

A new construction of modified equations for variational integrators

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Abstract

The construction of modified equations is an important step in the backward error analysis of symplectic integrator for Hamiltonian systems. In the context of partial differential equations, the standard construction leads to modified equations with increasingly high frequencies which increase the regularity requirements on the analysis. In this paper, we consider the next order modified equations for the implicit midpoint rule applied to the semilinear wave equation to give a proof-of-concept of a new construction which works directly with the variational principle. We show that a carefully chosen change of coordinates yields a modified system which inherits its analytical properties from the original wave equation. Our method systematically exploits additional degrees of freedom by modifying the symplectic structure and the Hamiltonian together.

1 Introduction

Over the last two decades, backward error analysis has emerged as a useful tool for proving conservation properties of numerical time integrators for differential equations. In a nutshell, one constructs a modified differential equation which is approximated by the numerical method to some higher order than the original equation and which possesses analogous conservation laws. Thus, the numerical scheme is nearly conservative on time scales over which it approximates the solution of the modified equation. Some of the strongest and most general results for ordinary differential equations were obtained by Benettin and Giorgilli [2] and Hairer and Lubich [14], using ideas which go back to Neishtadt [23], who optimally truncate an asymptotic series for the modified vector field to prove that a class of symplectic schemes when applied to Hamiltonian ordinary differential equations preserve the energy exponentially well over exponentially long times in the step size. Similar ideas appear in [15, 18, 29].

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While this construction formally extends to Hamiltonian partial differential equations, in this case the asymptotic series for the modified equation will generally contain arbitrary powers of unbounded operators, thereby breaking the natural ordering of the terms in the asymptotic series. In particular, the standard construction in the context of hyperbolic equations such as the semilinear wave equation, fails in the practically relevant regime when the scaling of time vs. space step is close to the CFL limit. This problem has been partially addressed in a number of ways. Cano [5] proves an exponential backward error analysis result conditional on a number of conjectures. Moore and Reich [22] and Islas and Schober [17] provide a formal backward error analysis in a multisymplectic setting. Under strong regularity assumptions on the true solution, [32] show that the occurrence of unbounded operators in the modified vector field only leads to loss of order in the exponents of the backward error estimates. Sometimes, non-standard modified equations can be helpful, such as in the result of [27] on the approximate numerical preservation of the momentum invariant. Cohen, Hairer, and Lubich [6] obtained results on polynomially long times for weakly nonlinear wave equations using the method of modulated Fourier expansions. Finally, there is a large body of recent work on the backward error analysis of splitting methods applied to partial differential equations [8, 9, 10, 11, 12]. However, the question whether strong results for generic solutions, i.e. solutions which are neither small nor analytic, can be obtained remains open.

Modified equations are clearly not unique. Various expressions appearing beyond the leading order of the asymptotic series can be consistently replaced by using the modified equation itself. In principle, one can use such substitutions to remove the occurrence of high frequencies at high orders of the modified system. Unfortunately, this process will generally break the Hamiltonian structure.

This paper is motivated by the observation that a large class of symplectic integrators can be derived via a discrete variational principle. Elementary examples appear in Wendlandt and Marsden [31] and Marsden and West [21] who, in particular, show that the implicit midpoint rule arises via a simple finite difference approximation of the action integral. More generally, a large number of symplectic schemes arises as variational integrators [19, 21]; in particular, Leok and Zhang [20] show that it is also possible to obtain variational integrators on the Hamiltonian side, which extends the concept to systems with degenerate Hamiltonians.

In this paper, we demonstrate that it is possible to construct modified equations via the variational principle. A naive variational construction has the apparent drawback that the order of time derivatives in the modified equations increases with the order to which the modified equations are constructed, i.e., the phase space gets increasingly bigger. Since the higher time derivatives appear at higher orders of the expansion, this construction leads to singular perturbation problems with multiple fast time scales. Still, the original slow dynamics lives on a submanifold in this larger phase space. Our main point is that we can approximately restrict to this submanifold by the use of a near-identity change of variables which moves all fast degrees of freedom beyond the truncation order of the asymptotic expansion. We call this approach the *method of degenerate variational asymptotics*; it is motivated by earlier work on model reduction for rapidly rotating fluid flow [24, 25].

