangle + \left\langle z^{n+1/2,i}, L z^{n,i+1/2} \right\rangle \right.
- \left. \left\langle z^{n+1/2,i+1}, L z^{n,i+1/2} \right\rangle - \left\langle z^{n+1/2,i}, L z^{n,i+1/2} \right\rangle \right)
\]
\[
= \delta \left( \left\langle z^{n+1,i+1} + z^{n,i+1}, L \left( z^{n+1,i+1} + z^{n,i+1} \right) \right\rangle + \left\langle z^{n+1,i} + z^{n,i}, L \left( z^{n+1,i} + z^{n,i} \right) \right\rangle \right.
- \left. \left\langle z^{n+1,i+1} + z^{n,i+1}, L \left( z^{n+1,i+1} + z^{n,i+1} \right) \right\rangle - \left\langle z^{n+1,i} + z^{n,i}, L \left( z^{n+1,i} + z^{n,i} \right) \right\rangle \right)
\]
\[
= 2\delta \left( \left\langle z^{n+1,i+1} + z^{n,i+1}, L z^{n,i+1} \right\rangle + \left\langle z^{n,i} + z^{n,i}, L z^{n,i+1} \right\rangle \right.
- \left. \left\langle z^{n+1,i+1} + z^{n,i+1}, L z^{n,i+1} \right\rangle - \left\langle z^{n,i} + z^{n,i}, L z^{n,i+1} \right\rangle \right).
\]

Now, by noting that
\[
\frac{1}{2} \delta_t^+ \left\langle z^{n+1/2,i}, L \delta_x^+ z_{n,i} \right\rangle
= \delta \left( \left\langle z^{n+1,i+1} + z^{n,i+1}, L \left( z^{n+1,i+1} - z^{n,i+1} \right) \right\rangle \right.
- \left. \left\langle z^{n+1,i} + z^{n,i}, L \left( z^{n+1,i} - z^{n,i} \right) \right\rangle \right)
\]
\[
= -2\delta \left( \left\langle z^{n+1,i+1} + z^{n,i+1}, L z^{n,i+1} \right\rangle + \left\langle z^{n,i} + z^{n,i}, L z^{n,i+1} \right\rangle \right.
- \left. \left\langle z^{n+1,i+1} + z^{n,i+1}, L z^{n,i+1} \right\rangle - \left\langle z^{n,i} + z^{n,i}, L z^{n,i+1} \right\rangle \right),
\]
and
\[
\frac{1}{2} \delta_x^+ \left\langle z^{n,i+1/2}, L \delta_t^+ z_{n,i} \right\rangle
= \delta \left( \left\langle z^{n+1,i+1} + z^{n,i+1}, L \left( z^{n+1,i+1} - z^{n,i+1} \right) \right\rangle \right.
- \left. \left\langle z^{n+1,i} + z^{n,i}, L \left( z^{n+1,i} - z^{n,i} \right) \right\rangle \right)
\]
\[
= -2\delta \left( \left\langle z^{n+1,i+1} + z^{n,i+1}, L z^{n+1,i} \right\rangle + \left\langle z^{n,i} + z^{n,i}, L z^{n+1,i} \right\rangle \right.
- \left. \left\langle z^{n+1,i+1} + z^{n,i+1}, L z^{n+1,i} \right\rangle - \left\langle z^{n,i} + z^{n,i}, L z^{n+1,i} \right\rangle \right),
\]
and by making the proper substitutions, we obtain the desired result. Then, to get the discrete momentum conservation law, simply take the inner product of $\delta_x^+ z_{n,i+1/2}^+$ with (3.19) and follow the same procedure. This completes the proof. \( \square \)
For nonlinear systems in general, exact conservation of discrete energy and momentum conservation laws cannot be guaranteed. The understanding of the energy and momentum conservation of fully discretized equations can only be achieved by some other means, and this is the subject of later chapters. However, certain semi-discretized energy and momentum conservation laws are still preserved exactly.

Proposition 3.6 Using the implicit midpoint scheme to discretize in space, leaving time continuous, yields a semi-discrete energy conservation law

$$\partial_t E^{n+1/2} + \delta_{\Delta x}^+ P^n = 0$$

with

$$E^{n+1/2} = S(z^{n+1/2}) - \frac{1}{2} \left< z^{n+1/2}, L \delta_{\Delta x}^+ z^n \right> \quad \text{and} \quad P^n = \frac{1}{2} \left< z^n, L z^n \right>.$$  

Using the implicit midpoint scheme to discretize in time only, gives a semi-discrete momentum conservation law

$$\partial_t G^{i+1/2} + \delta_i^+ I^i = 0,$$

which is satisfied for

$$G^{i+1/2} = S(z^{i+1/2}) - \frac{1}{2} \left< z^{i+1/2}, K \delta_{\Delta x}^+ z^n \right> \quad \text{and} \quad I^i = \frac{1}{2} \left< z^i, K z^n \right>.$$  

Proof We take the inner product of $z_i^{n+1/2}$ with the spatially discrete equation

$$K z_i^{n+1/2} + L \delta_{\Delta x}^+ z^n = \nabla_x S(z^{n+1/2})$$

to get

$$\left< z_i^{n+1/2}, L \delta_{\Delta x}^+ z^n \right> = \partial_t S(z^{n+1/2}).$$

because $K$ skew-symmetric implies $\left< z_i^{n+1/2}, K z_i^{n+1/2} \right> = 0$. Now write the identity

$$2 \left< z_i^{n+1/2}, L \delta_{\Delta x}^+ z^n \right> = \partial_t \left< z_i^{n+1/2}, L \delta_{\Delta x}^+ z^n \right> + \left< z_i^{n+1/2}, L \delta_{\Delta x}^+ z^n \right> - \left< z_i^{n+1/2}, L \delta_{\Delta x}^+ z_i^n \right>,$$

and notice that,

$$\delta_{\Delta x}^+ \left< z^n, L z_i^n \right> = \frac{1}{\Delta x} \left( \left( z_i^{n+1}, L z_i^{n+1} \right) - \left( z^n, L z_i^n \right) \right)$$

$$= \frac{1}{2\Delta x} \left( \left( \left( z_i^{n+1} - z^n \right), L \left( z_i^{n+1} + z_i^n \right) \right) + \left( \left( z_i^{n+1} + z^n \right), L \left( z_i^{n+1} - z_i^n \right) \right) \right)$$

$$= -\left< z_i^{n+1/2}, L \delta_{\Delta x}^+ z^n \right> + \left< z_i^{n+1/2}, L \delta_{\Delta x}^+ z_i^n \right>.$$
This leads to the spatially discrete energy conservation law. A semi-discrete momentum conservation law is derived in the same way by reversing the roles of space and time, i.e. discretize the PDE in time only and take the inner product of the resulting equation with $z_i^{n+1/2}$.

To make these results more clear, we consider the simple example of the wave equation. We also use this example to demonstrate the difference between local and global properties of the scheme, as well as the effects of the boundary conditions on the results.

### 3.2.2 The Wave Equation

Consider the simple wave equation

$$u_{tt} = u_{xx}, \quad x \in [0, 1]$$

with the absorbing boundary conditions

$$u_t(0,t) = u_x(0,t), \quad u_t(1,t) = -u_x(1,t).$$

We know that this equation, written as the system

$$v_t = u_{xx}, \quad u_t = v,$$

possesses an associated energy functional

$$H = \int_0^1 E dx \quad \text{for} \quad E = \frac{1}{2} \left(v^2 + (u_x)^2\right).$$

Taking the time derivative, we get

$$\partial_t E = vv_t + u_x u_{xt} = u_t u_{xx} + u_x u_{xt} = \partial_x (u_x u_z),$$

but

$$\frac{d}{dt} H = u_t(1,t)u_x(1,t) - u_t(0,t)u_x(0,t)$$

$$= -u_x^2(1,t) - u_x^2(0,t) \leq 0.$$

Thus, energy is conserved locally inside the domain, but energy is generally not conserved globally due to the boundary conditions. This emphasizes the difference between global and local conservation, as well as how the boundary conditions effect the results. In this case, the boundary conditions have no effect on the local properties.
Figure 3.1: Snapshots of the numerical solution of the wave equation using the Preissman box scheme with a Gaussian initial condition with zero velocity and absorbing boundary conditions.

Figure 3.2: The $\ell_\infty$-norm of the total energy $H$ (Left), and the $\ell_\infty$-norm of the residual in the discrete local energy conservation law (Right) plotted against time for the wave equation with absorbing boundary conditions.
Discretizing this equation with the Preissman box scheme yields

\[ \delta^+_t u_n^{i+1/2} = -\delta^+_n w_n^{i+1/2}, \]
\[ \delta^+_t u_n^{i+1/2} = w_n^{i+1/2}, \]
\[ \delta^+_n u_i^{n+1/2} = -w_i^{n+1/2}. \]

and using the discrete energy density

\[ E_{n+1/2} = \frac{1}{2} \left( (v_n^{i+1/2})^2 + (w_n^{i+1/2})^2 \right), \]

we find that

\[ \delta^+_t E_{n+1/2} = \frac{1}{2\Delta t} \left( (v_n^{i+1/2})^2 - (v_{n+1}^{i+1/2})^2 + (w_n^{i+1/2})^2 - (w_{n+1}^{i+1/2})^2 \right) \]
\[ = \frac{1}{2\Delta t} \left( v_n^{i+1/2} - v_{n+1}^{i+1/2} + w_n^{i+1/2} - w_{n+1}^{i+1/2} \right) \]
\[ = (v_n^{i+1/2} + w_n^{i+1/2} + \cdots) - (v_{n+1}^{i+1/2} + w_{n+1}^{i+1/2} + \cdots) \]
\[ = \delta^+_\omega w_n^{i+1/2} \]
\[ = -\delta^+_\omega \left( w_n^{i+1/2} \right), \]

which is just the discrete energy conservation law (3.18). However, by summing this over all \( n \) and using the discrete boundary conditions

\[ \delta^+_t u^0 = -w_0^{i+1/2} \]
\[ \delta^+_t u^j = w_{j+i+1/2} \]

we find that globally

\[ \delta^+_t \sum_n E_{n+1/2} = - (\delta^+_t u^j)^2 - (\delta^+_t u^0)^2 \leq 0. \]

Thus, the Preissman discretization also yields local energy conservation, but not necessarily global energy conservation, emphasizing the strength behind a multi-symplectic approach.

This is easily demonstrated through a numerical experiment. We use the Preissman box scheme to discretize the wave equation with absorbing boundary conditions and a Gaussian initial condition with zero velocity, on a boundary domain of \([0,40]\) and a time domain of \([0,30]\). In Figure 3.1, we plot snapshots of the numerical solution, showing that the oscillations are absorbed into the boundary. Then, Figure 3.2 shows that the total energy decreases to zero when the wave hits the boundary wall, while the local energy conservation law is conserved (up to round-off error) over the entire interval.
3.3 The Explicit Midpoint Scheme

Finally, applying the explicit midpoint rule in both space and time yields the simple two-step method given by

\[ \mathbf{K} \delta_t^{1/2} z^{n,i} + \mathbf{L} \delta_x^{1/2} z^{n,i} = \nabla_z S(z^{n,i}), \tag{3.21} \]

where we introduce

\[ \delta_t^{1/2} = \frac{1}{2} (\delta_t^+ + \delta_t^-) \quad \text{and} \quad \delta_x^{1/2} = \frac{1}{2} (\delta_x^+ + \delta_x^-), \]

in order to simplify notation.

3.3.1 Conservation Properties

Considering this method as a geometric integrator, it has several properties that make it comparable to the Euler and Preissman schemes, the first of which is the preservation of a multi-symplectic conservation law.

**Proposition 3.7** The explicit midpoint scheme (3.21) satisfies a discrete multi-symplectic conservation law (3.2) for

\[ \omega^{n,i} = dz^{n,i} \wedge K dz^{n,i-1} \quad \text{and} \quad \kappa^{n,i} = dz^{n,i} \wedge L dz^{n-1,i}. \]

**Proof** The variational equation associated with (3.21) is given by

\[ \mathbf{K} \delta_t^{1/2} dz^{n,i} + \mathbf{L} \delta_x^{1/2} dz^{n,i} = S_z(z^{n,i}) dz^{n,i}. \]

After taking the wedge product with \( dz^{n,i} \), we get

\[ dz^{n,i} \wedge K \delta_r^{1/2} dz^{n,i} + dz^{n,i} \wedge L \delta_x^{1/2} dz^{n,i} = 0, \]

which is equivalent to

\[ 0 = \frac{1}{\Delta t} (dz^{n,i} \wedge K (dz^{n,i+1} - dz^{n,i-1})) + \frac{1}{\Delta x} (dz^{n,i} \wedge L (dz^{n+1,i} - dz^{n-1,i})). \]

Since

\[ dz^{n,i} \wedge K (dz^{n,i+1} - dz^{n,i-1}) = dz^{n,i} \wedge K dz^{n,i+1} - dz^{n,i} \wedge K dz^{n,i-1} = dz^{n,i+1} \wedge K dz^{n,i} - dz^{n,i} \wedge K dz^{n,i-1}, \]
This raises questions regarding the definition for a multi-symplectic integrator, and these issues are discussed in more detail in the following chapters. Essentially, this issue arises due to the "non-compact" differencing resulting from the two-step nature of the scheme, such that

$$\delta_{1/2} z^{n,t} = \frac{1}{2\Delta t} (z^{n,t+1} - z^{n,t-1}).$$

Even though this method satisfies a discrete multi-symplectic conservation law we will not consider it to be a multi-symplectic discretization. Reasons for this become more apparent in the next chapter, but we include it here because it does satisfy a discrete multi-symplectic conservation law (3.2).

Moreover, this method can be obtained through a Lagrangian approach. Consider the discrete Lagrangian "density"

$$L^{n,i} = \frac{1}{2} \left( \left< z^{n,i}, \delta_{1/2} z^{n,i} \right> + \left< z^{n,i}, L \left( \delta_{1/2} z^{n,i} \right) \right> \right) - S(z^{n,i}),$$

which can also be stated

$$L^{n,i} = \frac{1}{4\Delta t} \left< z^{n,i}, K \left( z^{n,i+1} - z^{n,i-1} \right) \right> + \frac{1}{4\Delta x} \left< z^{n,i}, L \left( \delta_{n+1} z^{n,i} - \delta_{n-1} z^{n,i} \right) \right> - S(z^{n,i}).$$

Taking the variational derivative gives

$$\nabla_z S(z^{n,i}) = \frac{1}{2\Delta t} \left( K z^{n,i+1} + K z^{n,i-1} \right) + \frac{1}{2\Delta x} \left( L z^{n+1,i} + L z^{n-1,i} \right),$$

but this is just (3.21).

It can also be shown that this scheme preserves semi-discrete conservation laws of energy and momentum.

**Proposition 3.8** Discretizing the PDE (1.14) in space using the explicit midpoint rule implies a spatially discrete energy conservation law

$$\delta_t E^n + \delta_x E^{n-1/2} = 0$$

for

$$E^n = S(z^n) - \frac{1}{2} \left< z^n, L \delta_{1/2} z^n \right>$$

and

$$E^{n-1/2} = \frac{1}{4} \left( \left< z^n, L z^{n-1} \right> + \left< z^{n-1}, L z^n \right> \right),$$
and discretizing (1.14) in time with the explicit midpoint rule yields a semi-discrete momentum conservation law
\[ \partial_t G^i + \delta^i_{t-1} I^{t-1/2} = 0 \]
for
\[ G^i = S(z^i) - \frac{1}{2} \left\langle z^i, K \delta_t^{1/2} z^i \right\rangle \]
and
\[ I^{t-1/2} = \frac{1}{4} \left( \left\langle z^i, K z_x^{i-1} \right\rangle + \left\langle z^{i-1}, K z_x^i \right\rangle \right). \]

**Proof** We first derive the semi-discrete energy conservation law using the semi-discrete equation
\[ K z_t^n + L \delta_t^{1/2} z^n = \nabla_z S(z^n). \]
Taking the inner product of this equation with \( z^n_t \) gives
\[
\partial_t S(z^n) = \left\langle z^n_t, L \delta_t^{1/2} z^n \right\rangle \\
= \frac{1}{2} \left( \partial_t \left\langle z^n, L \delta_t^{1/2} z^n \right\rangle + \left\langle z^n_t, L \delta_t^{1/2} z^n \right\rangle - \left\langle z^n, L \delta_t^{1/2} z^n_t \right\rangle \right).
\]
Since
\[
\left\langle z^n_t, L \delta_x^{1/2} z^n \right\rangle - \left\langle z^n, L \delta_x^{1/2} z^n_t \right\rangle \\
= \frac{1}{2 \Delta x} \left( \left\langle z^n_t, L (z^{n+1} - z^{n-1}) \right\rangle - \left\langle z^n, L (z^{n+1} - z^{n-1}) \right\rangle \right) \\
= \frac{1}{2 \Delta x} \left( \left\langle z^{n+1}, L z^n_t \right\rangle + \left\langle z^{n-1}, L z^n_t \right\rangle - \left\langle z^n, L z_t^{n+1} \right\rangle + \left\langle z^n, L z_t^{n-1} \right\rangle \right) \\
= \frac{1}{2} \delta^i_{x^n} \left( \left\langle z^n, L z_t^{n-1} \right\rangle + \left\langle z^{n-1}, L z_t^n \right\rangle \right),
\]
we obtain the spatially discrete energy conservation law. Then the semi-discrete momentum conservation law is found in the same way using the time-discrete equation and taking the inner product with \( z^n_x \), and this completes the proof. \( \square \)

### 3.3.2 The Nonlinear Wave Equation

Applying the discretization (3.21) to the nonlinear wave equation gives
\[
-\delta_t^{1/2} u^{n,i} - \delta_x^{1/2} p^{n,i} = f'(u^{n,i}), \quad \delta_t^{1/2} u^{n,i} = v^{n,i}, \quad p^{n,i} = -\sigma' \left( \delta_x^{1/2} u^{n,i} \right),
\]
which is equivalent to
\[
\left( \delta_t^{1/2} \right)^2 u^{n,i} = \delta_x^{1/2} \sigma' \left( \delta_x^{1/2} u^{n,i} \right) - f'(u^{n,i}). \quad (3.22)
\]
On the other hand, applying this discretization to the Lagrangian functional (1.15) gives (3.3), where

$$L_{n,i} = L \left( \delta_t^{1/2} u^{n,i}, \delta_x^{1/2} u^{n,i}, u^{n,i} \right) = \frac{1}{2} \left( \delta_t^{1/2} u^{n,i} \right)^2 - \sigma \left( \delta_x^{1/2} u^{n,i} \right) - f(u^{n,i}).$$

Now, using the discrete variational principle, we get the Euler-Lagrange equation

$$\delta_t^{1/2} L_{\delta_t^{1/2} u^{n,i}} + \delta_x^{1/2} L_{\delta_x^{1/2} u^{n,i}} - L_{u^{n,i}} = 0,$$

which implies the equation (3.22).
Thus far, multi-symplectic equations have been presented along with some important properties, written as conservation laws, which have a significant role in determining the dynamics of the system. We have also discussed three numerical schemes and have shown how some of these conservation laws are preserved exactly by the scheme. However, there are still many questions concerning the behavior of these schemes. For example, in every case, the energy and momentum conservation laws could not be preserved exactly for general nonlinear problems using any of these schemes. To understand what happens to these conservation laws after discretization we must resort to the concept of modified equations through backward error analysis, and this is the subject of later chapters.

We also know nothing of the solution behavior for these schemes, and an analysis of this sort for nonlinear problems is beyond the scope of this thesis. However, for linear problems the exact solution of the PDE can be found, making a comparison of the exact solution and the numerical solution more straightforward. Hence, this chapter is devoted to an extensive analysis of linear equations, meaning we consider (1.14) such that

\[ S(z) = \frac{1}{2} (z, Az), \]

(4.1)

where \( A \) is symmetric. This implies the linear multi-symplectic PDE

\[ Kz_t + Lz_x = Az. \]

(4.2)

Here we discuss solutions and dispersion relations for both the continuous and discrete versions of this equation, giving a thorough understanding of the behavior of our three numerical methods for linear problems. Then we discuss two model problems, known as the linearized Boussinesq and KdV equations, in light of these results.
4.1 Dispersion Relations

Using standard Fourier analysis [30, 53, 56], the elementary single mode solution of (4.2) can be written

\[ z(x, t) = \Re \left\{ a e^{i(kx - \omega t)} \right\} \]  

(4.3)

where \( a = a(k) \) and \( \Re \{ \cdot \} \) indicates the real part. Here, \( k \) denotes the wave number, \( \omega \) denotes the wave frequency. Notice that we use the standard notation for the frequency, not to be confused with the two-form given by \( \omega \) in the previous sections.

Substituting this solution into the linear PDE (4.2) leads to the linear system

\[ (-i\omega K + ikL - A) a = 0. \]

Since we seek solutions such that \( a \) is non-zero, \( k \) and \( \omega \) must satisfy the dispersion relation [10]

\[ D_A(\omega, k) := \det (-i\omega K + ikL - A) = 0, \]  

(4.4)

which is used to characterize the PDE. It is important to note that the matrix used in this calculation is self-adjoint. This implies a real dispersion relation, meaning there is no diffusion [56, Chapter 11].

With the dispersion relation, one can write the frequency as a function of the wave number, such that \( \omega = \omega(k) \), at least locally. Then, for every \( k \) there may be several different frequencies \( \omega_j(k) \) corresponding to different modes. In many cases, the solution admits two modes such that \( \omega_1 = -\omega_2 \), corresponding to right and left traveling waves. This can be made more precise for a particular problem, and can be readily observed for an example in the final section of this chapter.

This dispersion relation is not specific to the single mode solution (4.3). In fact, the most general solution of the linear PDE (4.2) can be stated as a super-position of solutions

\[ z(x, t) = \int_{-\infty}^{\infty} a(k)e^{i(kx - \omega(k)t)} dk, \quad -\infty < x < \infty, \]

which is obtained through Fourier analysis [56, Chapter 11]. For example, the general solution of a typical one-dimensional problem with two modes, such as the wave equation, is given by

\[ z(x, t) = \int_{-\infty}^{\infty} a_1(k)e^{i(kx - \omega(k)t)} dk + \int_{-\infty}^{\infty} a_2(k)e^{i(kx + \omega(k)t)} dk. \]

Setting \( a_1 = a_1a \) and \( a_2 = a_2a \), such that \( a \) has been normalized, the constants \( a_1 \) and \( a_2 \) are determined by initial data, but the dispersion relation must still hold. Thus, we only consider the single mode solution (4.3) for the sake of simplicity.
Similar to (4.3), the solution of the spatially discrete equation can be written
\[ z^n(t) = R \left\{ \hat{a} e^{i(Kx - \Omega t)} \right\}, \]
and we take the numerical solution of (4.2) to be
\[ z^{n,i} = R \left\{ \hat{a} e^{i(Kx - \Omega t)} \right\}, \tag{4.5} \]
where \( K \) is the numerical wave number and \( \Omega \) is the numerical frequency (sometimes called the Nyquist frequency) such that
\[ -\pi \leq \Delta x K \leq \pi \quad \text{and} \quad -\pi \leq \Delta t \Omega \leq \pi, \tag{4.6} \]
because \( x_n = n\Delta x \) and \( t_i = i\Delta t \) (cf. [8, Chapter 11]). Notice that the wave number will remain the same for each solution, but the wave frequency and the vector multiplying the exponential function, which depends on the initial data, are different for each solution because their dependency on the wave number changes according to the discretization. This will become evident in the following subsections, where we apply these ideas to our three numerical discretizations. The numerical solution (4.5) can be used to derive numerical dispersion relations for each of these schemes based on the multi-symplectic structure.

4.1.1 The Euler Box Scheme

The Euler box scheme applied to the linear equation (4.2) gives
\[ (K_+ \delta_t^+ + K_- \delta_t^- + L_+ \delta_x^+ + L_- \delta_x^-) z^{n,i} = A z^{n,i}, \tag{4.7} \]
and by definition we have
\[ \delta_t^+ z^{n,i} = e^{-i\Omega \Delta t} - 1 z^{n,i}. \]
Using this and similar identities, we get the linear system
\[ \left( K_+ \frac{e^{-i\Omega \Delta t} - 1}{\Delta t} + K_- \frac{1 - e^{i\Omega \Delta t}}{\Delta t} + L_+ \frac{e^{iK \Delta x} - 1}{\Delta x} + L_- \frac{1 - e^{-iK \Delta x}}{\Delta x} - A \right) \tilde{a} = 0, \]
and defining
\[ M = (K_+ - K_-) \quad \text{and} \quad N = (L_+ - L_-), \tag{4.8} \]
this is equivalent to
\[ \left( -\frac{1}{\Delta t} \sin(\Delta t \Omega) K + \frac{1}{\Delta x} \sin(\Delta x K) L \right) \tilde{a} \]
\[ + \left( \frac{\cos(\Delta t \Omega) - 1}{\Delta t} M + \frac{\cos(\Delta x K) - 1}{\Delta x} N - A \right) \tilde{a} = 0, \tag{4.9} \]
because
\[ e^{\pm i\theta} = \cos \theta \pm i \sin \theta. \]

This implies an implicit numerical dispersion relation [53]
\[ D_{\tilde{A}}(\Omega_{\Delta t}, K_{\Delta x}) = \det \left( -i\Omega_{\Delta t} K + i K_{\Delta x} L - \tilde{A} \right) = 0, \]

where we define
\[ \Omega_{\Delta t} = \frac{\sin(\Delta t \Omega)}{\Delta t}, \quad K_{\Delta x} = \frac{\sin(\Delta x K)}{\Delta x}, \]
and
\[ \tilde{A} = A - M r - N_s, \]
for
\[ r = \frac{\cos(\Delta t \Omega) - 1}{\Delta t}, \quad \text{and} \quad s = \frac{\cos(\Delta x K) - 1}{\Delta x}. \]

Notice that the dispersion relation here is also found by taking the determinant of a self-adjoint matrix, meaning there is no diffusion induced by the numerical scheme. The same can be done for the semi-discrete equation
\[ K z^n + L_+ \delta^+ z^n + L_- \delta^- z^n = A z^n, \]
and we get the dispersion relation
\[ \det \left( -i\tilde{\omega} K + i \tilde{K} L - \tilde{A} \right) = 0, \]
for \( \tilde{A} = A - N_s. \)

### 4.1.2 The Preissman Box Scheme

Applying the Preissman box scheme to the linear PDE (4.2) yields (3.19), and using (4.5) we get
\[
\delta^+ \bar{z}^{n+1/2,i} = \frac{1}{2\Delta t} \left( z^{n+1,i+1} + z^{n+1,i-1} - z^{n,i+1} + z^{n,i-1} \right) = \frac{1}{2\Delta t} \left( \left( -i\Omega_{\Delta t} + K_{\Delta x} \right) + \left( -i\Omega_{\Delta t} - K_{\Delta x} \right) \right) \bar{z}^{n+1/2,i+1/2} + \frac{1}{2\Delta t} \left( \left( i\Omega_{\Delta t} - K_{\Delta x} \right) + \left( i\Omega_{\Delta t} + K_{\Delta x} \right) \right) z^{n+1/2,i-1/2} \]
\[
= \frac{1}{2\Delta t} \left( \left( -i\Omega_{\Delta t} + K_{\Delta x} \right) \left( -1 \right) \left( -i\Omega_{\Delta t} - K_{\Delta x} \right) \right) \bar{z}^{n+1/2,i+1/2} + \frac{1}{2\Delta t} \left( \left( i\Omega_{\Delta t} - K_{\Delta x} \right) \left( -1 \right) \left( i\Omega_{\Delta t} + K_{\Delta x} \right) \right) z^{n+1/2,i-1/2} \]
\[
= \frac{1}{2\Delta t} \left( \sin \left( \frac{\Omega_{\Delta t}}{2} \right) \cos \left( \frac{K_{\Delta x}}{2} \right) \bar{z}^{n+1/2,i+1/2} + \sin \left( \frac{\Omega_{\Delta t}}{2} \right) \cos \left( \frac{K_{\Delta x}}{2} \right) z^{n+1/2,i-1/2} \right). \]
and similarly
\[ \phi_z^{n,i+1/2} = \frac{2i}{\Delta x} \sin \left( \frac{K \Delta x}{2} \right) \cos \left( \frac{\Omega \Delta t}{2} \right) z^{n+1/2,i+1/2}. \]

Notice that we use
\[ \bar{z}^{n+1/2,i+1/2} = \bar{a} e^{i(Kz_{n+1/2}-\Omega t_{i+1/2})}, \]

which is related to the approximation \( z^{n+1/2,i+1/2} \) through the relation
\[ z^{n+1/2,i+1/2} = \frac{1}{4} \left( z^{n+1,i+1} + z^{n,i+1} + z^{n+1,i} + z^{n,i} \right) \]
\[ = \frac{1}{4} \left( e^{iK\Delta x} e^{-i\Omega \Delta t} + e^{-i\Omega \Delta t} + e^{iK\Delta x} + 1 \right) z^{n,i} \]
\[ = \frac{1}{4} \left( e^{-i\Omega \Delta t} + 1 \right) \left( e^{iK\Delta x} + 1 \right) e^{i\Omega \Delta t/2} e^{-iK\Delta x/2} z^{n+1/2,i+1/2} \]
\[ = \cos \left( \frac{\Omega \Delta t}{2} \right) \cos \left( \frac{K \Delta x}{2} \right) z^{n+1/2,i+1/2}. \]

After substituting these equalities into (3.19), we get the linear system
\[ \left( -iK \frac{2 \tan(\Omega \Delta t/2)}{\Delta t} + iL \frac{2 \tan(K \Delta x/2)}{\Delta x} - A \right) \bar{a} = 0. \]

Now, define the pseudo frequency and pseudo wave number for the Preissman box scheme by
\[ \Omega_P = \frac{2 \tan(\Omega \Delta t/2)}{\Delta t} \quad \text{and} \quad K_P = \frac{2 \tan(K \Delta x/2)}{\Delta x}, \]
respectively. This implies that the numerical dispersion relation is just
\[ (-i\Omega_P K + iK_P L - A) \bar{a} = 0, \]
which is the exact dispersion relation evaluated at the pseudo frequency and pseudo wave number, i.e.
\[ D_A (\Omega_P, K_P) = 0, \]
where \( D_A \) is given in (4.4). Further results concerning numerical dispersion relations for the Preissman box scheme have also been presented and discussed by Ascher and McLachlan [5].

4.1.3 The Explicit Midpoint Scheme

Substituting the numerical solution (4.5) into the scheme (3.21) gives
\[ \left( K \frac{e^{-i\Omega \Delta t} - e^{i\Omega \Delta t}}{2\Delta t} + L \frac{e^{iK \Delta x} - e^{-iK \Delta x}}{2\Delta x} - A \right) \bar{a} = 0. \]
Now, using the trigonometric identities
\[ e^{-i\Omega \Delta t} - e^{i\Omega \Delta t} = -2i \sin(\Delta t \Omega), \quad \text{and} \quad e^{iK \Delta x} - e^{-iK \Delta x} = 2i \sin(\Delta x K), \]
we get the linear equation
\[ \left( \frac{-i \sin(\Delta t \Omega)}{\Delta t} K + \frac{i \sin(\Delta x K)}{\Delta x} L - A \right) \hat{a} = 0, \tag{4.15} \]
and this matrix is again self-adjoint, implying there is no numerical diffusion. Thus, the dispersion relation
\[ \mathcal{D}_A(\Omega_{\Delta t}, K_{\Delta x}) = 0 \]
holds for \( \Omega_{\Delta t} \) and \( K_{\Delta x} \) given by (4.11). Notice here that \( \Omega_{\Delta t} \) and \( K_{\Delta x} \) are not 'invertible', because \( \sin(\Delta t \Omega) \), for example, is not invertible for \(-\pi \leq \Delta t \Omega \leq \pi\).

4.1.4 Mixed Discretizations

For reasons that become apparent in the following section, where we consider a specific model problem, suppose we discretize the linear PDE (4.2) in space with the explicit midpoint scheme and in time with the implicit midpoint scheme. Then we obtain
\[ K \delta_t^+ z^{n,i} + L \delta_x^{1/2} z^{n,i+1/2} = A z^{n,i+1/2}. \]
Then using the identities
\[ \delta_t^+ z^{n,i} = \frac{1}{\Delta t} (e^{-i\Omega \Delta t} - 1) z^{n,i} = \frac{-2i}{\Delta t} \sin \left( \frac{\Omega \Delta t}{2} \right) z^{n,i+1/2}, \]
and
\[ \delta_x^{1/2} z^{n,i+1/2} = \frac{1}{4\Delta x} \left( e^{-i\Omega \Delta t} + 1 \right) \left( e^{iK \Delta x} - e^{-iK \Delta x} \right) z^{n,i} \]
\[ = \frac{1}{\Delta x} \cos \left( \frac{\Omega \Delta t}{2} \right) \sin(K \Delta x) z^{n,i+1/2} \]
with
\[ z^{n,i+1/2} = \frac{1}{2} (e^{-i\Omega \Delta t} + 1) z^{n,i} = \cos \left( \frac{\Omega \Delta t}{2} \right) z^{n,i+1/2}, \]
gives the linear system
\[ \left( \frac{-2i}{\Delta t} \sin \left( \frac{\Omega \Delta t}{2} \right) K + \frac{i}{\Delta x} \cos \left( \frac{\Omega \Delta t}{2} \right) \sin(\Delta x K) L - \cos \left( \frac{\Omega \Delta t}{2} \right) A \right) \hat{a} = 0, \]
and we obtain the numerical dispersion relation
\[ \mathcal{D}_A(\Omega_P, K_{\Delta x}) = 0. \tag{4.16} \]
In the same manner, discretizing in space with the implicit scheme and in time with the explicit scheme yields
\[ K \delta^{1/2}_{x} z^{n+1/2,i} + L \delta^{+}_{x} z^{n,i} = A z^{n+1/2,i}, \]
and we find the numerical dispersion relation
\[ D_{\Lambda}(\Omega_{\Delta t}, K_p) = 0. \] (4.17)

4.2 Examples

For a better understanding of these numerical dispersion relations we consider two model problems, the Boussinesq equation and the KdV equation.

4.2.1 The Boussinesq Equation

For another example in second-order field theory, consider the Lagrangian functional (1.15) with
\[ L = L(u, u_{t}, u_{xx}, u_{x}) = \frac{1}{2} u_{t}^{2} + \frac{\alpha^{2}}{2} u_{xx}^{2} - g(u_{x}) - f(u), \]
where \( \alpha \) is a small parameter, and \( g \) is a smooth function. Using the variational principle
\[ \delta_{t} L_{ut} - \delta_{x} \delta_{x} L_{ux} + \delta_{x} L_{ux} - L_{u} = 0, \]
we obtain a Boussinesq wave model of the form
\[ (1 - \alpha^{2} \partial^{2}_{x}) u_{tt} = \delta_{xx} g'(u_{x}) - f'(u). \] (4.18)

We note here that the nonlinear wave equation is just a special case of this equation with \( \alpha = 0 \). In addition, for \( f(u) = 0 \) and \( g(v) = a_{g}/2\nu \) such that \( a_{g} \) is acceleration due to gravity, (4.18) becomes a regularized model for shallow water flow, and a multisymplectic spectral discretization for this problem has been discussed by Bridges and Reich [16]. After defining the linear operator \( B = (1 - \alpha^{2} \partial^{2}_{x}) \) and letting \( v = B u_{t} \), equation (4.18) can be written in the form
\[ v_{t} = \partial_{xx} g'(u_{x}) - f'(u), \quad u_{t} = B^{-1} v. \]

Hence, similar to the nonlinear wave equation, (4.18) can also be written as a Hamiltonian PDE in the form (1.10) with Hamiltonian functional
\[ H(u, v) = \int_{0}^{1} \left\{ \frac{v^{T} B^{-1} v}{2} + g(u_{x}) + f(u) \right\} dx \]
for a periodic domain $x \in [0, 1)$. Equation (4.18) can in turn be written as the first-order system of equations

$$
\begin{align*}
-v_t - w_x &= f'(u), \\
-\alpha v_x &= u_t, \\
\alpha \beta x &= v - u, \\
v_x &= u, \\
0 &= w + g'(v), \\
-\alpha \mu_x &= \beta,
\end{align*}
$$

and after taking

$$
K = \begin{pmatrix}
0 & -1 & 0 & 0 & 0 & 0 \\
1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0
\end{pmatrix}
\quad \text{and} \quad
L = \begin{pmatrix}
0 & 0 & 0 & -1 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & \alpha \\
0 & 0 & 0 & 0 & 0 & 0 \\
1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0
\end{pmatrix},
$$

(4.19)

this system is equivalent to (1.14) for $z = (u, v, \mu, w, \nu, \beta)^T$ and

$$
S(z) = \frac{\beta^2 - \mu^2}{2} + \mu v + \nu w + g(v) + f(u).
$$

With this multi-symplectic formulation we can apply the discretizations of the previous chapter maintaining each of the discrete conservation laws, reemphasizing the point that this approach to multi-symplectic integration is not limited to first order field theories.

To continue with our linear analysis, let $g(v) = \gamma v^2/2$ and $f(u) = \varepsilon u^2/2$ for some constants $\gamma$ and $\varepsilon$. This implies the linear Boussinesq equation

$$
(1 - \alpha^2 \partial^2_x)u_{tt} = (\gamma \partial^2_x - \varepsilon)u.
$$

Here, $\alpha$ is given by

$$
\alpha = \begin{pmatrix}
1 \\
-i\omega (1 + \alpha^2 k^2) \\
-i\omega \\
-i k \\
1 k \\
-\alpha \omega k
\end{pmatrix},
$$

where the constant $\alpha$ is determined by the initial conditions, and we have

$$
(-i\omega K + ikL - A) = \begin{pmatrix}
-\varepsilon & 1 \omega & 0 & -1 k & 0 & 0 \\
-1 i\omega & 0 & -1 & 0 & 0 & 0 \\
0 & -1 & 1 & 0 & 0 & i\alpha k \\
i k & 0 & 0 & 0 & -1 & 0 \\
0 & 0 & 0 & -1 & -\gamma & 0 \\
0 & 0 & -i\alpha k & 0 & 0 & -1
\end{pmatrix}.
$$
Then taking the determinant of this matrix implies the dispersion relation

\[ \mathcal{D}(\omega, k) = \omega^2 + \alpha^2 \omega^2 k^2 - \gamma k^2 - \varepsilon = 0, \]

or equivalently \( \omega_1 = W(k) \) and \( \omega_2 = -W(k) \), where we define the function

\[ W(k) := \left( \frac{\gamma k^2 + \varepsilon}{1 + \alpha^2 k^2} \right)^{\frac{1}{2}}. \tag{4.20} \]

This makes the two solution branches evident. For every wave number \( k \), there are two frequencies satisfying \( \omega_1 = -\omega_2 \), which correspond to two equivalent waves traveling in opposite directions.

Applying the multi-symplectic Euler scheme to this equation implies the numerical dispersion relation (4.10) with

\[
\tilde{A} = \begin{pmatrix}
\varepsilon & r & 0 & s & 0 \\
r & 0 & 1 & 0 & 0 \\
0 & 1 & -1 & 0 & 0 \\
s & 0 & 0 & 0 & 1 \\
0 & s & 0 & 0 & 1
\end{pmatrix},
\]

and the numerical dispersion relation becomes

\[
(\Omega^2_{\Delta t} + r^2) + \alpha^2 (\Omega^2_{\Delta t} + r^2) (K^2_{\Delta x} + s^2) - \gamma (K^2_{\Delta x} + s^2) - \varepsilon = 0.
\]

Using the identities

\[
\Omega^2_{\Delta t} + r^2 = \frac{1}{\Delta t^2} (\sin^2(\Delta t \Omega) + \cos^2(\Delta t \Omega) - 2 \cos(\Delta t \Omega) + 1)
\]
\[
= \frac{2}{\Delta t^2} (1 - \cos(\Delta t \Omega))
\]
\[
= \frac{4}{\Delta t^2} \sin^2\left(\frac{\Delta t \Omega}{2}\right)
\]
\[
:= \Omega^2_{\Delta t/2}
\]

and similarly

\[
K^2_{\Delta x} + s^2 = \frac{4}{\Delta x^2} \sin^2\left(\frac{\Delta x K}{2}\right) := K^2_{\Delta x/2},
\]

where the final equations here are assumed to be the definitions of \( \Omega_{\Delta t/2} \) and \( K_{\Delta x/2} \), this is equivalent to

\[
\frac{4}{\Delta t^2} \sin^2\left(\frac{\Delta t \Omega}{2}\right) + \frac{16\alpha^2}{\Delta t^2 \Delta x^2} \sin^2\left(\frac{\Delta t \Omega}{2}\right) \sin^2\left(\frac{\Delta x K}{2}\right) - \frac{4\gamma}{\Delta x^2} \sin^2\left(\frac{\Delta x K}{2}\right) - \varepsilon = 0.
\]

This is just

\[
\mathcal{D} (\Omega_{\Delta t/2}, K_{\Delta x/2}) = 0,
\]
which is equivalent to \( \Omega_{\Delta t/2} = \pm W(K_{\Delta x/2}) \), by (4.20). Therefore, the numerical dispersion relation for the symplectic Euler discretization of the linear Boussinesq equation can be written
\[
\frac{\Omega_{\Delta t}}{2} = \sin^{-1}\left(\pm \frac{\Delta t}{2} W(K_{\Delta x/2})\right), \quad \text{for} \quad -\pi \leq \Omega_{\Delta t} \leq \pi,
\]
because \( \sin(\eta) \) is invertible for \(-\pi/2 \leq \eta \leq \pi/2\). For the Preissman discretization, we simply use (4.14) and (4.20) to get
\[
\frac{\Omega_{\Delta t}}{2} = \tan^{-1}\left(\pm \frac{\Delta t}{2} W(K_P)\right) \quad \text{for} \quad -\pi \leq \Omega_{\Delta t} \leq \pi, \quad (4.21)
\]
because the \( \tan(\eta) \) is invertible for \(-\pi/2 \leq \eta \leq \pi/2\).

To find the numerical dispersion relation for the explicit midpoint scheme, one only needs to evaluate \( D \) at the pseudo frequency \( \Omega_{\Delta t} \) and pseudo wave number \( K_{\Delta x} \) given in (4.11). This gives
\[
\frac{1}{\Delta t^2} \sin^2(\Delta t \Omega) + \frac{\alpha^2}{\Delta t^2 \Delta x^2} \sin^2(\Delta t \Omega) \sin^2(\Delta x K) - \frac{\gamma}{\Delta x^2} \sin^2(\Delta x K) - \varepsilon = 0, \quad (4.22)
\]
which implies

\[ \Omega \Delta t = \begin{cases} 
-\pi - \sin^{-1}(\pm \Delta t \omega (K_{\Delta x})) & \text{for } -\pi \leq \Omega \Delta t \leq -\pi/2 \\
\sin^{-1}(\pm \Delta t \omega (K_{\Delta x})), & \text{for } -\pi/2 \leq \Omega \Delta t \leq \pi/2 \\
\pi - \sin^{-1}(\pm \Delta t \omega (K_{\Delta x})) & \text{for } \pi/2 \leq \Omega \Delta t \leq \pi 
\end{cases} \]  

(4.23)

In the same way, the numerical dispersion relations for the mixed discretizations are found using (4.16) and (4.17). Discretizing in space with the explicit midpoint scheme (EMP) and in time with the implicit midpoint scheme (IMP) implies

\[ \frac{\Omega \Delta t}{2} = \tan^{-1}(\pm \frac{\Delta t}{2} \omega (K_{\Delta x})), \quad \text{for } -\pi \leq \Omega \Delta t \leq \pi, \]

and using EMP in time and IMP in space implies

\[ \Omega \Delta t = \begin{cases} 
-\pi - \sin^{-1}(\pm \Delta t \omega (K_P)) & \text{for } -\pi \leq \Omega \Delta t \leq -\pi/2 \\
\sin^{-1}(\pm \Delta t \omega (K_P)), & \text{for } -\pi/2 \leq \Omega \Delta t \leq \pi/2 \\
\pi - \sin^{-1}(\pm \Delta t \omega (K_P)) & \text{for } \pi/2 \leq \Omega \Delta t \leq \pi 
\end{cases} \]

In Figure 4.1 we compare each of these numerical dispersion relations with the exact dispersion relation. We note first of all that the exact dispersion relation gives two frequencies for every wave number as expected. The plot shows that the dispersion relations for the Euler and Preissman schemes are very close to the exact relation. However, for the explicit midpoint scheme there are four frequencies for every wave number and four wave numbers for every frequency, making it impossible to decipher which is the correct approximation. We also notice that if we use the implicit method in time and the explicit method in space we get four wave numbers for each frequency, and using the implicit method in space and the explicit method in time there are four frequencies for every wave number. Hence, the explicit midpoint discretization produces some undesirable affects.

This behavior for the explicit midpoint scheme is due to the fact that the discretization introduces computational modes. These are produced when the discretization yields different branches in the dispersion relation, which is precisely what takes place in the lower middle plot of Figure 4.1. In other words, there are modes produced by this scheme that yield a good approximation to the solution, but there are also modes giving poor approximations, and care must be taken to ensure that these modes are not stimulated during numerical applications for nonlinear problems (cf. [46]).

It seems from these plots that computational modes are only introduced when we use the explicit midpoint discretization in time. However, it becomes apparent from equation (4.22), that plotting \(K \Delta x\) as a function of \(\Omega \Delta t\) would also yield different branches of
Figure 4.2: For $\alpha = .01$, $\Delta t = \Delta x = .1$ and $\gamma = \varepsilon = 1$, exact (crosses) and numerical (solid) dispersion relations for a linear Boussinesq equation using implicit (IMP) and explicit (EMP) midpoint discretizations.

Figure 4.3: For $\alpha = .5$, $\Delta t = \Delta x = .1$ and $\gamma = \varepsilon = 1$, exact (crosses) and numerical (solid) dispersion relations for a linear Boussinesq equation using implicit (IMP) and explicit (EMP) midpoint discretizations.
the dispersion relation due to the space discretization, because \( \sin(K \Delta x) \) is still non-
invertible.

Since \( \alpha \) is in no way related to \( \Delta t \) and \( \Delta x \), it is interesting to know how the dispersion
relations change as the parameter \( \alpha \) changes. In Figures 4.2 and 4.3, we plot the numerical
and exact dispersion relations for \( \alpha > \Delta t = \Delta x = .1 \) and for \( \alpha < \Delta t = \Delta x = .1 \). For
\( \alpha = .01 \), in Figure 4.2, we find that as the equation approaches the Klein-Gordon equation
the difference between the Euler and Preissman scheme becomes greater, even though
they are still both close to the exact dispersion relation. We also find that the explicit
midpoint discretization still yields computational modes, but at least one of these is still
close to the exact dispersion relation. The mixed discretizations, on the other hand, give
poor approximations to the frequency for \( K \Delta x \) sufficiently large, as well as computational
modes. For \( \alpha = .5 \), in Figure 4.3, the dispersion relations become more 'flattened' and as
a result each plot shows a close correlation between the numerical and exact dispersion
relations. The difference between the Euler and Preissman schemes is much smaller in
this case, but similar to the case \( \alpha = .1 \) there are computational modes for the explicit
midpoint and mixed discretizations.

4.2.2 The Korteweg-de Vries Equation

For another example, where we find slightly different results, consider a linearization of
the KdV equation (3.11) written in the form

\[
    u_t + \lambda_1 u_x + \lambda_2 u_{xxx} = 0,
\]

such that \( \lambda_1 \) and \( \lambda_2 \) are constants. This equation can also be written as the linear
multi-symplectic PDE (4.2) for \( z = (\phi, u, v, w)^T \),

\[
    A = \begin{pmatrix}
        0 & 0 & 0 & 0 \\
        0 & 2\lambda_1 & 0 & -1 \\
        0 & 0 & \frac{1}{2\lambda_2} & 0 \\
        0 & -1 & 0 & 0
    \end{pmatrix},
\]

and \( K \) and \( L \) given in (3.13). Thus, finding the determinant of the matrix

\[
    (-i\omega K + ikL - A) = \begin{pmatrix}
        0 & -i\omega & 0 & ik \\
        i\omega & -2\lambda_1 & -ik & 1 \\
        0 & ik & \frac{1}{2\lambda_2} & 0 \\
        -ik & 1 & 0 & 0
    \end{pmatrix},
\]

implies the dispersion relation

\[
    D(\omega, k) = \omega k - \lambda_1 k^2 + \lambda_2 k^4 = 0,
\]
which is equivalent to \( \omega = W(k) \) for
\[
W(k) := \lambda_1 k - \lambda_2 k^3.
\]
Thus, for every wave number there is one frequency.

To find the numerical dispersion relation for the Euler scheme we must first find \( \tilde{A} \), which is given by
\[
\tilde{A} = \begin{pmatrix}
0 & -r & 0 & -s \\
-r & 2\lambda_1 & s & -1 \\
0 & s & \frac{1}{2\lambda_2} & 0 \\
-s & -1 & 0 & 0 \\
\end{pmatrix}
\]
Hence, the numerical dispersion relation can be written
\[
\Omega_{\Delta t} K_{\Delta x} - rs + \lambda_1 s^4 - \lambda_1 s^2 + 2\lambda_2 K_{\Delta x}^2 s^2 - \lambda_1 K_{\Delta x}^2 + \lambda_2 K_{\Delta x}^4 = 0,
\]
which is just
\[
0 = \frac{1}{\Delta t \Delta x} (\sin(\Delta t \Omega) \sin(\Delta x K) - (\cos(\Delta t \Omega) - 1)(\cos(\Delta x K) - 1)) - \frac{4 \lambda_1}{\Delta x^2} \sin^2 \left(\frac{\Delta x K}{2}\right) + \frac{16 \lambda_2}{\Delta x^4} \sin^4 \left(\frac{\Delta x K}{2}\right),
\]
(4.25)
where we have used the identities
\[ \Omega_{\Delta t}^2 + s^2 = \Omega_{\Delta t/2}^2 \quad \text{and} \quad K_{\Delta x}^2 + s^2 = K_{\Delta x/2}^2. \tag{4.26} \]
For the Preissman box scheme the dispersion relation [5] is given by
\[ D(\Omega, K) = \Omega K - \lambda_1 K^2 + \lambda_2 K^4 = 0, \]
which is equivalent to
\[ \frac{\Delta t \Omega}{2} = \tan^{-1} \left( \frac{\Delta t \lambda_1}{\Delta x} \tan \left( \frac{\Delta x K}{2} \right) - \frac{4 \Delta t \lambda_2}{\Delta x^4} \tan^3 \left( \frac{\Delta x K}{2} \right) \right), \quad -\pi \leq \Delta t \Omega \leq \pi. \]
Similarly, the numerical dispersion relation for the explicit midpoint scheme is given by
\[ D(\Omega_{\Delta t}, K_{\Delta x}) = \Omega_{\Delta t} K_{\Delta x} - \lambda_1 K_{\Delta x}^2 + \lambda_2 K_{\Delta x}^4 = 0, \]
which is just (4.23) for \( W(K_{\Delta x}) \) defined in (4.24).

These numerical dispersion relations have been plotted over the exact dispersion relation in Figure 4.4. For the Preissman and explicit midpoint schemes, they can be plotted directly using (4.21) and (4.23) along with (4.24), and we find results similar to the linear Boussinesq equation. There are no computational modes for the Preissman scheme, and the numerical and exact dispersion relations are very close together. The explicit midpoint scheme does have computational modes, just as we would expect. In the case of the Euler scheme, writing the numerical frequency as a function of the wave number is more complicated. However, using (4.25), one can numerically find \( \Omega \) for any given \( K \), and this gives an approximation to the numerical dispersion relation, which is plotted in Figure 4.4. We find in this case that the Euler scheme also admits computational modes, because for every wave number there are two frequencies.

It has become clear that if the identities (4.26) can be used to completely re-describe the numerical dispersion relation for the Euler scheme, which is the case for the linear Boussinesq equation, then there are no computational modes. We expect that this is the case for any problems described by first order field theory, such as the nonlinear wave equation, but it is possible that the Euler scheme admits computational modes for other types of problems. However, we also observe that the Preissman box scheme does not have computational modes for any problems based on the relation (4.14), because \( \tan(\Omega_{\Delta t}/2) \) is always invertible for \(-\pi/2 < \Omega_{\Delta t}/2 < \pi/2\). By the same argument, we expect the explicit midpoint scheme will always have computational modes for every problem of the form (4.2).
There are, in fact, two characteristics that we expect a multi-symplectic numerical method to have. The first involves the absence of numerically induced diffusion, which is implied by a discrete multi-symplectic conservation law and is also apparent from the real numerical dispersion relations. The second characteristic expected of a multi-symplectic method, which has not been included in the current definition of a multi-symplectic integrator, is the nonexistence of computational modes. For this reason we will not consider the explicit midpoint scheme to be a multi-symplectic integrator, and in some cases we will not consider the Euler box scheme to be a multi-symplectic integrator.
In this chapter, we begin to investigate the behavior of multi-symplectic numerical methods applied to nonlinear Hamiltonian PDEs by analyzing the effects of the scheme on the energy and momentum conservation laws. A most useful method for this investigation is backward error analysis, which uses simple Taylor series expansions to find the equation, known as the modified equation, that is solved to higher order by the numerical solution.

Backward error analysis was first introduced by Wilkinson [57] for the purpose of understanding the propagation of rounding errors in computational linear algebra. More recently, the ideas of backward error analysis have been applied to ordinary differential equations and have been found to be very useful for understanding the behavior of numerical schemes as well as solution error for Hamiltonian ODEs. Our aim is to extend these ideas to numerical methods for Hamiltonian PDEs, but we must first introduce the standard analysis for ODEs.

5.1 Backward Error Analysis for ODEs

Since the expansions used in backward error analysis are dependent upon the scheme used to discretize a differential equation, we must use a specific method in order to demonstrate how the analysis is done. However, the following can be done for any finite difference method, and the techniques are described by Hairer, Lubich and Wanner [28, Chapter 9] and Sanz-Serna and Calvo [52, pages 129-131]. Consider the ODE

$$\dot{y} = g(y(t)),$$  \hspace{1cm} (5.1)

and discretize using the first order explicit Euler method to get

$$y^{i+1} = y^i + \Delta t g(y^i).$$  \hspace{1cm} (5.2)
Computing the first two terms of the Taylor series expansion of \( y(t_i + \Delta t) \) about \( t_i \) gives
\[
y(t_{i+1}) = y(t_i) + \Delta t \dot{y}(t_i) + \frac{\Delta t^2}{2} \ddot{y}(t_i) + O(\Delta t^3),
\]
and using the original equation (5.1), this is equivalent to
\[
y(t_{i+1}) = y(t_i) + \Delta t g(y(t_i)) + \frac{\Delta t^2}{2} \partial_y g(y(t_i)) g(y(t_i)) + O(\Delta t^3),
\]
where \( \partial_y g(y(t_i)) \) denotes the Jacobian of \( g \).

Now, ignoring all terms of order \( \Delta t^3 \) and higher in the expansion (5.4) and comparing it to the Euler scheme (5.2), we write the modified differential equation
\[
y = \bar{g}(y) := g(y) - \frac{\Delta t}{2} \partial_y g(y) g(y).
\]
This is called a first modification because we have added one term to the original equation in order to define the modified equation. Using Taylor again for the modified equation, this implies
\[
y(t_{i+1}) = y(t_i) + \Delta t \bar{g}(y(t_i)) + \Delta t^2 \frac{\partial_y \bar{g}(y(t_i)) \bar{g}(y(t_i))}{2} + O(\Delta t^3)
\]
\[
= y(t_i) + \Delta t \left( g(y(t_i)) - \frac{\Delta t}{2} \partial_y g(y(t_i)) g(y(t_i)) \right)
\]
\[
+ \frac{\Delta t^2}{2} \partial_y g(y(t_i)) g(y(t_i)) + O(\Delta t^3)
\]
\[
= y(t_i) + \Delta t g(y(t_i)) + O(\Delta t^3),
\]
and this shows that the explicit Euler scheme (5.2) solves the modified equation (5.5) to second order accuracy. Clearly, the numerical method will solve the modified equation to higher accuracy if more terms from the Taylor series are used. In fact, the modified equation can be written more generally with
\[
\bar{g}_j(y) = g(y) + \Delta t g_1(y) + \Delta t^2 g_2(y) + \ldots + \Delta t^p g_p(y),
\]
such that the explicit Euler method applied to this equation becomes
\[
y^{i+1} = y^i + \Delta t \bar{g}(y^i) + O(\Delta t^{p+1}),
\]
and provided the limit as \( p \to \infty \) exists, we can find the differential equation that is exactly solved by the numerical method.

For the Hamiltonian system (1.5), we have
\[
g(y) = J^{-1} \nabla_y H(y).
For the sake of simplicity let $y = (p, q)^T$ and assume the Hamiltonian is the sum of kinetic and potential terms such that $H(p, q) = T(p) + V(q)$. Then the system of equations is written

$$
\dot{p} = -\nabla_q V(q), \quad \dot{q} = \nabla_p T(p),
$$

and discretizing with the symplectic Euler method yields

$$
\begin{align*}
p^{i+1} &= p^i - \Delta t \nabla_q V(q^{i+1}) \\
q^{i+1} &= q^i + \Delta t \nabla_p T(p^i)
\end{align*}
$$

(5.6)

which is clearly just implicit Euler for the first equation and explicit Euler for the second. Note that this method is still explicit when $q$ is updated before $p$, and it can be written in a similar form to the symplectic Euler method of Chapter 3. By shifting the indicies of the first equation, we get

$$
p^i = p^{i-1} - \Delta t \nabla_q V(q^i),
$$

and we find that the resulting discretization is equivalent to

$$
J_+ \delta^i y^i + J_- \delta^i y^i = \nabla_y H(y^i),
$$

(5.7)

for

$$
J_- = \begin{pmatrix} 0 & 0 \\ -1 & 0 \end{pmatrix} \quad \text{and} \quad J_+ = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix},
$$

which is a general form of the symplectic Euler scheme for the system (1.5).

Using the Taylor series expansions as in (5.4), we get

$$
p(t_i) = p(t_{i+1}) + \Delta t \nabla_q V(q(t_{i+1})) - \frac{\Delta t^2}{2} V_{qq}(q(t_{i+1})) \nabla_p T(p(t_{i+1})) + O(\Delta t^3),
$$

and

$$
q(t_{i+1}) = q(t_i) + \Delta t \nabla_p T(p(t_i)) - \frac{\Delta t^2}{2} T_{pp}(p(t_i)) \nabla_q V(q(t_i)) + O(\Delta t^3),
$$

which implies the modified equations

$$
\dot{p} = -\nabla_q V(q) - \frac{\Delta t}{2} V_{qq}(q) \nabla_p T(p) \\
\dot{q} = \nabla_p T(p) + \frac{\Delta t}{2} T_{pp}(p) \nabla_q V(q),
$$

neglecting higher order terms. This system of equations is, in fact, Hamiltonian and can be derived from the modified Hamiltonian function

$$
\tilde{H} = H + \frac{\Delta t}{2} \nabla_p T(p) \nabla_q V(q),
$$
or more generally
\[ \hat{H} = H + \frac{\Delta t}{2} \{ V, T \}, \]
where \( \{ , \cdot \} \) denotes the canonical bracket also known as the Poisson bracket, which is defined
\[ \{ F, G \} = \sum_{j=1}^{d} \left( \frac{\partial F}{\partial q_j} \frac{\partial G}{\partial p_j} - \frac{\partial F}{\partial p_j} \frac{\partial G}{\partial q_j} \right). \]

In general, the modified Hamiltonian for the symplectic Euler method can be written
\[ \hat{H}_\rho = H + \frac{\Delta t}{2} \{ V, T \} + \frac{\Delta t^2}{12} \left( \{ T, \{ T, V \} \} + \{ V, \{ V, T \} \} \right) + \ldots, \]
where \( \rho \) is the number of modifications and the expansion terms are found using the BCH formula (cf. [28, Chapter 9] and [52, Chapter 12]). A modified Hamiltonian system of equations can also be obtained for inseparable Hamiltonians, but we only consider separable Hamiltonians for this introduction to backward error analysis. More general results are found in the next two chapters.

Unfortunately, this series is only an asymptotic expansion and does not always converge as \( \rho \to \infty \). However, it can be shown that the series converges before it starts to diverge, and by using an optimal choice for \( \rho \), the difference in the flow maps of the modified equation and the numerical method is exponentially small. In order to make this point more clear, let \( \Phi_{\Delta t} \) be the flow map of some numerical method and let \( \Phi_{\Delta t, \rho} \) be the flow map of the truncated modified equation such that
\[ y^{i+1} = \Phi_{\Delta t}(y^i), \]
and
\[ y(t_{i+1}) = \Phi_{\Delta t, \rho}(y^i) = y^i + \Delta t g_1(y^i) + \Delta t^2 g_2(y^i) + \ldots + \Delta t^\rho g_\rho(y^i), \]
where the coefficients \( g_j \) are defined by the original differential equation and the numerical method. Then one trivially derives the difference
\[ \| \Phi_{\Delta t, \rho}(y^i) - \Phi_{\Delta t}(y^i) \| \leq C_\rho(y^i) \Delta t^{\rho+1}, \]
when the maps involved are smooth, and typically one cannot expect to get a better estimate than
\[ C_\rho(y^i) \leq c_1(c_2 \rho)^\rho \]
for real analytic functions \( y \). This upper bound is minimal when
\[ \rho = (c_2 \Delta t)^{-1}, \]
and this choice of $\rho$ yields the exponential estimate

$$\|\Phi_{\Delta t, \rho}(y^i) - \Phi_{\Delta t}(y^i)\| \leq c_1 \Delta t e^{-1/(c_1 \Delta t)},$$

which shows that the solution of modified equation is exponentially close to the numerical solution.

**The Kepler Problem**

To demonstrate this more explicitly, we return to the Kepler problem with the Hamiltonian (1.8). Splitting the Hamiltonian such that $H(p, q) = T(p) + V(q)$ with

$$T(p) = \frac{(p_1^2 + p_2^2)}{2} \quad \text{and} \quad V(q) = \frac{-1}{(q_1^2 + q_2^2)^{1/2}},$$

and discretizing with the symplectic Euler scheme (5.6) implies

$$\dot{H}_1 = \frac{1}{2} (p_1^2 + p_2^2) - \frac{1}{(q_1^2 + q_2^2)^{1/2}} + \frac{\Delta t}{2} \left( \frac{p_1 q_1 + p_2 q_2}{(q_1^2 + q_2^2)^{3/2}} \right),$$

and

$$\dot{H}_2 = \dot{H}_1 + \frac{\Delta t^2}{12} \left( \frac{p_1^2 + p_2^2}{(q_1^2 + q_2^2)^{3/2}} - \frac{6p_1 p_2 q_1 q_2}{(q_1^2 + q_2^2)^{5/2}} + \frac{q_1^2 + q_2^2}{(q_1^2 + q_2^2)^{3}} \right).$$

Then the corresponding differential equations are satisfied by the numerical solution to second and third order, respectively. This higher order convergence is easily recognized in the lower right hand plot of Figure 1.1 where we plot the Hamiltonians $H$ and $\dot{H}_1$ along the numerical solution.

### 5.2 Standard Backward Error for the Wave Equation

It is now possible to formally apply these ideas to PDEs, and we do so here in an example. For the semi-linear wave equation we can discretize in space in order to obtain a large system of Hamiltonian ODEs. Then we can perform a backward error analysis for this system, deriving a modified Hamiltonian system of ODEs, which in turn gives modified semi-discrete conservation laws.

Consider the Hamiltonian ODE (3.7) with periodic boundary conditions

$$u^0(t) = u^f(t), \quad v^0(t) = v^f(t),$$
and for the sake of simplicity let $\sigma(w) = w^2/2$, which yields the spatially discrete system of equations

$$v^n_i = \delta_x^2 u^n_i - f'(u^n_i), \quad u^n_i = v^n_i.$$  

Then re-scaling the velocities $v^n = \phi^n/\Delta x$ and discretizing in time by a symplectic Euler method yields the equations

$$\phi^{n+1}_i - \phi^n_i = \varepsilon(u^{n+1,i} - 2u^{n,i} + u^{n-1,i}) - \varepsilon\Delta x^2 f'(u^{n,i}),$$

$$u^{n+1,i} - u^{n,i} = \varepsilon\phi^{n+1,i},$$

with the periodic boundary conditions

$$u^0_i = u^J_i, \quad \phi^0_i = \phi^J_i,$$

where $\varepsilon = \Delta t/\Delta x$, which is equivalent to the equations (3.10) for this choice of $\sigma(w)$. Now if we let $y^i = (u^i, \phi^i)^T$, where $u^i$ and $\phi^i$ are defined to be the vectors containing $u^{n,i}$ and $\phi^{n,i}$ respectively for all $n$, then these equations define a map denoted by

$$y^{i+1} = \Psi_\varepsilon(y^i).$$

This symplectic map is $\varepsilon$-close to the identity. Thus, one can find an approximate Hamiltonian flow map according to the results in [6, 50]. The difference between these maps can be made exponentially small in terms of the parameter $\varepsilon$ which implies near conservation of total energy over exponentially long time intervals. The validity of this statement depends crucially upon letting $\varepsilon \to 0$, and this is obviously a much stronger requirement than the usual CFL stability condition $\varepsilon \leq 1$, which often implies excellent conservation of energy even for nonlinear problems.

On the other hand, one could formally apply standard backward error analysis to (3.7) based on the fact that the time discretization is a simple splitting method (cf. [28]). We refer to this formal method of backward error analysis as BEA-1. A spatial discretization of a Hamiltonian PDE, using a symplectic integrator, yields a Hamiltonian system of ODEs. Thus, BEA-1 can be used to formally derive the modified equations. Choose a splitting of the Hamiltonian (3.9) such that $H = T + V$ with

$$T = \frac{1}{2} \sum_{n=1}^J (v^n)^2 \quad \text{and} \quad V = \sum_{n=1}^J \frac{\delta_x^2 u^n}{2} + f(u^n).$$

This implies, for example,

$$\{V, T\} = \sum_{n=1}^J (v^n \delta_x^2 u^n - v^n f'(u^n)).$$

(5.11)
To get a second modification, one would need the additional terms
\[ \{T, \{T, V\}\} = \sum_{n=1}^{J} (v^n)^2 f''(u^n) + v^n \delta_x^2 v^n \]
and
\[ \{V, \{V, T\}\} = \sum_{n=1}^{J} ((\delta_x^2 u^n)^2 - (f'(u^n))^2). \]
Higher order modifications are found in a similar manner.

Upon first observation we see that the modification terms also depend on powers of \(1/\Delta x\), which are all hidden in finite difference approximations. Hence, we must make the following necessary but reasonable assumptions, in order to guarantee that the associated modified Hamiltonian (5.8) indeed depends only on \(\Delta t\).

A1: The solutions of the given PDE remain smooth over the time interval of interest.
A2: For \(\Delta x\) sufficiently small and \(\Delta t\) satisfying a CFL stability condition, all necessary finite difference approximations can be bounded by a constant that does not depend on \(\Delta x\) and \(\Delta t\) (discrete smoothness).

This implies, for example, the estimate
\[ |\delta_x^2 u^n| \leq \text{constant}, \]
which implies \(\{V, T\} = \mathcal{O}(1)\) and the first modification term is \(\mathcal{O}(\Delta t)\). Naturally, A1 and A2 imply that the \(j\)th modification term in (5.8) is indeed \(\mathcal{O}(\Delta t^j)\). Unfortunately, the rigorous proof of A2 is strongly problem dependent for nonlinear PDEs, and it is a proof beyond the scope of this thesis. Clearly, a CFL stability argument is a necessary condition to ensure that A2 holds, but it is not sufficient. Some nonlinear stability argument is needed. In a similar context, Oliver, Wulff, and West [47] assume the solutions of the semi-linear wave equation are analytic to prove results concerning the conservation of momentum for the modified equations. The assumptions A1 and A2 do allow a formal application of BEA-1 to these types of problems where the small parameter \(\varepsilon\) just becomes \(\Delta t\). Hence, we assume they hold throughout the text.

5.3 Modified Conservation Laws for the Wave Equation

After one finds a modified Hamiltonian, the modified equations of motion are easily obtained. With this, it is possible to find semi-discrete modified conservation laws of
energy and momentum, which are satisfied by the numerical solution to higher order.

If we can write
\[ T = \sum_{n=1}^{J} T^n \quad \text{and} \quad V = \sum_{n=1}^{J} V^n, \]
then, e.g.,
\[ \{V, T\} = \sum_{n=1}^{J} \left( \sum_{m=1}^{J} \{V^m, T^n\} \right), \]
and more generally a modified Hamiltonian, which is well defined due to the periodic boundary conditions, can be written
\[ \hat{H}_\rho = \sum_{n=1}^{J} \hat{E}_\rho^n, \quad (5.12) \]
where \( \hat{E}_\rho^n \) is a semi-discrete modified energy density. Using this energy density and the corresponding equations of motion, we can obtain the semi-discrete conservation laws of energy and momentum. This is the subject of

**Theorem 5.1** Given a Hamiltonian system of the form (3.8) with a Hamiltonian of the general form
\[ H = \sum_{n=1}^{J} E^n, \quad \text{where} \quad E^n = E(u^n, v^n, \delta_x^{-}u^n, \delta_x^{-}v^n, \delta_x^{2}u^n, \delta_x^{2}v^n, \ldots), \quad (5.13) \]
is a semi-discrete energy density, then there is a corresponding flux \( F^n \) satisfying a semi-discrete energy conservation law (3.4).

Proof of this result and a constructive method for finding \( F^n \) are found in Appendix B.

Notice that the energy density given in (5.13) is the most general form that is possible for the modified equation in this case because the modified Hamiltonian is found using (5.8), and the terms \( T \) and \( V \) only depend upon \( u^n, v^n \), and their discrete spatial derivatives. Furthermore, this result holds for finite \( J \) and for periodic boundary conditions on the interior of the given region, as well as for an infinite domain. Hence, the same could formally be done for a momentum conservation law, and this is now demonstrated for the nonlinear wave equation.

The spatially discrete energy density in (3.9) can be differentiated with respect to time yielding
\[ \partial_t E^n = v^n u^n_t + \sigma'((\delta_x^{-}u^n))\delta_x^{-}u^n_t + f'(u^n), \]
and using the equations (3.7) we get
\[ v^n u^n = u^n \delta^+ \sigma'(\delta^- u^n) - f'(u^n) u^n. \]

This implies
\[
\partial_t E^n = u^n \delta^+ \sigma'(\delta^- u^n) + \delta^- u^n \sigma'(\delta^- u^n)
\]
\[ = \frac{1}{\Delta_x} (u^n \sigma'(\delta^- u^{n+1}) - \sigma'(\delta^- u^n)) + \sigma'(\delta^- u^n) (u^n - u^{n-1})
\]
\[ = \delta^+ (v^{n-1} \sigma'(\delta^- u^n)).
\]

Therefore, (3.4) is satisfied with the obvious substitution
\[ F^n = -v^{n-1} \sigma'(\delta^- u^n). \]

This conservation law and the one obtained using Proposition 3.2 are equivalent.

Taking \( \sigma(u) = u^2/2 \) and using (5.8) with (5.11), we find the modified Hamiltonian for \( \rho = 1 \) is given by (5.12) with
\[
E_1^n = \frac{1}{2} \left( (v^n)^2 + (\delta^- u^n)^2 + \Delta t (v^n \delta^2 u^n - v^n f'(u^n)) \right) + f(u^n), \tag{5.14}
\]
and the modified Hamiltonian system of ODEs becomes
\[
-\frac{\Delta t}{2} \delta^\pm u^n - \Delta^2 \delta^\pm \psi^n = f'(u^n) - \frac{\Delta^4}{2} f''(u^n) v^n,
\]
\[
u^n - \frac{\Delta^4}{2} \delta^2 u^n = v^n - \frac{\Delta^4}{2} f'(u^n). \tag{5.15}
\]

In fact, this system can be rewritten in the form
\[
-\frac{\Delta t}{2} \delta^\pm w^n - \Delta^2 \delta^\pm \psi^n = f'(u^n) - \frac{\Delta^4}{2} f''(u^n) v^n,
\]
\[
u^n - \frac{\Delta^4}{2} \delta^2 u^n = v^n - \frac{\Delta^4}{2} f'(u^n),
\]
\[-\delta^- u^n = -w^n,
\]
\[
\frac{\Delta^4}{2} \delta^- u^n = \frac{\Delta^4}{2} \psi^n,
\]
\[
\frac{\Delta^4}{2} \delta^- v^n = \frac{\Delta^4}{2} \phi^n,
\]

which is the symplectic Euler discretization in space for the multi-symplectic PDE (1.14) with \( z = (u, v, w, \phi, \psi)^T \) and
\[
S = \frac{v^2 - w^2}{2} + f(u) - \frac{\Delta t}{2} (f'(u) v - \phi \psi),
\]
for \( w = \psi = u_x \) and \( \phi = v_x \).

Now, a higher order semi-discrete modified energy conservation law
\[
\partial_t E^\rho_n + \delta^\pm F^\rho_n = 0 \tag{5.16}
\]
can be found through this modified multi-symplectic PDE, using (3.5) to find $\bar{E}^n_t$ and $\bar{G}^n_t$. However, this can become quite cumbersome as higher order derivatives are involved for higher order modifications and the phase space of the modified multi-symplectic PDE becomes very large. Furthermore, finding a canonical way to get a modified multi-symplectic PDE using BEA-1 is not straightforward. Therefore, it is useful to use Theorem 5.1 and differentiate the energy density given in the modified Hamiltonian with respect to time. Then one can use the modified equations to derive a modified energy conservation law.

The modified energy density (5.14) can be differentiated with respect to $t$ to give

$$\partial_t \bar{E}^n_t = \delta_+ \left\{ \delta^-_+ u^n \left( v^{n-1} + \frac{\Delta t}{2} \left( \delta^2 u^{n-1} - f'(u^{n-1}) \right) \right) \\
+ \frac{\Delta t}{2} u^n \left( \delta^-_+ v^n + \frac{\Delta t}{2} \left( \delta^-_+ \delta^2 u^n - \delta^-_+ f'(u^n) \right) \right) \\
- \frac{\Delta t}{2} \delta^-_+ v^n \left( v^n + \frac{\Delta t}{2} \left( \delta^-_+ \delta^2 u^n - f'(u^n) \right) \right) \right\},$$

which is found according to the results of Appendix B. Then the system of equations (5.15) implies

$$\partial_t \bar{E}^n_t = \delta_+ \left( u^{n-1} \delta^-_+ u^n + \frac{\Delta t}{2} \left( v^n \delta^-_+ u^n - u_t^n \delta^-_+ v^n \right) \right),$$

which shows that (5.16) is satisfied for $\rho = 1$.

Similar results can be derived formally concerning a momentum conservation law. First notice that the time discrete semi-linear wave equation (1.17) can be written

$$w_l^t = \partial u^t + f'(u^t), \quad u^t = w^t,$$  \hspace{1cm} (5.17)

disregarding stability issues. This is, in fact, also a Hamiltonian system in space where the Hamiltonian is given by

$$H = \sum_{i=0}^{\mathcal{N}_d} G^i, \quad \text{for} \quad G^i = \frac{1}{2} \left( (w^i)^2 + (\delta^-_t u^i)^2 \right) - f(u^i).$$  \hspace{1cm} (5.18)

We can differentiate the momentum flux given by $G^i$ to get

$$\partial_t G^i = w^t w^i_t + \delta^-_t u^t \delta^-_t w^i - f'(u^i) w^i_t = \delta^-_t \left( w^{i-1} \delta^-_t u^i \right),$$

where we have used (5.17), and this is just the semi-discrete momentum conservation law (3.6).
Consider a splitting of (5.18) such that \( H = T + V \) for

\[
T = \frac{1}{2} \sum_{i=1}^{N_{ts}} (w^i)^2 \quad \text{and} \quad V = \sum_{i=1}^{N_{ts}} \frac{1}{2} (\delta_i u^i)^2 - f(u^i).
\]

Then the first modification can be found by evaluating

\[
\{V, T\} = \sum_{i=1}^{N_{ts}} (w^i \delta_i^2 u^i + w^i f'(u^i)),
\]

which implies the modified momentum flux

\[
\tilde{G}_1^i = \frac{1}{2} \left( (w^i)^2 + (\delta_i u^i)^2 + \Delta x (w^i \delta_i^2 u^i + w^i f'(u^i)) \right) - f(u^i).
\]  \hspace{1cm} (5.19)

Thus, the modified semi-discrete equations of motion are given by

\[
\begin{align*}
\dot{w}^i & = \delta_i^2 u^i + f'(u^i) - \frac{\Delta x}{2} (\delta_i^2 w^i + w^i f''(u^i)) \\
\dot{u}^i & = w^i + \Delta x \left( \delta_i^2 u^i + f'(u^i) \right),
\end{align*}
\]

where the modification terms now contain corrections in space, rather than in time.

Writing this system as a multi-symplectic PDE would now lead to a semi-discrete modified momentum conservation law, but this again becomes very cumbersome for higher order modifications, so it is better to use an analog of Theorem 5.1. Hence, the semi-discrete modified momentum conservation law is obtained by differentiating \( \tilde{G}_1^i \), given in (5.19), with respect to \( x \) to get

\[
\partial_x \tilde{G}_1^i = \delta_i^+ u^i \delta_i^- w^i + w^i w^i - f'(u^i)u^i \\
+ \frac{\Delta x}{2} \left( w^i \delta_i^2 w^i + w^i \delta_i^2 u^i + w^i f'(u^i) + w^i f''(u^i) u^i \right).
\]

Then, using the modified equations and substituting

\[
\begin{align*}
\dot{w}^i & = u^i \delta_i^2 u^i + f'(u^i)u^i \\
& - \frac{\Delta x}{2} \left( w^i \delta_i^2 w^i + w^i \delta_i^2 u^i + w^i f''(u^i) u^i + w^i f''(u^i) u^i \right),
\end{align*}
\]

gives

\[
\partial_x \tilde{G}_1^i = \delta_i^- u^i \delta_i^- w^i + u^i \delta_i^2 u^i + \frac{\Delta x}{2} \left( w^i \delta_i^2 w^i - u^i \delta_i^2 w^i \right) \\
= \delta_i^+ \left( u^{i-1} \delta_i^- w^i \right) + \frac{\Delta x}{2} \delta_i^+ \left( w^i \delta_i^- u^i - u^i \delta_i^- w^i \right),
\]

and this is a semi-discrete modified momentum conservation law.
It is important to notice that there are two sets of modified equations here, one leading to a semi-discrete energy conservation law and the other leading to a semi-discrete momentum conservation law, depending on how we do the backward error analysis. In fact, the modified equations here are only for the systems of ODEs that result from a semi-discretization of the PDE. The advantage is that we can obtain semi-discrete conservation laws. However, the price paid for these is an incomplete picture of the modified equations for the PDE, and as a result, we get an incomplete understanding of the numerical solution behavior. However, this problem is addressed in Chapter 7.

5.4 Fully Discrete Conservation Laws

Now that the theory behind these ideas has been made clear, it is important to know how this works in practice.

Conservation of total energy can be monitored numerically by checking that the Hamiltonian converges to a constant value as $\Delta t \rightarrow 0$. For the modified equations, conservation of total energy can be checked directly because the modification terms contain no time derivatives, meaning no additional discretization error is introduced. Thus, the discrete Hamiltonian $\tilde{H}_p^i$, which is just the Hamiltonian evaluated at the numerical solution that is obtained using the symplectic Euler scheme, satisfies

$$\tilde{H}_p^i = \tilde{H}_p(t_i) + \mathcal{O}(\Delta t^{p+1})$$

(5.20)

where $\tilde{H}_p(t_i)$, the semi-discrete Hamiltonian given in (5.12) evaluated along the exact solution of the modified equation, is constant.

In contrast, the local energy conservation law does contain time derivatives, and in order to maintain the order of convergence of the modified conservation law numerically, we must use an approximation of the appropriate order for each time derivative. In general, we can derive a semi-discrete energy conservation law (5.16) for any number of modifications $\rho$, and we know that this conservation law is satisfied along the numerical solution up to an $\mathcal{O}(\Delta t^{p+1})$ error. Hence, to check the order of convergence numerically, this conservation law must be discretized using no less than an $\mathcal{O}(\Delta t^{p+1})$ method. As we consider the fully discrete conservation law, let

$$\delta_{t}^{(p+1)} z^m = \partial_t z^m(t_i) + \mathcal{O}(\Delta t^{p+1})$$

be any discretization of order $\rho + 1$. Then, we have the residual

$$r_{\rho}^m = \delta_{t}^{(p+1)} \tilde{E}_{\rho}^m + \delta_{x}^+ \tilde{F}_{\rho}^m = \mathcal{O}(\Delta t^{p+1})$$

(5.21)
provided each term containing time derivatives in $\tilde{F}_\rho^n$ is also discretized to the appropriate order. These higher order discretizations can be achieved in many ways, but one of the simplest and most practical is to use symmetric differencing (cf. [21, page 16]). The same analysis holds for discrete momentum conservation laws, where the spatial derivatives in (3.6) with $\rho$ modifications must be approximated by a method of the appropriate order.

Again, this can be demonstrated with the nonlinear wave equation. Clearly, (5.20) is immediately satisfied for both the modified and unmodified equations. Moreover, (5.21) with $\rho = 0$ is satisfied for

$$E^{n,i} = \frac{1}{2} \left( (v^{n,i})^2 + (\delta_x u^{n,i})^2 \right) + f(u^{n,i})$$

and

$$\tilde{F}^{n,i} = - (\delta_t^{(1)} u^{n-1,i}) \delta_x u^{n,i},$$

and it is satisfied for $\rho = 1$ with

$$\tilde{E}^{n,i}_1 = \frac{1}{2} \left( (v^{n,i})^2 + (\delta_x u^{n,i})^2 + \Delta t \left( v^{n,i} \delta_x^2 u^{n,i} - v^{n,i} f'(u^{n,i}) \right) \right) + f(u^{n,i})$$

and

$$\tilde{F}^{n,i}_1 = -(\delta_t^{(2)} u^{n-1,i}) \delta_x u^{n,i} - \frac{\Delta t}{2} \left( v^{n,i} \delta_t^{(1)} \delta_x u^{n,i} - (\delta_t^{(1)} u^{n,i}) \delta_x u^{n,i} \right),$$

respectively, where one can use, for example, $\delta_t^{(1)} = \delta_t^+$ and $\delta_t^{(2)} = (\delta_t^+ + \delta_t^-)/2$. 
A Revised Modified Equations Approach

The standard method of backward error analysis, presented in the previous chapter, can only be applied to a system of ODEs. These ideas can formally be applied to PDEs by considering the lattice differential equations that result from a semi-discretization of the PDE. Then using these equations one can easily obtain modified conservation laws of energy and momentum, which in turn lead to a better understanding of the behavior of the numerical method.

Though this analysis proved to be useful, there are certain limitations, because the modified equations only represent a system of ODEs and as a result only give a partial description of the error induced by the scheme. We would like to suggest that one use the expansion (5.3) rather than (5.4) in order to find modified equations for PDEs. To make it clear how this should be done for multi-symplectic PDEs, we discuss Hamiltonian ODEs first. This chapter is devoted to the derivation of modified equations using this revised approach for ODEs, and to an analysis of their properties. Though this approach may be somewhat less practical for ODEs than the standard approach, it becomes more useful in the context of PDEs discussed in the next chapter.

6.1 The Symplectic Euler Method

Consider the Hamiltonian ODE (1.5) for \( y \in \mathbb{R}^n \), and the symplectic Euler scheme (5.7). Using the standard Taylor series expansion of a function \( y(t) \) given by (5.3), implies

\[
\frac{y(t_{i+1}) - y(t_i)}{\Delta t} = y(t_i) + \frac{\Delta t}{2} y_u(t_i) + \frac{\Delta t^2}{6} y_{uu}(t_i) + \ldots, \tag{6.1}
\]

and we also have

\[
\frac{y(t_2) - y(t_1)}{\Delta t} = y(t_1) - \frac{\Delta t}{2} y_u(t_1) + \frac{\Delta t^2}{6} y_{uu}(t_1) - \ldots. \tag{6.2}
\]

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Thus, we can replace $\delta_1^+ y^i$ and $\delta_1^- y^i$ in (5.7) by truncated versions of (6.1) and (6.2) respectively and obtain the modified system of equations

$$J_+ y_t + \frac{\Delta t}{2} J_+ y_{tt} + J_- y_t - \frac{\Delta t}{2} J_- y_{tt} = \nabla_y H(y),$$

which is equivalent to

$$J y_t + \frac{\Delta t}{2} P y_{tt} = \nabla_y H(y),$$

(6.3)

where

$$P = J_+ - J_-$$

is symmetric. This is a first modification because we have ignored all terms of order $\Delta t^2$ and higher. In general, we obtain the modified system of equations

$$J y_t + \frac{\Delta t}{2} P y_{tt} + \frac{\Delta t^2}{6} J y_{ttt} + \ldots + \frac{\Delta t^p}{(p+1)!} P J J y = \nabla_y H(y)$$

for $p$ modifications, which can also be stated in the compact form

$$\sum_{j=0}^{p} C_j(\Delta t) \Gamma_j \delta_t^{j+1} y = \nabla_y H(y),$$

(6.4)

where

$$\Gamma_j = \begin{cases} J, & \text{for } j \text{ even} \\ P, & \text{for } j \text{ odd} \end{cases}$$

and

$$C_j(\Delta t) = \frac{\Delta t^j}{(j+1)!}.$$  

Note that the equation obtained by differentiation of (1.5) with respect to $t$ can be used to recursively eliminate the higher order derivatives, and yield the modified equations obtained from BEA-1 in the previous chapter. However, this becomes increasingly more complicated for higher order modifications, and this revised approach gives a more natural way of writing the modified equation.

### 6.1.1 A Modified Hamiltonian System

This brings us to the first result concerning these new modified equations, where we use the following definition. Let the column vector $\vec{y} \in \mathbb{R}^{2d(p+1)}$ stand for

$$\vec{y} = \vec{y}_p = \begin{pmatrix} y^{(0)}, y^{(1)}, y^{(2)}, \ldots, y^{(p)} \end{pmatrix}^T$$

(6.6)

with $y^{(0)} = y$, and $y^{(j)} = \delta_t^j y$ for all $j = 1, 2, \ldots, p$. 

Lemma 6.1 The function $\bar{H}_p(y)$ defined by

$$\bar{H}_p = H + \sum_{k=1}^{p} C_k(\Delta t) \left( \sum_{j=1}^{[(k+1)/2]} h_j (-1)^j \left< y^{(j)}, \Gamma_k y^{(k+1-j)} \right> \right)$$

where $\lfloor \eta \rfloor$ is the greatest integer less than or equal to $\eta$ and

$$h_j := \begin{cases} \frac{1}{2}, & \text{for } j = (k + 1)/2 \\ 1, & \text{otherwise} \end{cases}$$

is a conserved quantity for the modified equation (6.4).

The following proof of this result exploits the fact that taking the inner product of $y_t$ with the modified equation (6.4) yields an equation of the form $d\bar{H}/dt = 0$. This idea is used several times in the remainder of the text, and we note the similarity of this approach to the proof of Theorem 2.1 in Hairer and Lubich [27].

Proof For $p = 1$ we have

$$\bar{H}_1 = H(y) - \frac{\Delta t}{4} \left< y_t, P y_t \right>,$$

and taking the derivative gives

$$\frac{d}{dt} \bar{H}_1 = \frac{d}{dt} H(y) - \frac{\Delta t}{4} \left( \left< y_u, P y_u \right> + \left< y_t, P y_{tt} \right> \right) = \left< y_t, \nabla_y H(y) \right> - \frac{\Delta t}{2} \left< y_t, P y_{tt} \right>.$$

Now take the inner product of the modified equations (6.3) with $y_t$ to obtain

$$0 = \left< y_t, J y_t \right> = \left< y_t, \nabla_y H(y) \right> - \frac{\Delta t}{2} \left< y_t, P y_{tt} \right>$$

and this shows that $\bar{H}_1$ is a conserved quantity for the equation (6.3).

Now assume the lemma is true for $p = m$. Then,

$$0 = \left< y_t, J y_t \right> = \left< y_t, \nabla_y H(y) \right> - \frac{\Delta t}{2} \left< y_t, P y_{tt} \right> - \ldots - \frac{\Delta t^m}{(m+1)!} \left< y_t, \Gamma_m \partial_t^m y \right>$$

and this shows that $\bar{H}_1$ is a conserved quantity for the equation (6.3).

Now assume the lemma is true for $p = m$. Then,

$$0 = \left< y_t, J y_t \right> = \left< y_t, \nabla_y H(y) \right> - \frac{\Delta t}{2} \left< y_t, P y_{tt} \right> - \ldots - \frac{\Delta t^m}{(m+1)!} \left< y_t, \Gamma_m \partial_t^m y \right>$$

and in order to prove the lemma by induction we must show that

$$\frac{d}{dt} \partial_m(y) = \frac{d}{dt} \sum_{j=1}^{[(m+2)/2]} h_j (-1)^j \left< y^{(j)}, \Gamma_{m+1} y^{(m+2-j)} \right> = -\left< y_t, \Gamma_{m+1} \partial_t^{m+2} y \right>$$

and

$$\frac{d}{dt} \bar{H}_m = \frac{d}{dt} H(y) + \sum_{k=1}^{m} C_k(\Delta t) \left( \sum_{j=1}^{[(k+1)/2]} h_j (-1)^j \left< y^{(j)}, \Gamma_k y^{(k+1-j)} \right> \right)$$

where $\lfloor \eta \rfloor$ is the greatest integer less than or equal to $\eta$ and

$$h_j := \begin{cases} \frac{1}{2}, & \text{for } j = (k + 1)/2 \\ 1, & \text{otherwise} \end{cases}$$

is a conserved quantity for the modified equation (6.4).
where the first equation here is recognized to be the definition of $\Theta_m$. Note that

$$\frac{d}{dt} \Theta_m(y) = \sum_{j=1}^{[(k+1)/2]} h_j (-1)^j \left( \langle y^{(j)}, \Gamma_{m+1} y^{(m+3-j)} \rangle + \langle y^{(j+1)}, \Gamma_{m+1} y^{(m+2-j)} \rangle \right).$$

Thus, we see that the first term of this sum is in fact

$$- \langle y^{(1)}, \Gamma_{m+1} y^{(m+3-1)} \rangle = - \langle y_t, \Gamma_{m+1} \partial_t y^{m+2} \rangle,$$

and all remaining terms cancel due to the alternating sign until we reach the final term.

If $m$ is odd, then $\Gamma_{m+1} = J$, $[(m + 2)/2] = (m + 1)/2$ and the final term is just

$$\langle y^{(m+1)}, J y^{(m+2-m+1)} \rangle = \langle y^{(m+1)}, J y^{(m+1)} \rangle = 0.$$

If $m$ is even, then $\Gamma_{m+1} = P$, $[(m + 2)/2] = (m + 2)/2$, and the final two terms are given by

$$\frac{1}{2} \left( \langle y^{(m+2)}, P y^{(m-3-m+2)} \rangle + \langle y^{(m+2+1)}, P y^{(m+2-m+2)} \rangle \right) = \langle y^{(m+2)}, P y^{(m+2)} \rangle,$$

because $h_j = 1/2$ in this case. Since this term cancels with the previous term, this completes the proof.

In fact, the modified equations (6.4) can be written as a Hamiltonian ODE over an enlarged phase space with Hamiltonian function $\tilde{H}_p$. This is the subject of the following theorem.

**Theorem 6.1** The modified system of equations (6.4) with $\rho$ modifications is equivalent to the Hamiltonian system

$$\ddot{\tilde{y}} = \nabla_{\tilde{y}} \tilde{H}_p(\tilde{y}),$$

(6.8)

for $\tilde{H}_p$ given in (6.7). Here, $\tilde{J}$ is the block matrix consisting of the matrix elements $J_{i,j}$, such that

$$J_{i,j} \in \mathbb{R}^{2d \times 2d} \quad \text{and} \quad \tilde{J} \in \mathbb{R}^{2d(\rho+1) \times 2d(\rho+1)}$$

where

$$J_{i,j} = \begin{cases} (-1)^i C_{i+j}(\Delta t) \Gamma_{i+j}, & 0 \leq i + j \leq \rho \\ 0, & i + j > \rho \end{cases}$$

for $i, j = 0, 1, 2, \ldots, \rho$.

Before proving this statement for any $\rho$, we first show that the modified equations can be written as a Hamiltonian system for a few specific cases, making the proof more straight
forward. In the case $p = 1$, the modified equation takes the form (6.3). Thus, defining $y^{(1)} = y$, this system is equivalent to

$$Jy_t + \frac{\Delta t}{2} Py^{(1)}_t = \nabla_y H(y).$$

But this is just (6.8) with

$$\bar{y} = \left( \begin{array}{c} y \\ y^{(1)} \end{array} \right) = \left( \begin{array}{c} y \\ y_t \end{array} \right), \quad \text{and} \quad \bar{J} = \left( \begin{array}{cc} J & \frac{\Delta t}{2} P \\ -\frac{\Delta t}{2} P & 0 \end{array} \right)$$

and

$$\bar{H}_1(\bar{y}) = H(y) - \frac{\Delta t}{4} \left\langle y^{(1)}, Py^{(1)} \right\rangle = H(y) - \frac{\Delta t}{4} \left\langle y_t, Py_t \right\rangle.$$

For $p = 2$, the modified equation becomes

$$Jy_t + \frac{\Delta t}{2} Py_{tt} + \frac{\Delta t^2}{6} Jy_{ttt} = \nabla_y H(y),$$

which can also be written

$$Jy_t + \frac{\Delta t}{2} Py^{(1)}_t + \frac{\Delta t^2}{6} Jy^{(2)}_t = \nabla_y H(y),$$

where we have set $y_t = y^{(1)}$ and $y_{tt} = y^{(2)}$. Using these new variables, we can also write

$$\frac{\Delta t^2}{6} Jy_t = \frac{\Delta t^2}{6} Jy^{(1)}$$

and

$$-\frac{\Delta t^2}{6} Jy^{(1)} = -\frac{\Delta t^2}{6} Jy^{(2)},$$

which also implies

$$\frac{\Delta t}{2} Py_t - \frac{\Delta t^2}{6} Jy^{(1)}_t = -\frac{\Delta t}{2} Py^{(1)}_t - \frac{\Delta t^2}{6} Jy^{(2)}.$$

Thus, equation (6.8) with $p = 2$ is satisfied for

$$\bar{y} = \left( \begin{array}{c} y \\ y^{(1)} \\ y^{(2)} \end{array} \right) \quad \text{and} \quad \bar{J} = \left( \begin{array}{ccc} J & \frac{\Delta t}{2} P & \frac{\Delta t^2}{8} J \\ -\frac{\Delta t}{2} P & -\frac{\Delta t^2}{6} J & 0 \\ \frac{\Delta t^2}{6} J & 0 & 0 \end{array} \right),$$

with

$$\bar{H}_2(\bar{y}) = H(y) - \frac{\Delta t}{4} \left\langle y^{(1)}, Py^{(1)} \right\rangle - \frac{\Delta t^2}{6} \left\langle y^{(1)}, Jy^{(2)} \right\rangle.$$

For $p = 3$, we find that the modified equation

$$Jy_t + \frac{\Delta t}{2} Py_{tt} + \frac{\Delta t^2}{6} Jy_{ttt} + \frac{\Delta t^3}{24} Py_{tttt} = \nabla_y H(y),$$

remains satisfied with

$$\bar{y} = \left( \begin{array}{c} y \\ y^{(1)} \\ y^{(2)} \\ y^{(3)} \end{array} \right) \quad \text{and} \quad \bar{J} = \left( \begin{array}{cccc} J & \frac{\Delta t}{2} P & \frac{\Delta t^2}{8} J & \frac{\Delta t^3}{24} P \\ -\frac{\Delta t}{2} P & -\frac{\Delta t^2}{6} J & 0 & 0 \\ \frac{\Delta t^2}{6} J & 0 & 0 & 0 \\ \frac{\Delta t^3}{24} P & 0 & 0 & 0 \end{array} \right).$$
A REVISED MODIFIED EQUATIONS APPROACH

is equivalent to (6.8) for

\[
\begin{pmatrix}
y \\
y^{(1)} \\
y^{(2)} \\
y^{(3)}
\end{pmatrix},
\]
and

\[
J = \begin{pmatrix}
J & \frac{\Delta t}{2} P & \frac{\Delta t}{6} J & \frac{\Delta t^2}{24} P \\
\frac{\Delta t}{2} P & \frac{\Delta t}{6} J & \frac{\Delta t^2}{24} P & 0 \\
\frac{\Delta t}{2} J & \frac{\Delta t}{6} P & \frac{\Delta t^2}{24} P & 0 \\
\frac{\Delta t}{2} J & \frac{\Delta t}{6} P & \frac{\Delta t^2}{24} P & 0
\end{pmatrix},
\]

using similar manipulations. Continuing in this manner, one finds a Hamiltonian formulation for the modified equation over an enlarged phase space, as stated in Theorem 6.1. Now we prove this result.

Proof First, consider \( \tilde{H}_p(\tilde{y}) \) given in Lemma 6.1. Denote the vector elements of the vector \( \nabla \tilde{y} \tilde{H}_p \) by \( \zeta \), so that

\[
\nabla \tilde{y} \tilde{H}_p(\tilde{y}) = \zeta = (\zeta_0, \zeta_1, \ldots, \zeta_p)^T,
\]

with

\[
\zeta_0 = \nabla \tilde{y} \tilde{H}(\tilde{y}^{(0)}) = \nabla \tilde{y} H(y),
\]

and

\[
\zeta_j = (-1)^j \sum_{k=j}^p C_k(\Delta t) \Gamma_{k} y^{(k+1-j)} \quad \text{for} \quad j = 1, 2, 3, \ldots, p.
\]

Therefore, since (6.8) implies \( \tilde{J} \tilde{y}_t = \zeta \), we have

\[
\sum_{k=0}^p J_{0,k} y_t^{(k)} = \sum_{k=0}^p C_k(\Delta t) \Gamma_{k} y_t^{(k)} = \nabla \tilde{y} H(y) = \zeta_0
\]

and

\[
\sum_{k=j}^p J_{j,k-j} y_t^{(k-j)} = (-1)^j \sum_{k=j}^p C_k(\Delta t) \Gamma_{k} y_t^{(k-j)} = (-1)^j \sum_{k=j}^p C_k(\Delta t) \Gamma_{k} y_t^{(k+1-j)} = \zeta_j
\]

for \( j = 1, 2, 3, \ldots p \). Then this can be used recursively to get the equations

\[
\partial_{y} y^{(k)} = y^{(k+1)} \quad \text{for} \quad k = 0, 1, 2, \ldots, p,
\]

which are then used successively to yield (6.4). This proves the theorem. \( \square \)

This modified Hamiltonian \( \tilde{H}_p \) is equivalent to the modified Hamiltonian derived using standard backward error analysis up to \( O(\Delta t^{p+1}) \). The only difference here is that
the modification terms contain explicit time derivatives, and this has implications for checking the conservation of total energy numerically. To make this clear, notice that the discrete modified Hamiltonian must satisfy
\[ \tilde{H}_p^i = \tilde{H}_p(t_i) + O(\Delta t^{p+1}), \]
similar to (5.20). Thus, it is a necessary condition that each time derivative of \( \tilde{E}_p \) is approximated to the appropriate order to ensure the desired order of convergence, and this is easily done using symmetric differencing (cf. [21, page 16]).

6.1.2 Lagrangian Formulation

The modified equations are also equivalent to an Euler-Lagrange equation which is derived from the appropriate Lagrangian. For example, if \( \rho = 1 \), the modified equations can be derived from the Lagrangian density
\[ \mathcal{L}_1 = \mathcal{L}_1(y, y_t) = H(y) + \frac{1}{2} (y_t, Jy) + \frac{\Delta t}{4} (y_t, Py_t). \]  
(6.9)
In this case, the associated Euler-Lagrange equation is given by
\[ 0 = \partial_t \partial_{y_t} \mathcal{L}_1 - \partial_y \mathcal{L}_1 = \partial_t \left( \frac{1}{2} Jy + \frac{\Delta t}{2} Py_t \right) + \frac{1}{2} Jy_t - \nabla_y \mathcal{H}(y), \]
but this is just (6.3). The following proposition shows that this can be done for any number of modifications.

**Proposition 6.1** The modified equation (6.4) is equivalent to the Euler-Lagrange equation associated with the modified Lagrangian density
\[ \tilde{L}_\rho = H(y) + \sum_{j=0}^{[\rho/2]} \left( \begin{array}{c} -1 \\ \frac{1}{2} \end{array} \right)^j \left( C_{2j}(\Delta t) \left( \partial_t^{j+1} y, J\partial_t^j y \right) + C_{2j+1}(\Delta t) \left( \partial_t^{j+1} y, P\partial_t^j y \right) \right). \]

**Proof** The Lagrangian density is of the form
\[ \tilde{L}_\rho = \tilde{L}_\rho \left( y, y_t, y_{tt}, \ldots, \partial_t^{[\rho/2]+1} y \right). \]
Hence, the associated Euler-Lagrange equation is given by
\[ 0 = \left( -\partial_y + \partial_t \partial_{y_t} - \partial_{tt} \partial_{y_{tt}} + \ldots + (-1)^{[\rho/2]} \partial_t^{[\rho/2]+1} \partial_{\partial_t^{[\rho/2]+1} y} \right) \tilde{L}_\rho \\
\sum_{k=0}^{[\rho/2]+1} (-1)^{k+1} \partial_t^k \partial_{\partial_t^k y} \tilde{L}_\rho. \]
Now substitute for $\bar{L}_p$, and consider individual terms. First, for terms containing $J$, notice that $\rho$ is even. Thus, for each $t$ we have

$$\frac{1}{2} \left( \partial_t^{k+1} \partial_t^{k+1} J \partial_t y - \partial_t^k \partial_t^k J \partial_t y \right) = \frac{1}{2} \left( \partial_t^{k+1} J \partial_t y + J \partial_t^k \partial_t^{k+1} J \right) = J \partial_t^{2k+1} y. \quad (6.10)$$

For the terms containing $P$ we get

$$\frac{1}{2} \left( (-1)^{k+1} (-1)^{k-1} \partial_t^k \partial_t^k \partial_t^k \partial_t^k J \partial_t^k y, P \partial_t^k y \right) = (-1)^{2k} \partial_t^k \partial_t^k P \partial_t^k y = P \partial_t^{2k} y,$$

and this implies

$$\nabla_y J(y) = \sum_{k=0}^{[\rho/2]} \left( C_{2k} (\Delta t) J \partial_t^{2k+1} y + C_{2k+1} (\Delta t) P \partial_t^{2k} y \right).$$

Since this is just (6.4), the proof is complete. \(\square\)

In order to relate this result back to the modified Hamiltonian formulation of the previous subsection, we note that (6.8) can be derived from a Lagrangian formulation with

$$\bar{L}_p = \frac{1}{2} \left( \dot{y}, \dot{y} \right) - \bar{H}_p(y).$$

Yet this is just $\bar{L}_p$ given in Proposition 6.1.

We strictly consider the ODE case here, but we can apply these ideas to Hamiltonian PDEs in the following way. First, we can use the semi-discretized Hamiltonian system of PDEs then apply the revised backward error analysis to the resulting system of ODEs to obtain a modified Hamiltonian system similar to (6.8). We refer to this method as BEA-2, and note that the results are similar to the application of BEA-1, as is demonstrated in the following examples.

6.1.3 Model Problems

To demonstrate this new modified equations approach for ODEs we return to the Kepler problem, and then consider an application of these ideas to the nonlinear wave equation.

The Kepler Problem

Discretizing the Kepler problem (1.7) with the symplectic Euler method (5.6) implies the modified equations

$$q_t = p - \frac{\Delta t}{2} q_{tt} - \frac{\Delta t^2}{6} q_{ttt},$$
Figure 6.1: Comparison of modified Hamiltonians such that $H_j$ and $H_{j,*}$ are obtained using BEA-1 and BEA-2, respectively.

Figure 6.2: Order of convergence in energy conservation where the unmodified (crosses) and modified Hamiltonians, obtained using BEA-1 (solid) and BEA-2 (dashed), are evaluated along the numerical solution.
and

\[ p_t = -\frac{q}{\|q\|_2^3} + \frac{\Delta t}{2} p_t - \frac{\Delta t^2}{6} \text{,} \]

where \( p, q \in \mathbb{R}^2 \). Taking the inner product of the first equation with \( p_t \) and of the second equation with \( q_t \) and taking the difference of the two resulting equations yields

\[ (p_t)^T p + \frac{(q_t)^T q}{\|q\|_2^3} - \frac{\Delta t}{2} (p_t)^T q_t + \frac{\Delta t^2}{6} ((q_t)^T p_{tt} - (p_t)^T q_{tt}) = 0. \]

But this is just

\[ \frac{d}{dt} \tilde{H}_2 = 0 \]

for

\[ \tilde{H}_2 = H - \frac{\Delta t}{2} (p_t)^T q_t + \frac{\Delta t^2}{6} (p_t)^T q_{tt}, \]

and comparing this to the modified Hamiltonian given in (5.10) we find that they are equivalent up to order \( \Delta t^3 \) terms. In the same way, truncating the expansion after one term yields

\[ \tilde{H}_1 = H - \frac{\Delta t}{2} (p_t)^T q_t \]

and we find that this is equivalent to (5.9) up to an \( O(\Delta t^2) \) correction.

Now we demonstrate a comparison of BEA-1 and BEA-2 for the Kepler problem. In Figure 6.1, we plot the modified Hamiltonians \( \tilde{H}_1 \) and \( \tilde{H}_2 \) along the numerical solution, along with the modified Hamiltonians given in (5.9) and (5.10). With each successive modification the Hamiltonian is preserved to higher accuracy, and BEA-2 yields similar results to that of BEA-1. Figure 6.2 plots the norm of the residual in total energy conservation for different values of \( \Delta t \), showing again that BEA-1 and BEA-2 are equivalent up to higher order terms. This plot also reveals that the modified Hamiltonians are satisfied by the numerical solution to second order for one modification and to third order for two modifications for both BEA-1 and BEA-2.

The Nonlinear Wave Equation

These ideas can be applied to PDEs in a more complete manner, but first we apply these results to the nonlinear wave equation and discuss conservation of total energy using the Hamiltonian ODEs that result from a semi-discretization. After applying BEA-2 to (3.7), the modified equations of motion become

\[ u_t^n + \frac{\Delta t}{2} u_{tt}^n = \delta_x \sigma'(\delta_x u^n) - f'(u^n), \quad u_t^n - \frac{\Delta t}{2} u_{tt}^n = v^n, \]

(6.11)
and this implies an associated modified energy density

$$E_1^n = \frac{(v^n)^2}{2} + \sigma(\delta^+ u^n) + f(u^n) + \frac{\Delta t}{2} u^n v^n.$$

To show that the total energy $\bar{H}_1$, related to $E_1^n$ through (5.12), is conserved, we take the time derivative of $E_1^n$. This yields

$$\partial_t \bar{E}_1^n = v^n v^n + \sigma'(\delta^+ u^n)\delta^+ u^n + f'(u^n)u^n + \frac{\Delta t}{2} (u^n v^n + u^n v^n).$$

Since the equations (6.11) imply

$$v^n v^n = u^n \left( \delta^+ \sigma'(\delta^+ u^n) - f'(u^n) - \frac{\Delta t}{2} u^n \right) - \frac{\Delta t}{2} u^n v^n,$$

we get

$$\partial_t \bar{E}_1^n = u^n \delta^+ \sigma'(\delta_2 u^n) - f'(u^n) = \delta^+ \left( u^n \sigma'(\delta^+ u^n) \right),$$

and the total energy is clearly conserved under the assumed periodic boundary conditions.

It becomes apparent from (6.12) that we have a semi-discrete local energy conservation law in this case because the backward error analysis has been performed on a system of ODEs rather than the original PDE. Similar results hold for a momentum conservation law.

### 6.2 The Implicit Midpoint Rule

Discretizing the Hamiltonian system (1.5) with the implicit midpoint rule yields

$$\mathbf{J} \delta^+_t y^i = \nabla y H \left( y^{i+1/2} \right),$$

where

$$y^{i+1/2} = \frac{1}{2} (y^{i+1} + y^i).$$

Then, using the Taylor series expansions

$$y(t_{i+1}) = y(t_{i+1/2}) + \frac{\Delta t}{2} y_t(t_{i+1/2}) + \frac{\Delta t^2}{2^{2^2}2^{1}} y_{tt}(t_{i+1/2}) + \frac{\Delta t^3}{2^{2^3}3!} y_{ttt}(t_{i+1/2}) + \ldots$$

and

$$y(t_i) = y(t_{i+1/2}) - \frac{\Delta t}{2} y_t(t_{i+1/2}) + \frac{\Delta t^2}{2^{2^2}2^{1}} y_{tt}(t_{i+1/2}) - \frac{\Delta t^3}{2^{2^3}3!} y_{ttt}(t_{i+1/2}) + \ldots$$

we find that

$$\frac{y(t_{i+1}) - y(t_i)}{\Delta t} = y_t(t_{i+1/2}) + \frac{\Delta t^2}{2^{2^2}2^{1}} y_{ttt}(t_{i+1/2}) + \frac{\Delta t^3}{2^{2^3}3!} y_{ttt}(t_{i+1/2}) + \ldots.$$
and
\[ \frac{y(t_{i+1}) + y(t_i)}{2} = y(t_{i+1/2}) + \frac{\Delta t^2}{2} y_{tt}(t_{i+1/2}) + \frac{\Delta t^4}{24} y_{tttt}(t_{i+1/2}) + \ldots. \]

Taking the expansions out to \( O(\Delta t^{2\rho}) \) and defining
\[ A_k(\tau) = \frac{\tau^{2k}}{(2k)!} \quad \text{and} \quad B_k(\tau) = \frac{\tau^{2k}}{(2k + 1)!} \]
for
\[ \tau = \frac{\Delta t}{2}, \]
yields
\[ \delta^i_t y^i = \sum_{j=0}^{\rho} B_j(\tau) \delta^{2j+1}_i y \]
and
\[ y^{i+1/2} = \sum_{j=0}^{\rho} A_j(\tau) \delta^{2j}_i y. \]

Then substituting these expansions into (6.13) implies the general modified equation
\[ J \left( \sum_{j=0}^{\rho} B_j(\tau) \delta^{2j+1}_i y \right) = \nabla_y H \left( \sum_{j=0}^{\rho} A_j(\tau) \delta^{2j}_i y \right), \]
which can also be written as a modified Hamiltonian system of the form (6.8).

To demonstrate this, take \( \rho = 1. \) Then the modified equation becomes
\[ J \left( y_t + \frac{\tau^2}{3!} y_{ttt} \right) = \nabla_y H \left( y + \frac{\tau^2}{2!} y_{tt} \right). \]

Introducing the variable
\[ \dot{y} = y + \frac{\tau^2}{2!} y_{tt}, \]
implies
\[ y_t + \frac{\tau^2}{3!} y_{ttt} = y_t + \left( \frac{\tau^2}{2!} - \frac{2\tau^2}{3!} \right) y_{ttt} = \dot{y}_t - \frac{2\tau^2}{3!} y_{ttt} = \dot{y}_t - \frac{2\tau^2}{3!} \dot{y}_{ttt} + O(\tau^4). \]

Thus, if we ignore all \( O(\tau^4) \) terms, the modified equation is written
\[ J\ddot{y}_t - \frac{2\tau^2}{3!} J\dot{y}_{ttt} = \nabla_y H (\dot{y}). \]

Now, let \( y^{(0)} = \ddot{y}, y^{(1)} = y_t^{(0)} \) and \( y^{(2)} = y^{(1)}. \) Then the modified equation can be stated as a first order ODE
\[ Jy_t^{(0)} - \frac{\tau^2}{3} Jy_{t}^{(2)} = \nabla_y H \left( y^{(0)} \right), \]
which is equivalent to the modified Hamiltonian system (6.8) with

\[ \ddot{y} = \begin{pmatrix} y^{(0)}(t) \\ y^{(1)}(t) \\ y^{(2)}(t) \end{pmatrix} \quad \text{and} \quad \ddot{J} = \begin{pmatrix} J & 0 & -\frac{\tau^2}{3}J \\ 0 & \frac{\tau^2}{3}J & 0 \\ -\frac{\tau^2}{3}J & 0 & 0 \end{pmatrix}, \]

with

\[ \ddot{H}_1(y) = H(y^{(0)}) + \frac{\tau^2}{3} \left(y^{(1)}(t), J y^{(2)}(t) \right). \]

In order to show that this can be done for any number of modifications, we need the following lemma.

**Lemma 6.2** The modified equation (6.17) can be stated

\[ J \left( \sum_{j=0}^{p} C_j(\tau) \partial_{t}^{2j+1} \dot{y} \right) = \nabla_y H(\dot{y}), \quad (6.18) \]

where

\[ \dot{y} = \sum_{j=0}^{p} A_j(\tau) \partial_{t}^{2j} y. \quad (6.19) \]

and the coefficients \( C_k \) are defined by the recursion

\[ C_k(\tau) = B_k(\tau) - \sum_{j=1}^{k} A_j(\tau) C_{k-j}(\tau) \quad (6.20) \]

for \( k = 0, 1, 2, \ldots, p. \)

**Proof** Assuming the definitions (6.19) and (6.20), the lemma can be proved by showing that

\[ \sum_{j=0}^{p} C_j(\tau) \partial_{t}^{2j+1} \dot{y} = \sum_{j=0}^{p} B_j(\tau) \partial_{t}^{2j+1} y. \quad (6.21) \]

First, notice that

\[ \sum_{j=0}^{p} C_j(\tau) \partial_{t}^{2j+1} \dot{y} = \sum_{j=0}^{p} C_j(\tau) \partial_{t}^{2j+1} \left( \sum_{k=0}^{p} A_k(\tau) \partial_{t}^{2k} y \right) = \sum_{j=0}^{p} \sum_{k=0}^{p} C_j(\tau) A_k(\tau) \partial_{t}^{2(j+k)+1} y. \]

Now, if we ignore all \( O(\tau^{2(p+1)}) \) terms, then we can require \( j + k \leq p, \) and this implies

\[ \sum_{j=0}^{p} \sum_{k=0}^{p} C_j(\tau) A_k(\tau) \partial_{t}^{2(j+k)+1} y = \sum_{j=0}^{p} \sum_{k=0}^{j} \sum_{i=0}^{j} A_i(\tau) C_{j-i}(\tau) \partial_{t}^{2i+1} y. \]
By the definition (6.20), we have

\[ B_k(\tau) = \sum_{j=0}^{k} A_j(\tau) C_{k-j}(\tau) \]

because \( A_0 = 1 \) and \( C_0 = 1 \). Therefore, equation (6.21) holds, and making the appropriate substitutions into (6.17) yields the desired result. □

This result leads to the following theorem, which enables one to write the modified ODE (6.17) as a Hamiltonian system with an enlarged phase space.

**Theorem 6.2** The system of modified equations (6.17) is equivalent to the Hamiltonian system (6.8) where

\[ \tilde{\mathbf{y}} = \tilde{\mathbf{y}}_\rho = \left( y^{(0)}, y^{(1)}, y^{(2)}, \ldots, y^{(2\rho)} \right)^T \]

and

\[ \tilde{H}_\rho(\tilde{\mathbf{y}}) = H(\mathbf{y}^{(0)}) + \sum_{k=1}^{\rho} C_k(\tau) \left( \sum_{j=1}^{\rho} (-1)^j \left( y^{(j)}, \mathbf{J}y^{(2k+1-j)} \right) \right) \]

is a conserved quantity for (6.17). The block matrix \( \mathbf{J} \) consists of the matrix elements \( \mathbf{J}_{i,j} \), such that

\[ \mathbf{J}_{i,j} \in \mathbb{R}^{2d \times 2d} \quad \text{and} \quad \mathbf{J} \in \mathbb{R}^{2d(2\rho+1) \times 2d(2\rho+1)} \]

where

\[ \mathbf{J}_{i,j} = \begin{cases} (-1)^i C_k(\tau)\mathbf{J}, & i + j = 2k, \ k = 0, 1, 2, \ldots, \rho \\ 0, & \text{otherwise} \end{cases} \]

for \( i, j = 0, 1, 2, \ldots, \rho \).

**Proof** Using Lemma 6.2, we can write the system of modified equations (6.17) as (6.18). Now notice the similarity of this modified equation with (6.4). In fact, setting \( \mathbf{P} = 0 \) and substituting the coefficients \( C_j(\Delta t) \) for \( C_j(\tau) \) in (6.4) yields (6.18). Therefore, the proof of this result is the same as the proof of Theorem 6.1 with different coefficients and \( \mathbf{P} = 0 \). □

To demonstrate this further, consider the modified equation with \( \rho = 2 \), given by

\[ \mathbf{J} \left( \frac{\tau^2}{3!} \dddot{\mathbf{y}} + \frac{\tau^4}{5!} \dddot{\dddot{\mathbf{y}}} \right) = \nabla_y H \left( y + \frac{\tau^2}{2!} \dddot{\mathbf{y}} + \frac{\tau^4}{4!} \dddot{\dddot{\mathbf{y}}} \right). \]

Setting

\[ \mathbf{\tilde{y}} = y + \frac{\tau^2}{2!} \dddot{\mathbf{y}} + \frac{\tau^4}{4!} \dddot{\dddot{\mathbf{y}}}, \quad (6.22) \]
we find that
\[ y_t + \frac{\tau^2}{3!} y_{\mu\mu} + \frac{\tau^4}{5!} y_{\mu\mu\mu\mu} = y_t + \left(\frac{\tau^2}{2!} - \frac{2\tau^2}{3!}\right) y_{\mu\mu} + \left(\frac{\tau^4}{4!} - \frac{4\tau^4}{5!}\right) y_{\mu\mu\mu\mu} \]
\[ = \dot{y}_t - \frac{2\tau^2}{3!} y_{\mu\mu} - \frac{4\tau^4}{5!} y_{\mu\mu\mu\mu}. \]

Then, using (6.22), we get
\[ \frac{2\tau^2}{3!} y_{\mu\mu} = \frac{2\tau^2}{3!} \dot{y}_{\mu\mu} - \frac{\tau^4}{3!} y_{\mu\mu\mu\mu} + O(\tau^6), \]
which implies
\[ y_t + \frac{\tau^2}{3!} y_{\mu\mu} + \frac{\tau^4}{5!} y_{\mu\mu\mu\mu} = \dot{y}_t - \frac{2\tau^2}{3!} \dot{y}_{\mu\mu} + \left(\frac{\tau^4}{3!} - \frac{4\tau^4}{5!}\right) y_{\mu\mu\mu\mu} \]
\[ = \dot{y}_t - \frac{\tau^2}{3} \dot{y}_{\mu\mu} + \frac{2\tau^4}{15} y_{\mu\mu\mu\mu}, \]
where we have ignored all \( O(\tau^6) \) terms. Thus, the modified equation can be written
\[ \mathbf{J} \left( \dot{y}_t - \frac{\tau^2}{3} \dot{y}_{\mu\mu} + \frac{2\tau^4}{15} y_{\mu\mu\mu\mu} \right) = \nabla_\mathbf{y} H(\mathbf{y}). \]

Now this can be stated as a Hamiltonian system of the form (6.8) for
\[ \tilde{y} = \begin{pmatrix} y^{(0)} \\ y^{(1)} \\ y^{(2)} \\ y^{(3)} \\ y^{(4)} \end{pmatrix} \quad \text{and} \quad \tilde{\mathbf{J}} = \begin{pmatrix} \mathbf{J} & 0 & -\frac{\tau^2}{3} \mathbf{J} & 0 & \frac{2\tau^4}{15} \mathbf{J} \\ 0 & \frac{\tau^2}{3} \mathbf{J} & 0 & -\frac{2\tau^4}{15} \mathbf{J} & 0 \\ -\frac{\tau^2}{3} \mathbf{J} & 0 & \frac{2\tau^4}{15} \mathbf{J} & 0 & 0 \\ 0 & -\frac{2\tau^4}{15} \mathbf{J} & 0 & 0 & 0 \\ \frac{2\tau^4}{15} \mathbf{J} & 0 & 0 & 0 & 0 \end{pmatrix}, \]
with
\[ \tilde{H}(\tilde{y}) = H \left( y^{(0)} \right) + \frac{\tau^2}{3} \left( \langle y^{(1)}, \mathbf{J} y^{(3)} \rangle - \frac{2\tau^4}{15} \left( \langle y^{(1)}, \mathbf{J} y^{(4)} \rangle - \langle y^{(2)}, \mathbf{J} y^{(3)} \rangle \right) \right), \]
by setting \( y^{(0)} = \tilde{y} \).
In the previous chapter, we have developed a method for finding modified equations for symplectic discretizations of systems of Hamiltonian ODEs. This method is equivalent to the standard method of backward error analysis commonly used for Hamiltonian ODEs, and it was shown that the modified equations are also Hamiltonian.

Now these ideas can readily be applied to multi-symplectic PDEs. Ideally, one would like to obtain a modified PDE which fully describes the numerical method and has correction terms for both the time discretization and the space discretization, i.e. the modification terms contain powers of both $\Delta t$ and $\Delta x$. This is achieved through an application of this revised approach in both space and time, and we call this BEA-3.

### 7.1 The Euler Box Scheme

Now consider the numerical method (3.1). Using the Taylor series expansions (6.1)-(6.2), one can derive the modified PDE

$$K_z t + \frac{\Delta t}{2} (K_+ - K_-) z_{tt} + L z_z + \frac{\Delta x}{2} (L_+ - L_-) z_{xx} = \nabla_z S(z),$$

(7.1)

which can also be written as a multi-symplectic PDE. First, using the symmetric matrices $M$ and $N$ defined in (4.8) and setting $z^{(t,1)} = z_t$ and $z^{(x,1)} = z_x$ yields

$$K z_t + \frac{\Delta t}{2} M z^{(t,1)} + L z_z + \frac{\Delta x}{2} N z^{(x,1)} = \nabla_z S(z).$$

Then this is equivalent to

$$\ddot{\bar{z}} + \bar{L} \dot{z}_x = \nabla_{\bar{z}} S_{\bar{z}}(\bar{z}),$$

(7.2)

where $\bar{z} = (z, z^{(t,1)}, z^{(x,1)})^T$,

$$\bar{K} = \begin{pmatrix} K & \frac{\Delta t}{2} M & 0 \\ -\frac{\Delta t}{2} M & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad \bar{L} = \begin{pmatrix} L & 0 & \frac{\Delta x}{2} N \\ 0 & 0 & 0 \\ -\frac{\Delta x}{2} N & 0 & 0 \end{pmatrix},$$

(7.3)
and
\[ \tilde{S}_1(\tilde{z}) = S - \frac{\Delta t}{4} \left( z^{(t,1)} M z^{(t,1)} - \frac{\Delta x}{4} \left( z^{(x,1)} N z^{(x,1)} \right) \right). \]  
(7.4)

Higher order modifications are found in the same way. For \( p = 2 \) the modified equation is written
\[
K z_t + \frac{\Delta t}{2} M z_{tt} + \frac{\Delta t^2}{6} K z_{ttt} + L z_x + \frac{\Delta x}{2} N z_{xxx} + \frac{\Delta x^2}{6} L z_{xxx} = \nabla_z S(z).
\]

Then setting \( z^{(\eta,1)} = z_\eta \) and \( z^{(\eta,2)} = z_m \) for \( \eta = x, t \), this is equivalent to (7.2) for \( \tilde{z} = (z, z^{(t,1)}, z^{(t,2)}, z^{(x,1)}, z^{(x,2)})^T \),

\[
\tilde{K} = \begin{pmatrix}
K & \frac{\Delta t}{2} M & \frac{\Delta t^2}{6} K & 0 & 0 \\
-\frac{\Delta t}{2} M & -\frac{\Delta t^2}{6} K & 0 & 0 & 0 \\
\frac{\Delta t^2}{6} K & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 
\end{pmatrix},
\]

\[
\tilde{L} = \begin{pmatrix}
L & 0 & 0 & \frac{\Delta x}{2} N & \frac{\Delta x^2}{6} L \\
0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 \\
-\frac{\Delta x}{2} N & 0 & 0 & -\frac{\Delta x^2}{6} L & 0 \\
\frac{\Delta x^2}{6} L & 0 & 0 & 0 & 0 
\end{pmatrix},
\]

and
\[
\tilde{S}_2(\tilde{z}) = S - \frac{\Delta t}{4} \left( z^{(t,1)} M z^{(t,1)} - \frac{\Delta x}{4} \left( z^{(x,1)} N z^{(x,1)} \right) \right) - \frac{\Delta t^2}{6} \left( z^{(t,1)} K z^{(t,2)} - \frac{\Delta x^2}{6} z^{(x,1)} L z^{(x,2)} \right).
\]

A general formulation for \( \rho \) modifications is constructed in the proof of the following theorem.

**Theorem 7.1** For any number of modifications \( \rho \), the modified equation
\[
\nabla_z S(z) = \sum_{k=0}^{\rho} \left( C_k(\Delta t) \Gamma_k \partial_t^{\rho+1} z + C_k(\Delta x) \Lambda_k \partial_x^{\rho+1} z \right)
\]
(7.5)

for \( C_k(\cdot) \) defined in (6.5) and for
\[
\Gamma_\rho = \begin{cases} K, & \forall \rho \text{ even} \\ M, & \forall \rho \text{ odd} \end{cases} \quad \text{and} \quad \Lambda_\rho = \begin{cases} L, & \forall \rho \text{ even} \\ N, & \forall \rho \text{ odd} \end{cases},
\]
can be written as the multi-symplectic PDE (7.2), and the terms \( \tilde{S}, \tilde{z}, \tilde{K} \) and \( \tilde{L} \) are defined in the proof.
Proof As an easy extension of the proof for Theorem 6.1, let

\[ \bar{S}_\rho(\bar{z}) = S(z) + \sum_{k=1}^{\rho} C_k(\Delta t) \left( \sum_{j=1}^{[(k+1)/2]} h_j (-1)^j \left( \xi^{(t,j)} \Gamma_k x^{(t,k+1-j)} \right) \right) \]

\[ + \sum_{k=1}^{\rho} C_k(\Delta x) \left( \sum_{j=1}^{[(k+1)/2]} h_j (-1)^j \left( \xi^{(x,j)} \Lambda_k z^{(x,k+1-j)} \right) \right), \]

with

\[ \bar{z} = \left( z, z^{(t,1)}, z^{(t,2)}, \ldots, z^{(t,p)}, z^{(x,1)}, z^{(x,2)}, \ldots, z^{(x,p)} \right)^T, \] \hspace{1cm} (7.6)

Then defining \( \zeta \) such that

\[ \nabla_x \bar{S} = \zeta = (\zeta_0, \zeta_1^x, \zeta_2^x, \ldots, \zeta_p^x, \zeta_1^z, \zeta_2^z, \ldots, \zeta_p^z)^T, \]

implies

\[ \zeta_0 = \nabla_x S(z), \quad \zeta_j^x = (-1)^j \sum_{k=1}^{\rho} C_k(\Delta t) \Gamma_k x^{(t,k+1-j)} \]

and

\[ \zeta_j^z = (-1)^j \sum_{k=1}^{\rho} C_k(\Delta x) \Lambda_k z^{(x,k+1-j)} \]

for \( j = 1, 2, 3, \ldots, p \). Now, let \( K_{i,j} \) and \( L_{i,j} \) denote the matrix elements of the block matrices \( \bar{K} \) and \( \bar{L} \) respectively, such that

\[ K_{i,j} \in \mathbb{R}^{d \times d} \quad \text{and} \quad \bar{K} \in \mathbb{R}^{d(2\rho+1) \times d(2\rho+1)} \]

where

\[ K_{i,j} = \begin{cases} (-1)^i C_{i+j}(\Delta t) \Gamma_{i+j}, & i, j = 0, 1, 2, \ldots, \rho \text{ and } i + j \leq \rho \\ 0, & \text{otherwise} \end{cases} \]

and

\[ L_{i,j} \in \mathbb{R}^{d \times d} \quad \text{and} \quad \bar{L} \in \mathbb{R}^{d(2\rho+1) \times d(2\rho+1)} \]

where

\[ L_{i,j} = \begin{cases} (-1)^i C_{i+k}(\Delta x) \Lambda_{i+k}, & i = \rho + k, \ j = \rho + k \text{ and } i + j \leq 3\rho \\ 0, & \text{otherwise} \end{cases} \]

for \( k, k_j = 1, 2, \ldots, \rho \) with the requirements \( k_i = 0 \) for \( i = 0 \) and \( k_j = 0 \) for \( j = 0 \). Considering the first row of these matrices (the terms with \( j = 0 \)) and using \( \bar{K} \bar{z}_t + \bar{L} \bar{z}_x = \zeta \) implies

\[ \zeta_0 = \nabla_x S(z) = K_{0,1} \bar{z}_t + L_{0,1} \bar{z}_x + \sum_{k=1}^{\rho} \left( K_{0,k} \bar{z}_t^{(t,k)} + L_{0,k+\rho} \bar{z}_x^{(x,k)} \right) \]

\[ = \sum_{k=0}^{\rho} \left( C_k(\Delta t) \Gamma_k x^{(t,k)} + C_k(\Delta x) \Lambda_k z^{(x,k)} \right) \]
such that \( z(t,0) = z(x,0) = z \). Then the remaining equations containing \( t \) derivatives are

\[
\sum_{k=j}^{p} K_{j,k,j} z^{(t,k-j)} = (-1)^j \sum_{k=j}^{p} C_k (\Delta t) \Gamma_k z^{(t,k-j)} = (-1)^j \sum_{k=j}^{p} C_k (\Delta t) \Gamma_k z^{(t,k+1-j)} = \zeta_j
\]

for \( j = 1, 2, \ldots, p \), which implies

\[
\partial_t z^{(t,k)} = z^{(t,k+1)}, \quad k = 0, 1, 2, \ldots, p. \tag{7.7}
\]

We also have the \( x \) derivative equations

\[
L_{j,0} z_x + \sum_{k=j}^{2p-1} L_{j,k,j} z^{(x,k-j+1)} = (-1)^{j-p} C_{j-p} \Delta_{j-p} z_x + (-1)^{j-p} \sum_{k=j}^{2p-1} C_{k-p+1} (\Delta x) \Delta_{k-p+1} z^{(x,k-j+1)}
\]

for \( j = p + 1, p + 2, \ldots, 2p \). Then, by shifting this sum such that \( j = 1, 2, \ldots, p \) we get

\[
(-1)^j \sum_{k=j}^{p} C_k (\Delta x) \Delta_{k} z^{(x,k-j)} = (-1)^j \sum_{k=j}^{p} C_k (\Delta x) \Delta_{k} z^{(x,k-j+1)} = \zeta_j
\]

which implies

\[
\partial_x z^{(x,k)} = z^{(x,k+1)}, \quad k = 0, 1, 2, \ldots, p. \tag{7.8}
\]

Then the relations (7.7) and (7.8) are used recursively to obtain (7.5), completing the proof. \( \square \)

Since this theorem is such an easy extension of Theorem 6.1 for ODEs, it becomes clear that similar results are easily extended to problems with two and three space dimensions.

Notice, for the linear PDE (4.2), the modified equation takes the form

\[
\left( -i \omega K - \frac{\Delta t}{2} \omega^2 M + \frac{\Delta t^2}{6} i \omega^3 K + \cdots + i \hat{k} L - \frac{\Delta x}{2} \hat{k}^2 N - \frac{\Delta x^2}{6} i \hat{k}^3 L + \cdots \right) \bar{a} = A \bar{a},
\]

where we have substituted the solution

\[
z(x,t) = R \left\{ \bar{a} e^{i(\hat{k}x - \omega t)} \right\}, \tag{7.9}
\]

and if the series are not truncated we have simply

\[
A \bar{a} = -\frac{1}{\Delta t} \sum_{j=0}^{\infty} (-1)^j (\Delta t \omega)^{2j+1} \frac{}{(2j+1)!} K \bar{a} + \frac{1}{\Delta x} \sum_{j=0}^{\infty} (-1)^j (\Delta x \hat{k})^{2j+1} \frac{}{(2j+1)!} L \bar{a} + \frac{1}{\Delta t} \sum_{j=1}^{\infty} (-1)^j (\Delta t \omega)^{2j} \frac{}{(2j)!} M \bar{a} + \frac{1}{\Delta x} \sum_{j=1}^{\infty} (-1)^j (\Delta x \hat{k})^{2j} \frac{}{(2j)!} N \bar{a}.
\]
Since
\[
\sin \theta = \sum_{j=0}^{\infty} (-1)^j \frac{\beta^{2j+1}}{(2j+1)!}
\] (7.10)
and
\[
\cos \theta = \sum_{j=0}^{\infty} (-1)^j \frac{\beta^{2j}}{(2j)!},
\]
this is just (4.9) with \(\bar{\omega} = \Omega\) and \(\bar{k} = K\).

Remark: The modified equations approach of Chapter 5 is more useful in the context of ODEs because higher derivatives of the variable \(y\) can be expressed in terms of higher derivatives of the right hand side and visa versa. Based on the analyticity of the solution, this enables one to derive exponential estimates which relate the numerical solution to the exact solution of the modified equations. In the PDE context it is no longer possible to define the modification terms such that all higher derivatives in space and time of the solution are simultaneously eliminated. As a result, estimates relating the numerical solution to the exact solution of the modified equation are much harder to achieve, and this is, in fact, still an open problem.

Now we state the following result of Theorem 7.1.

Corollary 7.1 The modified PDE (7.5) satisfies local energy and momentum conservation laws.

Proof Clearly, this result can be obtained directly from the modified multi-symplectic formulation (7.2) in the enlarged phase space. For example, the energy conservation law is of the form
\[
\partial_t \bar{E}_p + \partial_x \bar{F}_p = 0,
\]
where
\[
\bar{E}_p = \bar{S}_p(\bar{z}) + \frac{1}{2} \langle \bar{z}, \bar{L}\bar{z} \rangle \quad \text{and} \quad \bar{F}_p = \frac{1}{2} \langle \bar{z}, \bar{L}\bar{z} \rangle
\]
are derived from (7.2) using the results of subsection 2.2, and the same can be done to get a modified momentum conservation law.

However, the result also holds in the original phase space. Taking the inner product of the modified equation (7.5) with \(z_t\) gives
\[
\partial_t S(z) = \sum_{k=0}^{p} \left( C_k(\Delta t) \langle z_t, \Gamma_k \sigma_k^h z \rangle + C_k(\Delta t) \langle z_t, \Lambda_k \sigma_k^h z \rangle \right).
\]
Then writing the terms of this sum as derivatives with respect to \( x \) or \( t \) and rearranging terms yields the desired result. For \( k = 2m - 1 \) for \( m = 1, 2, \ldots \), we have

\[
\langle z_t, \Gamma_k \partial_x^{k+1} z \rangle = \langle z_t, M \partial_x^{2m} z \rangle
\]

\[
= \partial_t \left( \frac{(-1)^{m+1}}{2} \langle \partial_x^m z, M \partial_x^m z \rangle + \sum_{j=1}^{m-1} (-1)^j \langle \partial_x^j z, M \partial_x^{2m-j} z \rangle \right)
\]

and

\[
\langle z_t, \Lambda_k \partial_x^{k+1} z \rangle = \langle z_t, N \partial_x^{2m} z \rangle
\]

\[
= \partial_x \left( \sum_{j=0}^{m-1} (-1)^j \langle \partial_x^{j+1} z, N \partial_x^{2m-1-j} z \rangle \right) + \frac{(-1)^{m+1}}{2} \partial_t \langle \partial_x^m z, N \partial_x^m z \rangle.
\]

For \( k = 2m \) for \( m = 1, 2, \ldots \), we have

\[
\langle z_t, \Gamma_k \partial_x^{k+1} z \rangle = \langle z_t, K \partial_x^{2m+1} z \rangle
\]

\[
= \partial_t \left( \sum_{j=1}^{m-1} (-1)^j \langle \partial_x^j z, K \partial_x^{2m+1-j} z \rangle \right)
\]

and

\[
\langle z_t, \Lambda_k \partial_x^{k+1} z \rangle = \langle z_t, L \partial_x^{2m+1} z \rangle
\]

\[
= \partial_x \left( \sum_{j=0}^{m-1} (-1)^j \langle \partial_x^{j+1} z, L \partial_x^{2m-j} z \rangle \right) + \frac{(-1)^m}{2} \left( \partial_x \langle \partial_x^m z, L \partial_x^m z \rangle + \partial_t \langle \partial_x^m z, L \partial_x^m z \rangle \right).
\]

Thus, simply rearranging terms yields a modified energy conservation law. Clearly, a modified local momentum conservation law is derived in the same way by taking the inner product of the modified equation with \( z_x \).

This approach provides us with a modified energy density \( \bar{E}_p \) and a modified energy flux \( \bar{F}_p \) without reference to a globally defined Hamiltonian, which makes this approach independent of the boundary conditions.

The modified equations in this case can also be obtained from a Lagrangian formulation. In fact, we have a general result similar to Proposition 6.1.

**Proposition 7.1** The modified equation (7.5) can be derived from the Lagrangian den-
This implies a variational principle which leads to higher order field theories.

The Nonlinear Wave Equation

Applying BEA-3 with $p = 1$, the modified equations of motion are equivalent to the system of PDEs

\[-u_t - \frac{\Delta t}{2} u_{tt} - p_x - \frac{\Delta x}{2} p_{xx} = f'(u),\]

\[u_x - \frac{\Delta x}{2} u_{xx} = w,\]

\[u_t - \frac{\Delta t}{2} u_{tt} = v,\]

\[-\sigma'(w) = p.\]

Using the energy density

\[\tilde{E}_1 = \frac{v^2}{2} + \sigma(w) + f(u) + \frac{\Delta t}{2} u_t v_t,\]

these equations imply

\[\partial_t \tilde{E}_1 = -u_t p_x - p u_{tx} + \frac{\Delta x}{2} (p u_{txx} - u_t p_{xx}),\]

because

\[m_t = \left( u_t - \frac{\Delta t}{2} u_{tt} \right) v_t \]
\[= u_t \left( -p_x - f'(u) - \frac{\Delta t}{2} u_{tt} - \frac{\Delta x}{2} p_{xx} \right) - \frac{\Delta t}{2} u_t v_t \]
\[= -u_t p_x - f'(u) u_t - \frac{\Delta t}{2} (u_t u_t + v_t u_t) - \frac{\Delta x}{2} u_t p_{xx},\]
and
\[ \sigma'(w)u_t = -pu_{xx} + \frac{\Delta x}{2}pu_{xxx}. \]

Therefore, the modified energy flux is
\[ \vec{F}_1 = u_t p + \frac{\Delta x}{2} (u_t p_x - pu_x). \]

### 7.2 The Preissman Box Scheme

We can also perform a useful backward error analysis for the discretization (3.15), such that the modified equations are also multi-symplectic and satisfy modified conservation laws. Introduce
\[ \tau = \frac{\Delta t}{2} \quad \text{and} \quad \chi = \frac{\Delta x}{2} \]

and define the notation
\[ [\mathcal{F}(z)]_{n+1/2} = \mathcal{F}(z_{n+1/2}, t_{i+1/2}). \]

Using Taylor series, we find the following expansions:
\[
z_{n+1/2} = [z + \tau z_t + \chi z_x + \tau \chi z_{tx} + \frac{\tau^2}{2} z_{tt} + \frac{\chi^2}{2} z_{xx} + \ldots]_{n+1/2},
\]
\[
z_{n+1} = [z - \tau z_t - \chi z_x - \tau \chi z_{tx} + \frac{\tau^2}{2} z_{tt} - \frac{\chi^2}{2} z_{xx} + \ldots]_{n+1},
\]
\[
z_{n+1,i} = [z - \tau z_t + \chi z_x - \tau \chi z_{tx} + \frac{\tau^2}{2} z_{tt} + \frac{\chi^2}{2} z_{xx} + \ldots]_{n+1/2},
\]

and
\[
z_{n,i} = [z - \tau z_t - \chi z_x + \tau \chi z_{tx} + \frac{\tau^2}{2} z_{tt} - \frac{\chi^2}{2} z_{xx} + \ldots]_{n+1/2},
\]

Then these are used to get
\[ z_{n+1/2,i+1/2} = [z + \frac{\tau^2}{2} z_{tt} + \frac{\chi^2}{2} z_{xx} + \frac{\tau^2 \chi^2}{4} z_{tttx} + \frac{\tau^4 x_{xxxx}}{4!} z_{ttttt} + \chi^4 x_{xxxxxx} + \ldots]_{n+1/2}, \]

as well as
\[ \delta_{n,i} z_{n+1/2} = [z_{n+1} + \frac{\chi^2}{3!} z_{xx} + \frac{\tau^2}{2} z_{ttt} + \frac{\tau^2 \chi^2}{2 \cdot 3!} z_{tttt} + \chi^4 x_{xxxx} + \frac{\tau^4}{4!} z_{tttttt} + \ldots]_{n+1/2}. \]
and

$$
\delta_+^i z^{n+1/2,i} = \left[ z_t + \frac{\tau^2}{3!} z_{ttt} + \frac{\chi^2}{2} z_{xxx} + \frac{\tau^2}{2} \frac{\chi^2}{3!} z_{txx} + \frac{\tau^4}{5!} z_{tttt} + \frac{\chi^4}{4!} z_{xxxx} + \ldots \right]_{n+1/2}.
$$

Together these expansions show that the scheme is second order in both space and time. In order to find a suitable truncation of these expansions we ignore all terms containing powers of $\tau$ and $\chi$ that are greater than $\rho$, and this enables us to use the the compact notation

$$
\delta_+^i z^{n+1/2,i} = \sum_{i,j=0}^\rho B_i(\tau) A_j(\chi) \delta_{w}^{2i} \delta_{z}^{2j} z,
$$

and

$$
\delta_+^i z^{n,i} = \sum_{i,j=0}^\rho A_i(\tau) B_j(\chi) \delta_{w}^{2i} \delta_{z}^{2j} z,
$$

and

$$
z^{n+1/2,i+1/2} = \sum_{i,j=0}^\rho A_i(\tau) A_j(\chi) \delta_{w}^{2i} \delta_{z}^{2j} z,
$$

where $A_j(\cdot)$ and $B_j(\cdot)$ are defined in (6.16). Substituting these expansions into (3.15) yields the general modified PDE

$$
\nabla_z S \left( \sum_{i,j=0}^\rho A_i(\tau) A_j(\chi) \delta_{w}^{2i} \delta_{z}^{2j} z \right) = K \left( \sum_{i,j=0}^\rho B_i(\tau) A_j(\chi) \delta_{w}^{2i} \delta_{z}^{2j+1} z \right) + L \left( \sum_{i,j=0}^\rho A_i(\tau) B_j(\chi) \delta_{w}^{2i} \delta_{z}^{2j+1} z \right). \quad (7.11)
$$

We note here that one could truncate the expansions such that we ignore all terms containing $\tau^j \chi^k$ if $j + k > \rho$. However, our final result, which is the derivation of a modified multi-symplectic PDE, remains the same in either case.

For $\rho = 1$, the modified equations become

$$
\nabla_z S \left( z + \frac{\tau^2}{2} z_{tt} + \frac{\chi^2}{2} z_{xx} + \frac{\tau^2 \chi^2}{4} z_{txx} \right) = K \left( z_t + \frac{\tau^2}{6} z_{ttt} + \frac{\chi^2}{2} z_{xxx} + \frac{\tau^2 \chi^2}{12} z_{txx} \right)
$$

$$
+ L \left( z_x + \frac{\chi^2}{6} z_{xxx} + \frac{\tau^2}{2} z_{att} + \frac{\tau^2 \chi^2}{12} z_{axxxt} \right),
$$

which can be viewed as a generalized (higher-order) multi-symplectic PDE and is satisfied by the numerical solution up to $\mathcal{O}(\tau^4 + \chi^4)$. This equation can also be written in the form of a standard (first-order) multi-symplectic PDE (7.2). First, define the new variable

$$
\dot{z} = z + \frac{\tau^2}{2} z_{tt} + \frac{\chi^2}{2} z_{xx} + \frac{\tau^2 \chi^2}{4} z_{txx},
$$
which implies
\[ z_t + \frac{\tau^2}{6} z_{ttt} + \frac{\chi^2}{2} z_{xxx} + \frac{\tau^2 \chi^2}{12} z_{tttxxx} = z_t + \left( \frac{\tau^2}{2} \right) z_{ttt} + \frac{\chi^2}{2} z_{xxx} + \left( \frac{\tau^2 \chi^2}{4} \right) z_{tttxxx} \]
\[ = \dot{z}_t - \frac{\tau^2}{3} z_{ttt} - \frac{\tau^2 \chi^2}{6} z_{tttxxx} \]
\[ = \dot{z}_t - \frac{\tau^2}{3} z_{ttt} + O(\tau^4), \]
and similarly
\[ z_x + \frac{\chi^2}{6} z_{xxx} + \frac{\tau^2}{2} z_{xxx} + \frac{\tau^2 \chi^2}{12} z_{xxx} = \dot{z}_x - \frac{\chi^2}{3} z_{xxx} + O(\chi^4). \]
Thus, by ignoring all \( O(\tau^4 + \chi^4) \) terms, the modified equation becomes
\[ K \left( \frac{\tau^2}{3} \dot{z}_{ttt} \right) + L \left( \frac{\chi^2}{3} \dot{z}_{xxx} \right) = \nabla_z S(\tilde{z}), \quad (7.12) \]
and this is equivalent to the multi-symplectic PDE (7.2) for \( \tilde{z} = (\tilde{z}, p, q, r, s)^T \), and
\[ \tilde{S} = S - \frac{\tau^2}{3} p^T K p - \frac{\chi^2}{3} s^T L s, \]
with
\[ \tilde{K} = \begin{pmatrix} K & 0 & \frac{-\chi^2}{3} K & 0 & 0 \\ 0 & \frac{\tau^2}{3} K & 0 & 0 & 0 \\ \frac{-\tau^2}{3} K & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix}, \]
and
\[ \tilde{L} = \begin{pmatrix} L & 0 & 0 & 0 & \frac{-\chi^2}{3} L \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{-\chi^2}{3} L & 0 \\ \frac{-\tau^2}{3} L & 0 & 0 & 0 & 0 \end{pmatrix}, \]
where \( p = \dot{z}_t, q = p_t, r = \dot{z}_x, \) and \( s = r_s \). Again, this can be achieved to arbitrary high order, and to show this we use the following lemma, which is an extension of Lemma 6.2.

**Lemma 7.1** The modified equation (7.11) can be written
\[ K \left( \sum_{k=0}^{\rho} C_k(\tau) \partial_t^{2k+1} \dot{z} \right) + L \left( \sum_{k=0}^{\rho} C_k(\chi) \partial_x^{2k+1} z \right) = \nabla_z S(\tilde{z}) \quad (7.13) \]
for
\[ \dot{\tilde{z}} = \sum_{i,j=0}^{\rho} A_i(\tau) A_j(\chi) \partial_t^i \partial_x^j z, \quad (7.14) \]
and for \( C_k(\cdot) \) defined in (6.20).
Proof. Similar to the proof of Lemma 6.2, we assume the definitions (7.14) and (6.20). Then we have

\[
\sum_{k=0}^{\rho} C_k(\tau)\partial_t^{2k+1}\zeta = \sum_{k=0}^{\rho} C_k(\tau)\partial_t^{2k+1}\left(\sum_{i,j=0}^{\rho} A_i(\tau)A_j(\chi)\partial_t^{2i}\partial_t^{2j}\zeta\right)
\]

\[
= \sum_{k=0}^{\rho} \sum_{i,j=0}^{\rho} C_k(\tau)A_i(\tau)A_j(\chi)\partial_t^{2i}\partial_t^{2j}\partial_t^{2k+1}\zeta + O\left(\tau^{2(\rho+1)}\right)
\]

\[
= \sum_{i,j=0}^{\rho} B_i(\tau)B_j(\chi)\partial_t^{2i}\partial_t^{2j}\partial_t^{2k+1}\zeta + O\left(\tau^{2(\rho+1)}\right),
\]

and following the same procedure yields

\[
\sum_{k=0}^{\rho} C_k(\chi)\partial_t^{2k+1}\zeta = \sum_{i,j=0}^{\rho} A_i(\tau)B_j(\chi)\partial_t^{2i}\partial_t^{2j}\partial_t^{2k+1}\zeta + O\left(\chi^{2(\rho+1)}\right).
\]

Thus, dropping higher order terms and making the appropriate substitutions in the modified equation (7.11), yields the desired result. \(\square\)

Now the modified equation can be written in multi-symplectic form according to the following theorem. Proof of this result is much the same as the proof of Theorem 6.2.

Theorem 7.2 The modified equation (7.11) for any \(\rho\) can be written as the multi-symplectic PDE (7.2), where \(\tilde{z}, \tilde{S}, \tilde{K}\), and \(\tilde{L}\) are given in the proof.

Proof. First, write the modified equation (7.11) in the form (7.13) using Lemma 7.1. Note that these modified equations are just the modified equations (7.5) in Theorem 7.1 with different coefficients on the higher order terms, i.e. \(C_j(\Delta t)\) and \(C_j(\Delta x)\) are replaced by \(C_j(\tau)\) and \(C_j(\chi)\) respectively, and all odd powers of \(\tau\) and \(\chi\) disappear. Thus, let

\[
\tilde{z} = \left(z^{(0)}, z^{(t,1)}, z^{(t,2)}, \ldots, z^{(t,2\rho)}, z^{(x,1)}, z^{(x,2)}, \ldots, z^{(x,2\rho)}\right)^T,
\]

for \(z^{(0)} = \bar{z}\), and define the block matrices \(\tilde{K}\) and \(\tilde{L}\) such that they consist of the matrix elements \(K_{i,j}\) and \(L_{i,j}\) respectively for

\[
K_{i,j} \in \mathbb{R}^{d \times d}\quad \text{and} \quad \tilde{K} \in \mathbb{R}^{d(4\rho+1) \times d(4\rho+1)}
\]

where

\[
K_{i,j} = \begin{cases} (-1)^i C_k(\tau)K, & i + j = 2k \text{ and } k = 0, 1, 2, \ldots, \rho \\ 0, & \text{otherwise} \end{cases}
\]

and

\[
L_{i,j} = \begin{cases} (-1)^i C_k(\chi)L, & i + j = 2k \text{ and } k = 0, 1, 2, \ldots, \rho \\ 0, & \text{otherwise} \end{cases}
\]

and

\[
\tilde{L} = \begin{cases} (-1)^i C_k(\chi)L, & i + j = 2k \text{ and } k = 0, 1, 2, \ldots, \rho \\ 0, & \text{otherwise} \end{cases}
\]

and

\[
\tilde{K} = \begin{cases} (-1)^i C_k(\tau)K, & i + j = 2k \text{ and } k = 0, 1, 2, \ldots, \rho \\ 0, & \text{otherwise} \end{cases}
\]
and

\[ L_{i,j} \in \mathbb{R}^{d \times d} \quad \text{and} \quad \tilde{L} \in \mathbb{R}^{d(2\rho+1) \times d(2\rho+1)} \]

where

\[ L_{i,j} = \begin{cases} (-1)^{k_i} C_{k_i+k_j}(\chi) L, & i = 2(\rho + k_i), \ j = 2(\rho + k_j) \text{ and } i + j \leq 6\rho \\ 0, & \text{otherwise} \end{cases} \]

for \( k_i, k_j = 1, 2, \ldots, \rho \) with the requirements \( k_i = 0 \) for \( i = 0 \) and \( k_j = 0 \) for \( j = 0 \). Hence, \( \tilde{S}_\rho = S + \sum_{k=1}^\rho C_k(\tau) \left( \sum_{j=1}^\rho (-1)^j \left( z^{(tj)}, K x^{(t,2k+1-j)} \right) \right) \]

\[ + \sum_{k=1}^\rho C_k(\chi) \left( \sum_{j=1}^\rho (-1)^j \left( z^{(x,j)}, L x^{(x,2k+1-j)} \right) \right), \]

the proof is the same as the proof of Theorem 7.1 with these new coefficients and with all terms containing the symmetric matrices \( M \) and \( N \) set to zero.

The modified conservation laws of energy and momentum are easily found using the modified multi-symplectic PDE. The modified form of the conservation law (2.6) can then be computed from these modified energy and momentum conservation laws.

For the linear PDE (4.2), the modified equation (7.13) can be stated explicitly as

\[ K \left( \tilde{z}_t - \frac{\tau^2}{3} \tilde{z}_{ttt} + \frac{2\tau^4}{15} \tilde{z}_{tttt} - \ldots \right) + L \left( \tilde{x}_x - \frac{x^2}{3} \tilde{x}_{xxx} + \frac{2x^4}{15} \tilde{x}_{xxxx} - \ldots \right) = A \tilde{z}. \]

Substituting the solution (7.9) into this equation yields

\[ \left( K \left( -1\tilde{\omega} - \frac{1}{3} \tilde{\omega}^3 - \frac{12\tau^4}{15} \tilde{\omega}^5 - \ldots \right) + L \left( i \tilde{k} + \frac{i}{3} \tilde{k}^3 + \frac{12x^4}{15} \tilde{k}^5 + \ldots \right) - A \right) \tilde{a} = 0. \]

Then, due to the identity

\[ \tan(\theta) = \theta + \frac{\theta^3}{3} + \frac{2\theta^5}{15} + \frac{17\theta^7}{315} + \ldots, \]

we obtain

\[ \left( \frac{-1}{\tau} \tan(\tau \tilde{\omega}) K + \frac{i}{\chi} \tan(\chi \tilde{k}) L - A \right) \tilde{a} = 0, \]

which is just the linear system (4.13) for \( \Omega = \tilde{\omega} \) and \( K = \tilde{k} \). Thus, the modified equation can be found exactly for linear problems because the expansions converge to the numerical method, and it satisfies modified energy/momentum conservation laws.
The modified PDE (7.12) can also be derived from a modified Lagrangian density
\[ \tilde{L}_1 = \frac{1}{2} \left( \langle \ddot{\tilde{z}}, K \tilde{z}_t \rangle + \frac{\tau^2}{3} \langle \dddot{\tilde{z}}, K \tilde{z}_{tt} \rangle + \langle \ddot{\tilde{z}}, L \tilde{z}_t \rangle + \frac{\chi^2}{3} \langle \dddot{\tilde{z}}, L \tilde{z}_{tt} \rangle \right) - S(\tilde{z}), \]
and just as one would expect, this can be done for any $\rho$.

**Proposition 7.2** The modified equations (7.13) for the Preissman box scheme can be obtained from the Euler-Lagrange equation given the Lagrangian density
\[ \tilde{L}_\rho = \sum_{j=0}^{\rho} \frac{(-1)^j}{2} \left( C_j(\tau) \langle \partial_t^j \tilde{z}, K \partial_t^{j+1} \tilde{z} \rangle + C_j(\chi) \langle \partial_t^j \tilde{z}, L \partial_t^{j+1} \tilde{z} \rangle \right) - S(\tilde{z}). \]

**Proof** Proof of this result can be done in the same manner as the proof of Proposition 6.1. In this case the Euler-Lagrange equation takes the form
\[ 0 = \sum_{k=0}^{\rho} (-1)^{k+1} \left( \partial_t^k \partial_t^{k+1} \tilde{z} + \partial_t^k \partial_t^{k+1} \tilde{z} \right) \tilde{L}_\rho. \]
Then, substituting $\tilde{L}_\rho$ and using the identity (6.10) yields the desired result. \( \square \)

Given a linear symmetry, this modified Lagrangian density is also invariant under the transformation (2.14). For example, the associated conservation law for $\rho = 1$ is easily obtained by taking the inner product of the modified equation (7.13) with $B \tilde{z}$, which yields
\[ \langle \ddot{\tilde{z}}, KB\tilde{z}_t \rangle - \frac{\tau^2}{3} \langle \dddot{\tilde{z}}, KB\tilde{z}_{tt} \rangle + \langle \ddot{\tilde{z}}, LB\tilde{z}_t \rangle - \frac{\chi^2}{3} \langle \dddot{\tilde{z}}, LB\tilde{z}_{tt} \rangle = 0. \]
Then the identity
\[ \langle \ddot{\tilde{z}}, KB\tilde{z}_t \rangle = \partial_t \left( \langle \ddot{\tilde{z}}, KB\tilde{z}_t \rangle - \frac{1}{2} \langle \dddot{\tilde{z}}, KB\tilde{z}_t \rangle \right), \]
and a similar identity for $\langle \ddot{\tilde{z}}, LB\tilde{z}_{tt} \rangle$, imply the modified conservation law
\[ 0 = \partial_t \left( \frac{1}{2} \langle \ddot{\tilde{z}}, KB\tilde{z} \rangle - \frac{\tau^2}{3} \langle \dddot{\tilde{z}}, KB\tilde{z}_t \rangle + \frac{\tau^2}{6} \langle \dddot{\tilde{z}}, KB\tilde{z}_t \rangle \right) + \partial_x \left( \frac{1}{2} \langle \ddot{\tilde{z}}, LB\tilde{z} \rangle - \frac{\chi^2}{3} \langle \dddot{\tilde{z}}, LB\tilde{z}_{tt} \rangle + \frac{\chi^2}{6} \langle \dddot{\tilde{z}}, LB\tilde{z}_t \rangle \right), \]
and we expect that this can be done for any number of modifications.

### 7.3 The Explicit Midpoint Scheme

We can also derive modified equations for the two-step method. (See Hairer [25] for results on backward error analysis of multi-step methods for ODEs.) The discretization
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(3.21) can be stated
\[
\frac{1}{2} \left( K \delta_t^2 z^n + K \delta_t^- z^n + L \delta_x^+ z^n + L \delta_x^- z^n \right) = \nabla_z S(z^n).
\]

Then using the Taylor series expansions (6.1)-(6.2) implies the modified equation
\[
K_x^t + \frac{\Delta t^2}{6} K_{x_{t+2}} + L_x + \frac{\Delta x^2}{6} L_{x_{max}} = \nabla_z S(z)
\]

with one modification term, and clearly this can be written as a modified multi-symplectic PDE (7.2) in the same way as (7.13) was for the Preissman box scheme. In fact, the modified equations for any \( \rho \) are
\[
\nabla_z S(z) = \sum_{k=0}^{\rho} \left( B_k(\Delta t) K \delta_t^{2k+1} z + B_k(\Delta x) L \delta_x^{2k+1} z \right),
\]

where \( B_k \) is given in (6.16). Since this equation has the same form as equation (7.13), Theorem 7.2 can be used to find a modified multi-symplectic PDE with different coefficients on the modification terms. Thus, we have the following corollary.

**Corollary 7.2** The modified equations associated with the explicit midpoint scheme (3.21) can be written as a multi-symplectic PDE of the form (7.2) for any number of modifications and this modified PDE can be derived from a discrete Lagrangian.

Thus, we can also find modified conservation laws. In addition, we find that for linear equations we get
\[
\left( K \left( -i \omega + \frac{i \Delta t^2 \omega^3}{6} + \ldots \right) + L \left( i k - \frac{i \Delta x^2 k^3}{6} + \ldots \right) L - A \right) \tilde{a} = 0.
\]

According to the identity (7.10), this formally converges to the linear system (4.15) which implies the numerical dispersion relation for this method.

Based on these results, one may be tempted to label the explicit midpoint scheme a multi-symplectic method. Yet, the simple fact that this scheme introduces computational modes for linear equations leads us to conclude that it should not be considered multi-symplectic. In fact, it is not all together clear when multi-step methods are symplectic in the context of ODEs (cf. [28, Chapter 14]). Thus, we should not expect it to be clear in the context of PDEs. Nevertheless, the issue of the present definition of a multi-symplectic integration method arises. The two approaches used to define multi-symplectic integrators thus far (the definition of Bridges and Reich [15], which says the integrator conserves the symplectic structure of the PDE, and the definition of Marsden, Patrick, and Shkoller [36], which uses a discrete variational principle) are not complete.
These ideas have been touched upon by Reich [51], who has discussed multi-symplectic Runge-Kutta/Gauss-Legendre collocation methods, which do not yield computational modes for linear problems. In this analysis, the discrete multi-symplectic conservation law is considered as an approximation of a contour integral along the boundary of the computation cell. This may be the way to resolve the issues concerning multi-symplectic methods and computational modes, but the answers are still not clear.
Since many applications involve dissipation, it is natural to ask if the ideas of previous chapters can be applied to problems with added dissipation. In this chapter we consider only a weak dissipation, which is sometimes known as Newtonian relaxation. This particular type of dissipation is, in fact, the only dissipation that is compatible with the symplectic structure in such a way that the results for the previous chapters are easily carried over to these new problems.

In the following sections, we discuss the dissipation properties associated with the differential equations. This is followed with an application of the Euler and Preissman schemes to PDEs with added dissipation, including a discussion on the numerical preservation of the dissipation properties. In the following chapter, these results are demonstrated numerically with a model problem.

8.1 Conformal Symplecticity

We consider differential equations for which the symplectic form dissipates exponentially. Systems of this type are said to be conformal symplectic, and examples of such problems are mechanical systems that include frictional forces. Many studies have been conducted for systems of this type. In fact, many aspects of conformal symplectic ODEs are well understood, including the derivation of numerical schemes that preserve the dissipation of the symplectic form. However, there is currently no extension of conformal symplecticity to PDEs. As a result there are no results concerning numerical schemes that preserve such properties for PDEs, and our aim in this chapter is to consider schemes of this type. With this in mind, we must define a conformal multi-symplectic property for PDEs and understand the other dissipation properties for such systems, but first we consider the ODE case.
8.1.1 Ordinary Differential Equations

We begin with the system of differential equations
\[ \dot{q} = \nabla_p \dot{H}(p, q), \quad \dot{p} = -\nabla_q \dot{H}(p, q) - cp, \]
where \( p, q \in \mathbb{R}^d \) and \( c \) is any constant. This system can also be written in the general form
\[ J\dot{y} = \nabla_y \dot{H}(y) + \tilde{D}y, \]
for \( y = (p, q)^T \), and
\[ \tilde{D} = c \begin{pmatrix} 0_d & 0_d \\ I_d & 0_d \end{pmatrix}, \]
which is just the Hamiltonian system (1.5) with added dissipation. In order to simplify the following derivations, notice that the matrix \( \tilde{D} \) can be written as the sum of a symmetric matrix and a skew-symmetric matrix, such that
\[ \tilde{D} = \frac{c}{2} \left[ \begin{pmatrix} 0_d & I_d \\ I_d & 0_d \end{pmatrix} + \begin{pmatrix} 0_d & -I_d \\ I_d & 0_d \end{pmatrix} \right] = \frac{c}{2} [P - J] \]
where \( P = J_+ - J_- \). Therefore, this system of equations is equivalent to
\[ J\dot{y} = \nabla_y H(y) - \frac{c}{2} Jy \quad (8.1) \]
for
\[ H(y) = \dot{H}(y) + \frac{c}{4} (y, Py), \]
also stated
\[ \dot{y} = J^{-1} \nabla_y H(y) - \frac{c}{2} y, \]
which is clearly just a Hamiltonian system with linear dissipation.

Now, we are interested in how this change in the equations of motion affect the symplectic form and the energy. First, consider the associated variational equation
\[ J\delta y = H_{yy}(y)\delta y - \frac{c}{2} J\delta y, \]
and take the wedge product with \( dy \) to get
\[ dy \wedge J\delta y = -\frac{c}{2} (dy \wedge J\delta y), \]
which implies
\[ \delta_t (dy \wedge J\delta y) = -c (dy \wedge J\delta y). \]
As a result, we use the following definition.
Definition 8.1 A differential equation \( \dot{y} = g(y) \) is said to be conformal symplectic or a conformal Hamiltonian system, if the relation
\[
\partial_t \omega = -c \omega
\]
is satisfied for \( \omega = dy \wedge Jdy \).

The energy dissipation of a conformal Hamiltonian system can be considered by taking the inner product of \( \dot{y}^T \) with (8.1), which gives
\[
\partial_t H(y) = \frac{c}{2} (\dot{y}, Jy),
\]
which can have any sign, and we refer to this as the energy dissipation property for (8.1). More on conformal Hamiltonian systems can be found in McLachlan and Perlmutter [39].

8.1.2 Partial Differential Equations

Based on Definition 8.1, it is reasonable to extend the idea of conformal symplecticity to PDEs in the following way.

**Definition 8.2** A PDE is called conformal multi-symplectic if it satisfies the relation
\[
\partial_t \omega + \partial_a \kappa = -c \omega - b \kappa \tag{8.2}
\]
for \( \omega = dz \wedge Kdz \) and \( \kappa = dz \wedge Ldz \).

In order to construct such a PDE, consider the multi-symplectic equation (1.14) with added dissipation written in the form
\[
Kz_t + Lz_x = \nabla_z S(z) - \frac{a}{2} Kz - \frac{b}{2} Lz. \tag{8.3}
\]

Then, taking the wedge product of \( dz \) with the variational equation
\[
Kdz_t + Ldz_x = S_{zz}(z)dz - \frac{a}{2} Kdz - \frac{b}{2} Ldz
\]
gives
\[
dz \wedge Kdz_t + dz \wedge Ldz_x = -\frac{a}{2} (dz \wedge Kdz) - \frac{b}{2} (dz \wedge Ldz).
\]
This implies
\[
\partial_t (dz \wedge Kdz) + \partial_a (dz \wedge Ldz) = -a (dz \wedge Kdz) - b (dz \wedge Ldz),
\]
which is just the conformal multi-symplectic condition (8.2).

Now the energy and momentum dissipation properties can be found in the obvious way. Taking the inner product of \( z_t \) with (8.3) yields
\[
\langle z_t, L z_t \rangle = \partial_t S(z) - \langle z_t, D z \rangle,
\]
where we define
\[
D = \frac{a}{2} K + \frac{b}{2} L.
\]
This implies that the dissipation equation has the property
\[
\partial_t E + \partial_x F = \langle z_t, D z \rangle,
\]
(8.4)
where \( E \) and \( F \) are given in (2.11), and we call this property the energy dissipation law. Similarly, one may take the inner product of \( z_w \) with (8.3) to get
\[
\partial_x G + \partial_t I = \langle z_w, D z \rangle,
\]
which we refer to as the momentum dissipation law.

8.2 Numerical Methods

Now we would like to construct numerical methods that preserve these dissipation properties. Results of McLachlan and Quispel [40, 41] show that splitting methods can be used to numerically preserve dissipation properties for conformal symplectic ODEs. Essentially, this is done by splitting the vector field of the differential equation into a non-Hamiltonian part, which can be solved exactly, and a Hamiltonian part, which can be solved using a symplectic integrator. Then the flow maps obtained through this computation are composed to yield a numerical method which preserves the conformal symplectic property exactly.

Unfortunately, it is not clear how this idea can be applied to a PDE of the form (8.3). In fact, there is no current notion of a splitting method for multi-symplectic PDEs, aside from the application of a splitting method to discretize in time with a standard method applied to the spatial variables, similar to the application of the Störmer/Verlet method to a multi-symplectic PDE discussed in [43]. It is possible to consider a conformal multi-symplectic PDE (8.3) with \( b = 0 \). Then one can discretize in space with any symplectic scheme and split the corresponding finite-dimensional vector field into Hamiltonian and non-Hamiltonian parts, in order to compose the resulting flow maps and obtain a method.
which satisfies a discrete conformal symplectic property. However it is not clear how this can be done for problems with \( b \neq 0 \).

We would like to find numerical schemes that preserve the conformal multi-symplectic property by satisfying a discrete version of (8.2). Hence, we use the following definition.

**Definition 8.3** A numerical method for solving the equation (8.3) is called a conformal multi-symplectic integrator if a relation of the form

\[
\delta_t \omega^{n,i} + \delta_x \kappa^{n,i} = -aw^{n,i} - b\kappa^{n,i}
\]

is satisfied, where the discretizations \( \delta_t \) and \( \delta_x \) depend on the numerical method.

Since it is not clear how to construct schemes that satisfy a discrete conformal multi-symplectic property, we consider an application of the Euler and Preissman schemes that have been used throughout this text, and we find remarkable behavior. Then we use a modified equations approach to understand the effects of the discretization on the energy and momentum dissipation.

### 8.2.1 The Euler Box Scheme

Using the symplectic Euler method to discretize (8.3) yields the scheme

\[
K_{+} \delta_i^+ z^{n,i} + K_{-} \delta_i^- z^{n,i} + L_{+} \delta_i^+ z^{n,i} + L_{-} \delta_i^- z^{n,i} = \nabla_z S(z^{n,i}) - Dz^{n,i}.
\]

Now taking the wedge product of \( dz^{n,i} \) with the associated variational equation yields

\[
\delta_i^+ (dz^{n,i-1} \wedge K_{+} dz^{n,i}) + \delta_i^+ (dz^{n,i-1} \wedge L_{+} dz^{n,i}) = -dz^{n,i} \wedge Dz^{n,i},
\]

where we have used the proof of Proposition 3.1. Thus, the multi-symplectic Euler scheme does not satisfy a discrete conformal multi-symplectic property in the strict sense of Definition 8.3, because the indices are staggered on the left hand side of this equation but not on the right.

Turning our attention to the energy/momentum dissipation, we find that certain semi-discrete properties are still satisfied exactly. Given the spatially discrete equation

\[
K \delta_i^+ z^n + L_{+} \delta_i^+ z^n + L_{-} \delta_i^- z^n = \nabla_z S(z^n) - Dz^n,
\]

we have a semi-discrete energy dissipation law

\[
\partial_t E^n + \delta_i^+ F^n = \langle x^n_i, Dz^n \rangle
\]
for $F^n$ given in (3.5). In the same way, we have
\[ \partial_t G^i + \delta_t^t F^i = \langle z^i, Dz^i \rangle, \]
which is the semi-discrete momentum dissipation law

In order to understand the effects of the full discretization on the energy dissipation law, we must consider the modified equations, and determine if they yield useful information. Using the Taylor series expansions (6.1)-(6.2) gives the modified equations
\[ K_\xi + \frac{\Delta t}{2} M_\xi + L_\xi + \frac{\Delta x}{2} N_\xi = \nabla_z S(z) - Dz. \quad (8.5) \]
Now this can clearly be written in the form
\[ K_\varepsilon + L_\varepsilon = \nabla_z \delta \varepsilon - \mathbf{D} \delta \varepsilon \quad (8.6) \]
for $\varepsilon = (z, z^{(t,1)}, z^{(x,1)})^T$ with the definitions (7.3)-(7.4) and
\[ \mathbf{D} = \begin{pmatrix} D & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \]
and this can, in fact, be done for the general modified PDE
\[ \sum_{k=0}^\rho \left( C_k (\Delta t) \Gamma_k \delta_k^{k+1} z + C_k (\Delta x) \Lambda_k \delta_k^{k+1} z \right) = \nabla_z S(z) - Dz, \]
using the proof of Theorem 7.1. Using the proof of Corollary 7.1, one can also show that the modified equation satisfies a modified energy dissipation property
\[ \partial_t \mathcal{E}_\rho + \partial_z \mathcal{E}_\rho = \langle z_t, Dz \rangle, \quad (8.7) \]
and a modified momentum dissipation property
\[ \partial_t \mathcal{E}_\rho + \partial_z \mathcal{E}_\rho = \langle z_{zt}, Dz \rangle. \quad (8.8) \]

8.2.2 The Preissmann Box Scheme

Applying the implicit midpoint rule to (8.3) yields the discretization
\[ K_\xi + L_\xi = \nabla_z S(z^{n+1/2, i+1/2}) - Dz^{n+1/2, i+1/2}. \]
Using the associated variational equation, we get
\[ dz^{n+1/2, i+1/2} \wedge \left( K_\xi^{+} dz^{n+1/2, i+1/2} + L_\xi^{+} dz^{n, i+1/2} \right) \]
\[ = -dz^{n+1/2, i+1/2} \wedge Dz^{n+1/2, i+1/2} \]
\[ = -dz^{n+1/2, i+1/2} \wedge \left( \frac{a}{2} K + \frac{b}{2} L \right) dz^{n+1/2, i+1/2}. \]
Now we can use the proof of Proposition 3.3 to show that this discretization satisfies a discrete conformal multi-symplectic condition

$$\delta_i^+ \omega^{n+1/2,i} + \delta_a^+ \kappa^{n,i+1/2} = -a\omega^{n+1/2,i+1/2} - b\kappa^{n+1/2,i+1/2}$$

for $\omega^{n+1/2,i}$ and $\kappa^{n,i+1/2}$ given in (3.16) and (3.17) respectively.

It is also possible to derive semi-discrete energy and momentum dissipation properties. Taking the inner product of $z_i^{n+1/2}$ with the spatially discrete equation

$$Kz_i^{n+1/2} + L\delta_a^+ z^n = \nabla S(z^n) - Dz^{n+1/2}$$

yields

$$\left\langle z_i^{n+1/2}, L\delta_a^+ z^n \right\rangle = \partial_t z_i^{n+1/2} - \left\langle z_i^{n+1/2}, Dz^{n+1/2} \right\rangle,$$

and just as in Proposition 3.6 we get a semi-discrete energy dissipation law

$$\partial_t E^{n+1/2} + \delta_a^+ F^n = \left\langle z_i^{n+1/2}, Dz^{n+1/2} \right\rangle.$$

Similarly, the semi-discrete momentum dissipation property

$$\partial_a G^{i+1/2} + \delta_i^+ T^i = \left\langle z_i^{i+1/2}, Dz^{i+1/2} \right\rangle$$

holds.

In order to understand the fully discrete energy and momentum dissipation properties, we turn our attention to the modified equations. The modified equation for any number of modifications is written

$$\sum_{j=0}^n \left( C_j(\tau)K\delta_z^{2j+1} + C_j(\chi)L\delta_a^{2j+1} \right) = \nabla \tilde{S}(\tilde{z}) - D\tilde{z},$$

which can also be written in the form (8.6). Taking the inner product of $\tilde{z}_i$ (resp. $\tilde{z}_a$) with the modified equation for any number of modifications in this case yields modified energy (resp. momentum) dissipation properties of the form (8.7) (resp. (8.8)), and similar results hold in this case as for the Euler method.
This chapter is devoted to numerical simulation. Our purpose here is simply to demonstrate the results achieved in this thesis, and provide numerical evidence which reinforce our formal analysis. We begin with experiments which show that the modified conservation laws of energy and momentum are satisfied by the numerical solution to higher order for the sine-Gordon equation. Then, taking a specific soliton solution of this equation, we give results demonstrating that the numerical scheme reproduces the qualitative solution behavior of the original equation. Finally, we consider a dissipative PDE, and demonstrate the numerical preservation of dissipative properties. All simulations were performed on a single processor using MATLAB, which made it possible to take advantage of the matrix-vector operations inherent in the problem for each discretization.

9.1 Conservation of Energy and Momentum

To check the preservation of the modified conservation law to higher order numerically, consider a specific case of (1.16), with $\sigma(w) = w^2/2$, and $f(u) = 1 - \cos(u)$ which gives the sine-Gordon equation

$$u_{tt} = u_{xx} - \sin(u).$$

(9.1)

For all simulations we use the periodic boundary conditions

$$u(x_0, t_i) = u(x_J, t_i), \quad u_x(x_0, t_i) = u_x(x_J, t_i)$$

for $x_0 = 0$ and $x_J = 1$, and the initial conditions are given by a standard Gaussian with zero velocity, though similar results hold for different initial and boundary conditions.

We use the Euler box scheme to discretize (9.1), then solve the system of equations

$$v^{i+1} = v^i - \Delta t (\delta_x w^i + \sin(u^i))$$

$$u^{i+1} = u^i + \Delta t v^{i+1}$$

$$w^{i+1} = -\delta_x u^{i+1}$$

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Figure 9.1: Residual in modified and unmodified energy conservation laws over 10 periods for $\Delta x = .01$ and $\Delta t = .005$.

Figure 9.2: Modified and unmodified total energy along the numerical solution over 40 periods for $\Delta x = .01$ and $\Delta t = .01$. 

where $\mathbf{u}^i = \mathbf{u}(t_i)$ is the vector whose entries are the values of $u$ at each of the grid points with analogous definitions for $\mathbf{v}$ and $\mathbf{w}$, and $\delta_n^i$ represents the matrix obtained by applying $\delta_n^i$ to each entry of a given vector. Using this notation, we solve for the vectors $\mathbf{u}$, $\mathbf{v}$, and $\mathbf{w}$ at each time step, then use this to evaluate the residual $\mathbf{r}^n_{m,i}$ given in (5.21). This in turn yields a residual matrix $\mathbf{r}^n_{m,i}$, which contains the values of $\mathbf{r}^n_{m,i}$ at each grid point and at each time step. The same is also done for the momentum conservation law where we represent the residual matrix by $\mathbf{r}^n_{m,i}$. Then we are able to plot the residual as a function of $x$ or $t$ by respectively taking

$$r_m(x_n) = \max_i |r^n_{m,i}| \quad \text{or} \quad r_m(t_i) = \max_n |r^n_{m,i}|.$$  \hspace{1cm} (9.2)

Similarly we can find $r_e(t_i)$ and $r_e(x_n)$, and we make constant use of these functions in the following simulations.

In Figure 9.1, we plot the residual in the modified (using BEA-2) and unmodified energy conservation laws $r_e(t)$. The modified conservation laws yield smaller residuals as $\rho$ increases, showing that they are better satisfied by the numerical solution. This simulation has also been performed over ten periods, showing that there is very little, if any energy
drift induced by the scheme for the local conservation law. Also to demonstrate this fact, we have plotted the modified and unmodified total energy along the numerical solution in Figure 9.2, and the residual in the modified and unmodified momentum conservation laws, first as a function of time and then as a function of space, in Figure 9.3. For each of these experiments we have plotted the results over forty periods, and once again we see no drift and better conservation by the modified energy/momentum.

It is important to notice at this point, that considering the energy conservation alone is not enough for these results, nor is the momentum conservation law alone. This is due to the modified equations approach that we use here and to the semi-discrete conservation laws that result from such an analysis. In fact, a measure of accuracy in time is only achieved through the energy conservation law, and the momentum conservation law only measures the accuracy in space. Yet, the backward error analysis performed still provides the useful information for understanding the behavior of the scheme.

The residuals in these plots may also seem relatively large. This is due to the size of \( \Delta t \) and \( \Delta x \), which were used based on the size of the time interval, and were sufficient.
Figure 9.5: \( r_e(\Delta t) \), for the following curves: BEA-2 (solid), and BEA-3 with \( \Delta x = .005 \) (dashed) and \( \Delta x = .0025 \) (chain).

for these experiments. Making these values smaller does in fact yield a smaller residual, and this can be seen in the following set of experiments.

To show that the modified conservation laws are, in fact, preserved to higher order by the numerical solution, we use \( r_e^{n,i} \) to compute

\[
\max_{n,i} |r_e^{n,i}| = r_e
\]

for each value of \( \Delta t \). This procedure is then repeated for different step sizes \( \Delta t \), in order to check the order of convergence for modified and unmodified energy conservation laws. The same is also done for the modified momentum conservation law where we evaluate \( r_m \) for \( \Delta t \) fixed, while we vary \( \Delta x \). We integrate over one period for each simulation.

Using log-log scale, Fig. 9.4a plots \( r_e \) as a function of \( \Delta t \) with \( \Delta x = 1/40 \) and \( \Delta t = 1/40, 1/80, 1/160, 1/400, 1/600, 1/1000, \) and \( 1/1500 \). Similarly, Fig. 9.4b plots \( r_m \) as a function of \( \Delta x \) for the momentum conservation law. In this case, backward error analysis in space requires that we keep \( \Delta t \) fixed while \( \Delta x \to 0 \). However, the condition \( \Delta t \leq \Delta x \) must be satisfied in order to ensure the stability of the Euler scheme. Therefore, we set \( \Delta t = 1/1500 \) for \( \Delta x = 1/40, 1/80, 1/160, 1/400, 1/600, 1/1000, \) and \( 1/1500 \). The figure clearly shows that the modified energy conservation laws, obtained using BEA-1, are conserved to higher order. For \( \rho = 0 \) the residual converges linearly for both energy
Figure 9.6: In log-log scale, \( r_e(\Delta t) \) for BEA-1 (crosses), BEA-2 (solid), and the shifted residual using BEA-3 with \( \Delta x = .005 \) (dashed) and \( \Delta x = .01 \) (circles).

and momentum conservation laws, while \( \rho = 1 \) gives second order convergence and \( \rho = 2 \) gives third order convergence.

Now consider the modified energy conservation law where the modified equations have been derived using the BEA-3. Then, evaluation of this conservation law along the numerical solution is accomplished using

\[
    r^n_{e,i} = \delta^{(\rho+1)}_t \hat{E}^n_{\rho,i} + \delta^{(\rho+1)}_x \hat{F}^n_{\rho,i} = \mathcal{O}(\Delta x^{\rho+1} + \Delta t^{\rho+1}),
\]

where each derivative of both \( \hat{E}_{\rho,i} \) and \( \hat{F}_{\rho,i} \) is approximated to the appropriate order. After discretizing the modified conservation law we get (9.3) for \( \rho = 1 \) with

\[
    \hat{E}^{n,i}_1 = \frac{(u^{n,i})^2}{2} + \sigma(u^{n,i}) + f(u^{n,i}) + \frac{\Delta t}{2} \delta^{(1)}_t u^{n,i} \delta^{(1)}_x v^{n,i},
\]

and

\[
    \hat{F}^{n,i}_1 = p^{n,i} \delta^{(2)}_t u^{n-1,i} + \frac{\Delta x}{2} \left( \delta^{(2)}_t u^{n+1,i} \delta^{(1)}_x p^{n,i} - p^{n,i} \delta^{(2)}_t \delta^{(1)}_x u^{n,i} \right).
\]

Once again we use, for example, \( \delta^{(1)}_t = \delta^{+}_t \), \( \delta^{(2)}_t = (\delta^{+}_t + \delta^{-}_t)/2 \), etc., to maintain the order of convergence.

For the following simulations we consider only the energy conservation law because the stability restriction \( \Delta t \leq \Delta x \) makes it difficult to analyze the results for the momentum
conservation law. Hence, each plot here gives $r_e$ as a function of $\Delta t$, but similar results also hold for the momentum conservation law. Unless stated otherwise, we set $\Delta x = 1/100$ with $\Delta t = 1/200, 1/250, 1/300, 1/400, 1/500, 1/600, 1/800, 1/1000, 1/1400, 1/2000$. Fig. 9.5 shows a clear difference between BEA-2 and BEA-3. (Note that, due to the stability restriction $\Delta t \leq \Delta x$, this plot can only be plotted for $\Delta x = 1/400$ with $\Delta t = 1/400, 1/500, 1/600, 1/800, 1/1000, 1/1400, 1/2000$.) For BEA-2, $r_e \to 0$ as $\Delta t \to 0$, but for BEA-3, $r_e \to C \Delta x^2$, for some constant $C$, as $\Delta t \to 0$. However, as $\Delta x \to 0$, we have $r_e \to 0$. This is made more clear in the following table, where we see that for $\Delta t \approx 0$, the residual converges to zero like $\Delta x^2$, i.e. $r_e = O(\Delta t^2 + \Delta x^2)$.

<table>
<thead>
<tr>
<th>$\Delta x$</th>
<th>.02</th>
<th>.01</th>
<th>.005</th>
<th>.0025</th>
</tr>
</thead>
<tbody>
<tr>
<td>Approx. $\lim_{\Delta t \to 0} r_e$</td>
<td>.3184</td>
<td>.0827</td>
<td>.0211</td>
<td>.0059</td>
</tr>
</tbody>
</table>

Table 9.1: Order ($\Delta t^2+\Delta x^2$) convergence of residual for fully discrete energy conservation law

Using log-log scale, Fig. 9.6 compares each method of backward error analysis. It shows that there is little, if any, difference between BEA-1 and BEA-2. If the $\Delta x^2$ dependence of the residual for BEA-3 is neglected, i.e. the parabolas of Fig. 9.5 are shifted to intercept the y-axis at zero, then we see that the residual is slightly smaller, and this is true regardless of our choice for $\Delta x$. Overall, BEA-3 gives a better understanding of the error due to discretization of a Hamiltonian PDE.

### 9.2 Computational Solitary Wave Solutions

The study of waves is one of the most important aspects of dynamical systems, and a particularly interesting type of wave, known as a traveling wave or soliton, is a solitary wave that travels without changing its speed or shape. The NLS equation has a family of solitary wave solutions, as do several other equations that can be written in the form (1.14), such as the KdV equation, Boussinesq equations, and nonlinear wave equations (cf. [9, 10, 11, 12, 56]).
9.2.1 General Theory

Generally, a traveling wave is given by the solution ansatz

\[ z(x,t) = \psi(x - ct), \]

where \( c \) denotes the wave speed. Letting \( \xi = x - ct \) and substituting this solution into (1.14) yields

\[ -cK\psi'(\xi) + L\psi'(\xi) = \nabla \psi S(\psi(\xi)), \]

which is a boundary value problem on an infinite domain and can be written

\[ J_c\psi' = \nabla \psi S(\psi), \tag{9.4} \]

where \( J_c = (L - cK) \) is skew-symmetric. If \( J_c \) is nonsingular, then this is just a Hamiltonian ODE similar to (1.5). The solution \( \psi(\xi) \) of this Hamiltonian system is defined as a soliton solution if

\[ \lim_{\xi \to \pm\infty} \psi'(\xi) = 0 \quad \text{and} \quad \lim_{\xi \to \pm\infty} \psi(\xi) = \psi_{\pm}, \tag{9.5} \]

such that \( \psi_{\pm} \) are equilibrium points of (9.4). By definition, if \( \psi_+ = \psi_- \) we have a homoclinic orbit and if \( \psi_+ \neq \psi_- \) we have a heteroclinic orbit. Our concern in this section is numerical computation of these orbits [7], because any orbit of these types gives rise to a (not necessarily stable) soliton solution for the nonlinear PDE (1.14).

A thorough analysis of the error growth due to time discretization for these solutions has been performed for the KdV equation [17] and the NLS equation [20]. Specifically, Durán and Sanz-Serna [20] have shown that the implicit midpoint time discretization has better error propagation mechanisms than other non-conservative schemes. In particular, they have shown that the time-discrete solutions of the NLS equation, which have been initialized with an exact soliton profile, are made up of a modified solitary wave, that have a different wave speed and amplitude than the exact soliton, as well as a complementary term that grows linearly in time and higher order terms.

Using the results of the previous sections, it may be possible to show that the numerical solutions of the fully discretized NLS equation initialized with an exact soliton profile are made up of a modified soliton, which has corrections in both space and time, along with the complementary error and higher order terms. From a slightly different perspective, one may be able to show that the modified equations have solitary wave solutions. Then, initializing the numerical scheme with the new modified soliton profile would yield numerical soliton solutions that are preserved to higher order in both space and time.
Substituting the solution

\[ z(x, t) = \mu(x - ct) = \mu(\xi) \]

into the modified equation (7.1) with one modification term where we have used the Euler box scheme to discretize (1.14), yields the ODE

\[ J_c \mu' + \varepsilon P_c \mu'' = \nabla_\mu S(\mu), \tag{9.6} \]

where \( \varepsilon = \Delta x \) and

\[ P_c = \frac{1}{2} \left( \frac{c^2 \Delta t}{\Delta x} M + N \right), \]

with \( c\Delta t/\Delta x \leq 1 \) for stability. Now, assuming that

\[ \mu(\xi) = \psi(\xi) + \varepsilon \phi(\xi), \tag{9.7} \]

such that \( \psi(\xi) \) is the exact soliton solution of the original PDE (1.14) and \( \phi \) depends on \( c, \Delta t, \) and \( \Delta x, \) implies

\[ \mu'' = \psi'' + \varepsilon \phi'' = J_c^{-1} S_{\psi\psi}(\psi) \psi' + \varepsilon \phi''. \]

Then substituting this into (9.6) yields the modified equation

\[ J_c \mu' = \nabla_\mu S(\mu) - \epsilon P_c J_c^{-1} S_{\psi\psi}(\psi) \psi', \tag{9.8} \]

where we have ignored \( O(\varepsilon^2) \) terms. Notice that (9.5) implies that the fixed points of this equation are those of the original equation.

Now, substituting (9.7) into (9.8) and ignoring again \( O(\varepsilon^2) \) terms gives the first-order system of linear ODEs

\[ J_c \phi' = S_{\psi\phi}(\psi) \phi - P_c J_c^{-1} S_{\psi\psi}(\psi) \psi'. \tag{9.9} \]

Therefore, a traveling wave solution for the modified equation can be found by solving of (9.9), subject to the boundary conditions

\[ \lim_{\xi \to \pm \infty} \phi(\xi) = 0. \]

To show well-posedness of this boundary value problem, one would need to use the exponential dichotomy estimates [4] for solutions of the homogeneous equation

\[ \phi' = J_c^{-1} S_{\psi\phi}(\psi) \phi, \]

which are known in principle based on the fact that, this is just a linearization of the ODE (9.4) about its soliton solution.
9.2.2 The Sine-Gordon Equation

Results in that spirit have been achieved concerning soliton solutions of the sine-Gordon equation (9.1), which can be written in the form (1.14) with $z = (u, v, w)^T$,

$$K = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad L = \begin{pmatrix} 0 & 0 & -1 \\ 0 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix},$$

and

$$S(z) = \frac{v^2}{2} + \frac{w^2}{2} + \cos u.$$

It is well known that there is a family of solitary wave solutions for (9.1) given by

$$u(x, t) = 4 \tan^{-1} \left( \pm \exp \left( \frac{\pm(x - ct)}{(1 - c^2)^{1/2}} \right) \right), \quad (9.10)$$

where $|c| < 1$ is the wave speed (cf. [19]).

A modified soliton

Using the multi-symplectic Euler box scheme to discretize gives

$$\delta_t^+ u^{n,i} + \delta_x^+ w^{n,i} = -\sin u^{n,i}, \quad \delta_t^- u^{n,i} = v^{n,i}, \quad \delta_x^- u^{n,i} = -w^{n,i}, \quad (9.11)$$

Notice that eliminating $v$ and $w$ gives the familiar second order scheme

$$\delta_t^2 u^{n,i} = \delta_x^2 u^{n,i} - \sin u^{n,i}, \quad (9.12)$$

where $\delta_\eta^2 = \delta_\eta^+ \delta_\eta^-$ for $\eta = x, t$. Hence, the numerical solution $u^{n,i}$ is accurate to second order in both $\Delta t$ and $\Delta x$, but using the scheme (9.11) yields first order error because $v$ and $w$ are only approximated to first order. This is demonstrated in following table.

<table>
<thead>
<tr>
<th>$\rho$</th>
<th>0</th>
<th>1</th>
<th>2</th>
<th>3</th>
</tr>
</thead>
<tbody>
<tr>
<td>$u$</td>
<td>2</td>
<td>2</td>
<td>4</td>
<td>4</td>
</tr>
<tr>
<td>$v, w$</td>
<td>1</td>
<td>2</td>
<td>3</td>
<td>4</td>
</tr>
</tbody>
</table>

Table 9.2: Order of convergence of $u$, $v$, and $w$ corresponding the the number of modifications

To make this more clear, the modified equations for (9.11) are

$$v_t + \frac{\Delta t}{2} v_{tt} + w_x + \frac{\Delta x}{2} w_{xx} = -\sin u, \quad (9.13)$$

$$u_t - \frac{\Delta t}{2} u_{tt} = v, \quad (9.14)$$

$$u_x - \frac{\Delta x}{2} u_{xx} = -w. \quad (9.15)$$
Figure 9.7: The difference between the numerical and exact solutions for modified and unmodified solitons, and a comparison of the modified and unmodified initial conditions (lower right) for \( c = .98, \Delta t = .005 \) and \( \Delta x = .01 \).

Since the numerical solution is already second order accurate in \( u \), only (9.14) and (9.15) need to be verified along the numerical solution to check for second order accuracy with respect to the modified equations. Computing higher order corrections gets increasingly more complicated.

However, the modified equation for (9.12), given by

\[
\frac{\Delta t^2}{12} u_{ttt} = u_{xx} + \frac{\Delta x^2}{12} u_{xxxx} - \sin u,
\]

(9.16)
is easily obtained using Taylor expansions and is satisfied by the numerical solution to fourth order. Now it is reasonable to ask if this modified system of equations has soliton solutions (related results are discussed by Mann [35]). This can be answered by setting \( u(x, t) = u(x - ct) = u(\xi) \) in (9.16) and finding solutions of the boundary value problem

\[
(c^2 - 1)u'' - \frac{1}{12} (\Delta x^2 - c^4 \Delta t^2) u''' = -\sin u.
\]

(9.17)

Though it is not obvious how to solve this equation for a heteroclinic connection, we were able to find such a connection to high accuracy numerically. This approximation
Figure 9.8: Solution error plotted in log-log scale against $\Delta t$ for Test 1 (dashed), Test 2 (chain), and Test 3 (solid).

can be used to initialize the scheme (9.12) and this in turn yields a numerical solution for the PDE that is accurate to fourth order in $u$ with respect to both $\Delta t$ and $\Delta x$.

Now we can discuss numerical simulations for a 'modified soliton'. In these simulations we set $c = .98$, $\Delta t = .005$ and $\Delta x = .01$, with a spatial domain of $[-5, 5]$, and we run three different tests.

**Test 1:** ($\rho = 0$) Initialize the numerical scheme (9.11) with $u^{n,0} = u(x_n, 0)$, $v^{n,0} = u_t(x_n, 0)$ and $w^{n,0} = -u_x(x_n, 0)$ for $u$ given in (9.10).

**Test 2:** ($\rho = 1$) Initialize the numerical scheme (9.11) with $u^{n,0} = u(x_n, 0)$, and $v$ and $w$ modified according to (9.14)-(9.15) for $u$ given in (9.10).

**Test 3:** ($\rho = 3$) Initialize the scheme (9.12) using a numerically computed solution of (9.17), which we denote $U^0(x)$.

The lower right hand plot of Figure 9.7, plots the difference between the initial conditions $u^0(x)$ and $U^0(x)$. (It is interesting to note that this difference takes the form of the second derivative of the solution times a small parameter.) The other plots of this figure show the difference between the exact soliton solution (found by translating the initial soliton
Figure 9.9: Snapshots of the exact solution (dashed) and the numerical solution (solid) for the collision of two solitons with $c = .9$, $\Delta t = .01$ and $\Delta x = .02$.

profile according to change in time) and the numerical soliton solution. We see that the error found in Test 2 is smaller than the error found in Test 1, and the error found in Test 3 is smaller still, showing that the solution of the modified equation satisfies the numerical scheme more accurately.

Using log-log scale in Fig. 9.8, we plot the solution error against $\Delta t$, to check the order of convergence. For these results we have kept the ratio $\Delta t/\Delta x$ fixed, so change in $\Delta t$ directly corresponds to change in $\Delta x$. The dashed line shows that the numerical solution, obtained in Test 1 is first order accurate. The chain line shows that Test 2 yields second order accuracy in both $\Delta t$ and $\Delta x$. Finally, the solid line shows approximately forth order convergence for Test 3. The accuracy in Test 3 is limited by the fact that the reference soliton solution had to be computed numerically, and this is a delicate procedure due to the heteroclinic nature of the solution.

This is numerical evidence that the modified equations have soliton solutions, meaning that the exact solution behavior may be reproduced by the numerical scheme, and initializing the numerical scheme appropriately yields a numerical solution that is close to
Figure 9.10: Modified and unmodified total energy along the numerical solution for a soliton collision with $\Delta x = .02$ and $\Delta t = .01$.

Figure 9.11: Residual in modified and unmodified energy conservation laws as a function of time for a soliton collision with $\Delta x = .02$ and $\Delta t = .01$. 
an exact soliton solution.

**Soliton collisions**

Here we consider energy/momentum estimates in the collision of two solitons. (Related results can be found in [42, 51].) In the following simulations we use BEA-2 to obtain the modified energy/momentum conservation laws. In addition, we initial the Euler box scheme with

\[ u^0(x) = 4 \tan^{-1} \left( \exp \left[ \frac{-(x - 5)}{(1 - c^2)^{1/2}} \right] \right) - 4 \tan^{-1} \left( \exp \left[ \frac{-(x + 5)}{(1 - c^2)^{1/2}} \right] \right) \]

and \( v^0(x) = u^0(x) \), using (9.10), on a spatial domain \([-12 12]\) and a time domain \([0 10]\), for \( c = .9 \).

In Figure 9.9, we plot the numerical solution and the exact solution at different times, showing the motion of these two solitons through their collision, which takes place shortly after time \( t = 5 \). In the lower right hand plot we see that the numerical soliton has the same shape as the exact soliton, but appears to be moving at a slightly different speed. We note here the similarity of this result with the work of Durán and Sanz-Serna [20], who show the numerical solution of the NLS equation, discretized in time with a symplectic
integrator, is made up of a soliton traveling at a different speed.

Now, consider the numerical conservation of energy. Figure 9.10 plots the total energy and the modified total energy along the numerical solution, showing a large disturbance in the energy when the collision occurs. Similarly, Figures 9.11, 9.12, and 9.13, plot the residuals in modified and unmodified local energy and momentum conservation laws along the numerical solution as functions of space and time separately using definitions of the form (9.2). This also shows large differences in the residual at the place and the time of collision. However, the residuals return to small oscillations close to zero after the collision, showing that the overall energy and momentum conservation remain the same. We also find in each plot that the modified conservation laws are preserved to higher accuracy by the numerical solution.
Consider the sine-Gordon equation with added dissipation given by
\[ u_{tt} + au_t = u_{xx} + bu_x - \sin(u). \]

Discretizing with the Euler box scheme to get
\[ \delta_t^+ v^n + \delta_x^+ w^n = -\sin(u^n) - av^n - bw^n, \]
\[ \delta_t^- v^n = v^n, \]
\[ \delta_x^- w^n = -w^n. \]

Since a spatially discrete energy dissipation property of the form
\[ \partial_t E^n + \delta_x^+ F^n + av^n v_t^n + bw^n w_t^n = 0 \]
is satisfied by the spatially discrete equations for
\[ E^n = \frac{1}{2} ((v^n)^2 + (w^n)^2) - \cos(u^n) \quad \text{and} \quad F^n = v^{n-1} w^n, \]
we only consider this property in the following analysis with the understanding that similar results hold for a semi-discrete momentum dissipation property. Additionally, we use only BEA-2 to obtain modified dissipation laws here, in order to check their higher order convergence along the numerical solution. However, results concerning fully discrete dissipation properties and an application of BEA-3 are easily carried over from the previous analysis.

With this in mind, we consider the modified equation
\[ v^n + \frac{\Delta t}{2} v^n + \frac{\Delta t^2}{6} w^n = \delta_x^2 u^n - \sin(u^n) - av^n + b\delta_x^- u^n \]
\[ u^n - \frac{\Delta t}{2} u_t^n + \frac{\Delta t^2}{6} u_{tt}^n = v^n \]
with two modifications. Using these equations, one can easily show that the modified energy dissipation property
\[ \partial_t \tilde{E}_2^n + \delta_x^+ \tilde{F}_2^n + av^n v^n - bu^n \delta_x^- u^n = 0 \]
is satisfied for
\[ \tilde{E}_2^n = \frac{1}{2} ((v^n)^2 + (w^n u^n)^2) - \cos(u^n) + \frac{\Delta t}{2} v^n v^n + \frac{\Delta t^2}{6} (u^n u_{tt}^n - v^n v_{tt}^n) \]
Figure 9.14: In log-log scale, the residual in energy dissipation plotted along the numerical solution using the Euler scheme.

and

\[ \tilde{F}_2^n = -v^{n-1} \delta_x u^n. \]

We note here that only the conserved quantities have changed while the amount of dissipation remains the same. Hence, the scheme in some way preserves the qualitative solution behavior of the PDE even for \( a \) and \( b \) large.

In log-log scale, Figure 9.14 plots the \( \ell_\infty \)-norm of the residual in the modified and unmodified dissipation properties evaluated along the numerical solution for different values of \( \Delta t \). For each simulation we set \( a = 1 \) and \( b = 1 \), and keep \( \Delta x = 1/100 \) fixed for \( \Delta t = 1/100, 1/200, 1/400, 1/800, 1/1600 \) and \( 1/3200 \). The plot shows first order convergence for the original dissipation property and higher order convergence for each successive modification.
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Closing Remarks

In closing, we first summarize the results of this thesis. Then we can make conclusions based on these results, and determine how the objectives of this work have been achieved. Finally, we discuss the problems that remain unresolved as well as ideas for future work in multi-symplectic integration.

10.1 Summary and Conclusions

Throughout this text we have discussed the multi-symplectic integration of general Hamiltonian PDEs on a multi-symplectic structure with applications to Boussinesq, Korteweg-de Vries, nonlinear Schrödinger, and nonlinear wave equations. In particular, we have considered several local conservation laws associated with multi-symplectic PDEs, and have analyzed the behavior of certain multi-symplectic integrators through the effects they have on these conservation laws. The three finite-difference numerical methods discussed are the first order, explicit, one-step, symplectic Euler scheme, the second order, implicit, Preissman box scheme, and the second order, two-step, explicit midpoint scheme, covering a wide range of different types of methods.

It was first shown that each of these methods preserve the symplectic structure of the PDE by satisfying discrete multi-symplectic conservation laws exactly. In addition, each of these schemes satisfy semi-discrete conservation laws of energy and momentum exactly. The Preissman box scheme also preserves fully discrete conservation laws of energy and momentum for linear PDEs, as well as conservation laws associated with linear symmetries, making it a special scheme, but it is also the most expensive scheme of the three.

For linear PDEs, we derived numerical dispersion relations, which describe the numerical method. It was shown that the explicit midpoint scheme and, in some cases, the
Euler scheme introduce computational modes, in which case they should indeed not be considered multi-symplectic schemes.

Since fully discrete energy/momentum conservation laws are not in general satisfied for nonlinear problems with these schemes, we used backward error analysis and the idea of modified equations to study the effects of the discretization on these properties. Using Taylor series expansions, one can find a modified differential equation that is solved by the numerical solution to higher order. Then this modified equation yields modified energy/momentum conservation laws, which are satisfied by the numerical solution to higher order. Thus, we obtain a description of the effects of the numerical scheme on the behavior of the differential equation.

More specifically, a semi-discretization of the PDE gives a system of ODEs. Then, performing a formal backward error analysis on this system of ODEs gave modified equations that could be used to get modified semi-discrete conservation laws, provided the appropriate assumptions are made with regard to the smoothness of the solutions. The strength of this approach lies in the fact that there are semi-discrete conservation laws for the modified equations.

Yet, this approach has a shortcoming in that the modified equations did not represent the PDE but the system of ODEs resulting from a semi-discretization. Hence, an alternative modified equations approach was introduced in which a modified multi-symplectic PDE could be derived and used to obtain conservation laws that were preserved to higher order in both space and time. This approach proved to be more natural and useful. However, the higher order derivatives in the modified equations in this case cannot be eliminated, making rigorous estimates relating the numerical solution to the solution of the modified equation difficult to achieve.

Concerning linear PDEs, one finds that the series expansions in the modified equations converge to the numerical scheme, provided there are no computational modes, showing that the numerical solution is in fact the solution of the modified equation. Unfortunately, this has no direct implications for the relation of the numerical solution and the solution of the modified equation for nonlinear problems, due to the difference between linear and nonlinear solution behavior.

Following this analysis, we considered multi-symplectic PDEs with linear dissipation. Using an appropriate definition of conformal multi-symplecticity, it was shown that the Preissman scheme preserves this property numerically. However, one also finds that semi-
discrete energy and momentum dissipation properties are satisfied by the Preissman and Euler schemes, and that the modified equations satisfy energy and momentum dissipation properties.

Finally, a thorough application of these results to the sine-Gordon equation was made through numerical simulation. Altogether, these results have yielded a better understanding of the geometric properties of multi-symplectic integrators through the development of a modified equations approach, thus achieving our objectives. Furthermore, this approach can be used in the future analysis of other unsolved problems.

10.2 Unresolved Problems and Future Work

Clearly, this has not been an exhaustive study. One major question that remains concerns rigorous estimates showing that the exact solution of the modified equations is, in fact, the numerical solution. One would hope to show that the difference between the numerical solution and the solution of a suitably truncated modified equation is exponentially small, similar to the results obtained for the backward error analysis of ODEs. However, due to the nature of the modified equations, and the complex behavior of PDEs, this endeavor has proved to be very difficult.

A first step in this direction has been made by Oliver, West, and Wulff [47], who have derived exponential estimates in relation to momentum conservation, but the remaining questions are far from being answered. Another starting point for this research would be to consider multi-symplectic elliptic PDEs, allowing one to make use of a maximum principle.

Another related question, which still remains, concerns using these results to derive estimates for the accuracy of numerical solutions. A first step in this direction is to consider solitary wave solutions in extension to the results of Chapter 9. Specifically, one could search for a modified soliton that is satisfied by the modified equations [45]. This proved to be difficult for the sine-Gordon equation, but may be achievable for another equation such as the KdV equation [17]. One may also be able to prove the existence of a modified soliton in general, which would lead to further implications concerning the numerical reproduction of the qualitative solution behavior. Alternatively, one may be able to find a modified soliton that better represents the numerical solution [20] in both space and time. Then additional questions to consider concern the stability of such solitons [11, 12, 13, 14].
Moreover, symplectic schemes are known to have certain instabilities due to numerical resonance. This is a result of taking large time steps such that the stability condition $c\Delta t/\Delta x$ is close to one, or in the case of implicit methods, when $c\Delta t > \Delta x$. Thus, these schemes may not always be the best methods for solving conservative systems, but there are other conservative methods that do not become unstable as a result of resonance. Such schemes are non-symplectic, but they do satisfy discrete conservation laws of energy and momentum exactly (cf. [23, 24, 32, 54]). Further questions to consider are those related to a theoretical and numerical juxtaposition of multi-symplectic schemes with non-symplectic energy/momentum conserving schemes, or with other non-conservative schemes, concerning the geometric properties of the equations (cf. [3, 31, 51, 58]). In addition, one may be able to develop new higher order numerical methods based on the results of this thesis through the development of composition or splitting methods for PDEs or by using the modified equations of existing schemes.

As noted in the introduction, multi-symplectic integration is a recent topic of research. In many respects we have only ‘scratched the surface’ in this area of research, and the remaining unsolved problems may keep researchers busy for many years to come. Hence, we can look forward to the future development of multi-symplectic integration and backward error analysis with great anticipation and high expectation.
Recall that in order to extremize a function $f(x)$, by which we mean, find the maximum or minimum obtained by the function for some vector $x_0$, we must have $\nabla_x f(x_0) = 0$. This is easily observed by noting that, for any small scalar $\epsilon \neq 0$ and for any $\eta \neq 0$, $f(x_0)$ is the smallest value of $f$, implies $f(x_0 + \epsilon \eta) > f(x_0)$. Now, Taylor's theorem gives

$$f(x_0 + \epsilon \eta) = f(x_0) + \epsilon \eta^T \nabla_x f(x_0) + O(\epsilon^2),$$

and this shows that for $\epsilon \eta^T \nabla_x f(x_0) \neq 0$, a change in the sign of $\epsilon$ implies a change in the sign of $f(x_0 + \epsilon \eta) - f(x_0)$. But this is a contradiction, so we must have $\nabla_x f(x_0) = 0$.

The same idea applies when one wants to extremize functionals rather than functions, and this is the problem of variational calculus (cf. [33, Chapter 5]). Suppose we want to minimize the functional

$$I[y] = \int F(x, y(x), y'(x)) \, dx.$$  

Then the first variation, also called the variational derivative, of $I$, must be zero, meaning we must have

$$\frac{\partial}{\partial \epsilon} \bigg|_{\epsilon=0} I[y + \epsilon \eta] = 0.$$

This is true if and only if

$$0 = \lim_{\epsilon \to 0} \left( \frac{1}{\epsilon} (I[y + \epsilon \eta] - I[y]) \right)$$

$$= \lim_{\epsilon \to 0} \left( \frac{1}{\epsilon} \int (F(x, y + \epsilon \eta, y_{\eta} + \epsilon y_{\eta_{\eta}}) - F(x, y, y_{\eta})) \, dx \right)$$

$$= \lim_{\epsilon \to 0} \left( \frac{1}{\epsilon} \int \left( \frac{\partial F}{\partial y} \epsilon \eta + \frac{\partial F}{\partial y_{\eta}} \epsilon y_{\eta} \right) \, dx \right),$$

$$= \int \left( \frac{\partial F}{\partial y} - \frac{\partial}{\partial x} \frac{\partial F}{\partial y_{\eta}} \right) \eta \, dx,$$

where we have used Taylor's theorem and integration by parts. Thus, by the standard continuity argument, we require

$$F_y - \frac{\partial}{\partial x} F_{y_{\eta}} = 0,$$

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which is just the Euler-Lagrange equation for the functional $I$. This is how we arrive at
the definition of the variational derivative given by (1.9).

The importance of variational calculus in the study of Hamiltonian ODEs becomes ap­
parent with the statement of

Hamilton’s Principle: The trajectories of an object, given by $q$ in Section 1.1, render
the functional $\mathcal{L} = \int L \, dt$ stationary.

In other words, the first variation of $\mathcal{L}$ must be zero, and the connection between La­
grange’s equation and Hamilton’s equations noted in the first chapter is immediately
obvious.

As we turn our attention to Hamiltonian PDEs, the same principle holds. Given the
general Lagrangian functional $\mathcal{L} = \int \int L \, dx \, dt$ for

$$L = L(z, z_t, z_x, z_{tt}, z_{tx}, z_{xx}, \ldots) ,$$

we find that the first variation of $\mathcal{L}$ is zero if and only if

$$0 = L_{z_t} - \frac{\partial_t L_{z_t}}{dt} + \frac{\partial_x L_{z_x}}{dx} + \frac{\partial_{tt} L_{z_{tt}}}{dt} + \frac{\partial_{tx} L_{z_{tx}}}{dx} + \frac{\partial_{xx} L_{z_{xx}}}{dx} - \ldots ,$$

where we must use integration by parts numerous times. This is how we arrive at
the Euler-Lagrange equations used throughout the text, and given the appropriate La­
grangian the derivation of the multi-symplectic formulation is clear.

Since there is a direct correlation between the Lagrangian and the multi-symplectic struc­
ture, it is natural to appeal to a discrete Lagrangian, and hence, a discrete variational
principle, in order to preserve the multi-symplectic structure of the related PDE. Given
the Lagrangian density

$$L = L(z, z_t, z_x) ,$$

we approximate the Lagrangian functional with

$$\mathcal{L} = \sum_{n,i} L^{n,i} \quad \text{for} \quad L^{n,i} = L(z^{n,i}, z^{n-\frac{1}{2},i}, z^{n-\frac{1}{2},i+1}, z^{n-\frac{1}{2},i-1}) \, \Delta t \Delta x \approx \int_{t_{n-1}}^{t_n} \int_{x_{n-1}}^{x_n} L \, dx \, dt ,$$

for small enough $\Delta t$ and $\Delta x$. In order to extremize this discrete functional, we set
$\partial \mathcal{L} / \partial z^{n,i} = 0$, which implies the discrete Euler-Lagrange equation (cf. [28, section 6.6])

$$0 = \partial_1 L(z^{n,i}, z^{n-\frac{1}{2},i}, z^{n-\frac{1}{2},i+1}, z^{n-\frac{1}{2},i-1}) + \partial_2 L(z^{n+\frac{1}{2},i}, z^{n,i}, z^{n-\frac{1}{2},i+1}) + \partial_3 L(z^{n+\frac{1}{2},i}, z^{n+\frac{1}{2},i-1}, z^{n,i}) ,$$

(A.2)
where \( \partial_j L \) is the partial derivative of \( L \) with respect to the \( j \)th argument. Given a particular Lagrangian and a particular discretization, this is then used to derive a numerical scheme for the associated PDE.

To demonstrate this for a specific discretization, discretize (A.1) by

\[
L^{n,i} = L \left( z^{n,i}, \delta_z^{-,n,i}, \delta_z^{+,n,i} \right) = L \left( z^{n,i}, x_{n-1,i}, z^{n+1,i} \right).
\]

Then by the discrete Euler-Lagrange equation (A.2) we get

\[
0 = \left( \frac{\partial L}{\partial z^{n,i}} + \frac{\partial L}{\partial \delta_z^{-,n,i}} \right) + \left( \frac{\partial L}{\partial \delta_z^{+,n,i}} + \frac{\partial L}{\partial \delta_x^{-,n,i}} \right)
+ \frac{\partial L}{\partial \delta_x^{+,n,i} + \frac{\partial L}{\partial \delta_z^{+,n,i} + \frac{\partial L}{\partial \delta_x^{+,n,i}}}.
\]

which implies

\[
0 = \frac{\partial L}{\partial z^{n,i}} + \frac{1}{\Delta t} \left( \frac{\partial L}{\partial \delta_t^{-,n,i}} - \frac{\partial L}{\partial \delta_t^{+,n,i}} \right) + \frac{1}{\Delta x} \left( \frac{\partial L}{\partial \delta_x^{-,n,i}} - \frac{\partial L}{\partial \delta_x^{+,n,i}} \right).
\]

Thus, we arrive at the discrete Euler-Lagrange equation

\[
\delta_t^+ L^{n,i} - \delta_x^- \left( \frac{\partial S}{\partial z^{n,i}} \right) = 0,
\]

which is used throughout the thesis.

To show this more explicitly for the Lagrangian

\[
L^{n,i} = \left( z^{n,i} + \delta_z^{-,n,i} \right) + \left( z^{n,i} + \delta_z^{+,n,i} \right) - S(z^{n,i}),
\]

we use the discrete variational principle to get

\[
\nabla_z S(z^{n,i}) = \frac{1}{\Delta t} \left( K_+ \left( z^{n,i} - z^{n-1,i} \right) - K_- \left( z^{n,i} - z^{n+1,i} \right) \right)
+ \frac{1}{\Delta x} \left( L_+ \left( z^{n,i} - z^{-1,i} \right) - L_- \left( z^{n,i} - z^{n+1,i} \right) \right)
= K_+ \delta_x^+ z^{n,i} + K_- \delta_x^- z^{n,i} + L_+ \delta_x^+ z^{n,i} + L_- \delta_x^- z^{n,i},
\]

which is the Euler box scheme, and we see that this is equivalent to the derivation in subsection 2.2.1. Alternatively, one could simply use the discrete Euler-Lagrange equation to get

\[
K_-^T \delta_t^+ z^{n,i} + L_-^T \delta_x^+ z^{n,i} - K_- \delta_t^- z^{n,i} - L_- \delta_x^- z^{n,i} + \nabla_z S \left( z^{n,i} \right) = 0,
\]

which is again just the Euler box scheme (3.1).
Proof of Theorem 5.1

Here we show that given any Hamiltonian of the form (5.13), a spatially discrete energy conservation law can be derived, and we show how to construct this conservation law through simple recursion. We first introduce the notation

\[
\delta_a^j := \begin{cases} 
\delta_a^{-1}, & \forall j \text{ even} \\
\delta_a^j, & \forall j \text{ odd}
\end{cases} \quad \text{and} \quad \delta_a^{j+} := \begin{cases} 
\delta_a^{j-1}, & \forall j \text{ odd} \\
\delta_a^{j+}, & \forall j \text{ even}
\end{cases}
\]

where \( j = 0, 1, 2, \ldots \) and \( \delta_a^0 = 1 \). To clarify, the operator \( \delta_a^{2j} \) is just the operator \( \delta_a^2 \) acting \( j \) times, e.g. \( \delta_a^4 = \delta_a^2 \delta_a^2 \). Based on these definitions, we have

\[
\delta_a^j \delta_a^{-j} = \begin{cases} 
1, & \forall j \text{ even} \\
0, & \forall j \text{ odd}
\end{cases}
\]

and similarly

\[
\delta_a^j \delta_a^{-j} = \begin{cases} 
1, & \forall j \text{ odd} \\
0, & \forall j \text{ even}
\end{cases}
\]

Therefore,

\[
\delta_a^j \delta_a^{-j} \mu^n = \delta_a^{-j+1} \mu^{n+1} = \delta_a^{j+1} \mu^{n+1} = \delta_a^{j+1} \mu^n
\]

and

\[
\delta_a^j \delta_a^{-j} \mu^n = \delta_a^{j+1} \mu^n,
\]

where we have used

\[
\delta_a^j \mu^n = \delta_a^{-j} \mu^{n+1} \quad \text{and} \quad \delta_a^{-j} \mu^n = \delta_a^j \mu^{n-1},
\]

and we make use of these identities throughout this section.

Now consider the Hamiltonian (5.13) with

\[
E^n = E(u^n, v^n, \delta_u^{-1} u^n, \delta_v^{-1} v^n, \delta_u^2 u^n, \delta_v^2 v^n, \ldots, \delta_u^M u^n, \delta_v^M v^n)
\]

for any \( M \) and \( N \). If we define

\[
\mu_j^n = E\delta_u^{-j} u^n \quad \text{and} \quad \nu_j^n = E\delta_v^{-j} v^n,
\]

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then, using the Hamiltonian equations (3.8), we find that the equations of motion are given by the system of ODEs
\[ \dot{u}^n = \sum_{k=0}^{N} (-1)^k \delta_2^k \mu_k^n, \quad \dot{\nu}^n = \sum_{k=0}^{M} (-1)^{k+1} \delta_2^{k+} \mu_k^n. \]

Then a conservation law is found by evaluating
\[ \partial_t E^n = \sum_{k=0}^{N} \nu_k^n \delta_2^{k-} \phi^n + \sum_{k=0}^{M} \mu_k^n \delta_2^{k+} \dot{u}^n. \]

A simple substitution yields
\[ \partial_t E^n = \sum_{j=0}^{N} \sum_{i=0}^{M} (-1)^{i+1} \nu_j^i \delta_2^{i-} \delta_2^{j+} \mu_i^j + \sum_{i=0}^{M} \sum_{j=0}^{N} (-1)^{j+1} \mu_i^j \delta_2^{i+} \delta_2^{j-} \nu_j^i, \]

which is equivalent to
\[ \partial_t E^n = \sum_{i=0}^{M} \sum_{j=0}^{N} \left( (-1)^j \mu_i^j \delta_2^{i+} \delta_2^{j+} \right) + \left( (-1)^i \nu_j^i \delta_2^{i+} \delta_2^{j-} \right), \]

where we use
\[ \delta_2^{i-} \delta_2^{j+} = \begin{cases} 
\delta_2^{i+j}, & i+j \text{ even} \\
\delta_2^{i+j+}, & i \text{ odd, } j \text{ even} \\
\delta_2^{i+j-}, & i \text{ even, } j \text{ odd}
\end{cases} \quad \text{and} \quad \delta_2^{i+} \delta_2^{j+} = \begin{cases} 
\delta_2^{i+j}, & i+j \text{ even} \\
\delta_2^{i+j+}, & i \text{ even, } j \text{ odd} \\
\delta_2^{i+j-}, & i \text{ odd, } j \text{ even}
\end{cases}
\]

along with
\[ \delta_2^{i-} = \delta_2^{i+} \quad \text{and} \quad \delta_2^{j-} = \delta_2^{j+}. \]

The spatially discrete energy conservation law can now be found by showing that the individual terms of (B.1) can be written as the sum of finite difference approximations. Consider individual terms of the double sum (B.1), and let \( m = i + j \). In order to derive a spatially discrete energy conservation law, we must be able to write
\[ \mu^n \delta_2^m (-1)^i \nu^n + (-1)^{m+1} \nu^n \delta_2^m (-1)^{i+1} \mu^n = \sum_k \delta_2^k g_2^k, \]

where \( g_2^k \) depends on \( \mu^n \) and \( \nu^n \) as well as \( i \) and \( j \). Here we compute these quantities for arbitrary values of \( m \), and write the appropriate recursion relation based on the patterns that develop.

First consider the case \( i + j \) even, with \( i < j \) and \( i, j = 0, 1, 2, \ldots, m \). Then we have
\[ \delta_2^+ \mu^n \delta_2^+ \nu^n - \delta_2^+ \nu^n \delta_2^+ \mu^n \]
\[ = \frac{1}{\delta_2^+} \left( \delta_2^+ \mu^n \delta_2^+ \nu^n - \delta_2^+ \nu^n \delta_2^+ \mu^n \right), \]
and by adding and subtracting the terms
\[ \delta_n^+ \nu^{n+1} \delta_n^{r-1,-\nu^n+1} \quad \text{and} \quad \delta_n^+ \nu^{n+1} \delta_n^{r-1,-\nu^n+1} \]
we obtain
\[ \delta_n^+ \mu_n \delta_n^+ \nu^n - \delta_n^+ \nu \delta_n^{r-1} \mu_n = \delta_n^+ \left( \delta_n^+ \mu_n \delta_n^{r-1,-\nu^n} - \delta_n^+ \delta_n^+ \nu \delta_n^{r-1,-\nu^n} \right) - \left( \delta_n^+ \mu_n \delta_n^{r-1,-\nu^n} - \delta_n^+ \nu \delta_n^{r-1,-\nu^n} \right). \]

Realizing that the last two terms on the right hand side of this equation are of the same form as the left hand side, we can continue in this manner until we reach the final term with \( r = j \), and we have in this case
\[ \delta_n^+ \mu_n \delta_n^+ \nu^n - \delta_n^+ \nu \delta_n^{r-1} \mu_n = 0. \]

Therefore, for \( m \) even
\[ \mu_n \delta_n^m \nu^n - \nu \delta_n^m \mu_n = \sum_{k=0}^{m} (-1)^k \left( \delta_n^+ \left( \delta_n^k \mu_n \delta_n^{m-k-1,-\nu^n} - \delta_n^+ \nu \delta_n^{m-k-1,-\nu^n} \right) \right). \]

Now consider the case \( r + j \) odd, with \( r < j \) and \( r, j = 0, 1, 2, \ldots, m \). Then we have
\[ \delta_n^+ \mu_n \delta_n^+ \nu^n + \delta_n^+ \nu \delta_n^{r-1,-\nu^n} \]
\[ = \frac{1}{\Delta x} \left( \delta_n^+ \mu_n \delta_n^{r-1,-\nu^n+1} - \delta_n^+ \mu_n \delta_n^{r-1,-\nu^n} + \delta_n^+ \nu \delta_n^{r-1,+\nu^n} - \delta_n^+ \nu \delta_n^{r-1,-\nu^n} \right) \]
and adding and subtracting the terms
\[ \delta_n^+ \nu^{n+1} \delta_n^{r-1,-\nu^n+1} \quad \text{and} \quad \delta_n^+ \nu^{n-1} \delta_n^{r-1,+\nu^n} \]
we get
\[ \delta_n^+ \mu_n \delta_n^+ \nu^n + \delta_n^+ \nu \delta_n^{r-1,-\nu^n} \mu_n = \delta_n^+ \left( \delta_n^+ \mu_n \delta_n^{r-1,-\nu^n} + \delta_n^+ \nu \delta_n^{r-1,+\nu^n} \right) - \left( \delta_n^+ \mu_n \delta_n^{r-1,-\nu^n} + \delta_n^+ \nu \delta_n^{r-1,+\nu^n} \right). \]

Just as before we see the beginning of a cycle, and this process can be repeated until we reach the final term. Setting \( r = k \) and \( j = k + 1 \) for some constant \( 0 < k < m \), the final term takes the form
\[ \delta_n^k \mu_n \delta_n^{k+1,-\nu^n} + \delta_n^k \nu \delta_n^{k+1,+\mu^n} \]
\[ = \frac{1}{\Delta x} \left( \delta_n^k \mu_n \delta_n^{k+1,-\nu^n+1} - \delta_n^k \nu \delta_n^{k+1,+\mu^n} + \delta_n^k \nu \delta_n^{k+1,-\nu^n} + \delta_n^k \nu \delta_n^{k+1,+\mu^n} - \delta_n^k \nu \delta_n^{k+1,-\nu^n} \right) \]
\[ = \frac{1}{\Delta x} \left( \delta_n^k \nu \delta_n^{k+1,+\mu^n} \right). \]
Hence, for $m$ odd we can write $m = 2\ell + 1$, and we have

\begin{align*}
\mu^n \delta_{m} + \nu^n + \nu^n \delta_{m+1} - \mu^n &= \delta_{m}^+ \left( \delta_{m}^+ - \nu^n \delta_{m}^+ + \mu^{n-1} \right) \\
&+ \sum_{k=1}^{\ell} (-1)^{k-1} \delta_{m}^+ \left( \delta_{m}^{k-1} + \nu^n \delta_{m-k-1} - \nu^n \right) \\
&+ \sum_{k=1}^{\ell} (-1)^{k-1} \delta_{m}^- \left( \delta_{m}^{k-1} + \nu^n \delta_{m-k+1} + \mu^n \right).
\end{align*}

Now, making the appropriate substitutions into \((B.1)\) yields a spatially discrete energy conservation law, and the proof is complete.