The current work is the first proof-of-concept for this approach. We consider a simple, yet nontrivial special case: the next-order modified equations for the implicit midpoint

scheme applied to the semilinear wave equation. We find that the new modified equations do not admit frequencies beyond the scale already present in the original partial differential equation. In particular, unlike the modified equations which arise from the conventional construction, they have a dispersion relation for linear waves which has a finite limit as the wave number k tends to infinity. This behavior coincides qualitatively with that of the implicit midpoint rule itself, which also possesses a finite highest numerical frequency in a time-semidiscrete analysis [3]. Moreover, we can show that the full nonlinear modified equations are well-posed—locally in time but for a time interval which is independent of the time step parameter—precisely in the energy space which arises naturally from the modified Hamiltonian.

The paper is structured as follows. After the introduction of the semilinear wave equation in Section 2, Section 3 gives a brief derivation of the implicit midpoint scheme as a variational integrator. In Section 4, we recall the standard Hamiltonian construction of the modified vector field and show that the result is only useful under restrictive time-step assumptions. Section 5 explains the naive variational construction; Section 6 introduces the method of degenerate variational asymptotics, which constrains the phase space of the modified equations to the slow degrees of freedom. After addressing the question of consistent initialization of the modified system in Section 7, in Section 8 we give a numerical evidence that the new modified equations indeed perform as claimed. In Section 9, we present an analytic framework in which the nonlinear elliptic operator which arises in the formulation of the new modified equations is invertible, and we recast them in the form of a semilinear evolution equation, thereby obtaining a proof of local well-posedness in the natural energy space. Section 10 discusses the extension of our ideas to higher order in the time step parameter. Finally, Section 11 concludes with a brief discussion of the results.

2 The semilinear wave equation

We consider the semilinear wave equation on the circle \mathbb{T} ,

$$\ddot{u} = \partial_{xx}u + f(u), \quad (1)$$

where $u = u(x, t)$ and we write $\dot{u} \equiv \partial_t u$. It arises as the Euler–Lagrange equation with Lagrangian $L: Q \times Q \rightarrow \mathbb{R}$ given by

$$L(u, \dot{u}) = \int_{\mathbb{T}} \frac{1}{2} \dot{u}^2 - \frac{1}{2} (\partial_x u)^2 + V(u) \, dx \quad (2)$$

with $f = V'$ and Q being a space of sufficiently smooth functions on \mathbb{T} ; we also assume that V is smooth.

Writing $p = \dot{u}$, the semilinear wave equation is Hamiltonian with conserved energy

$$H(p, u) = \int_{\mathbb{T}} \frac{1}{2} p^2 + \frac{1}{2} (\partial_x u)^2 - V(u) \, dx. \quad (3)$$

In addition, the Lagrangian is invariant under space translations. Hence, Noether’s theorem implies conservation of momentum

$$J(u, p) = \int_{\mathbb{T}} p \partial_x u \, dx. \quad (4)$$

It is often convenient to write the semilinear wave equation as a first order system: setting

$$U = \begin{pmatrix} u \\ p \end{pmatrix}, \quad A = \begin{pmatrix} 0 & 1 \\ \partial_{xx} & 0 \end{pmatrix}, \quad \text{and} \quad B(U) = \begin{pmatrix} 0 \\ f(u) \end{pmatrix}, \quad (5)$$

equation (1) takes the form

$$\dot{U} = AU + B(U). \quad (6)$$

3 Variational integrators

Consider uniform grid on time interval $[0, T]$ with mesh size $h = T/n$. Following [30, 31], we consider the discrete variational principle associated with the temporal semidiscretization, namely, find u_0, \dots, u_n which are a stationary point of the discrete action

$$\mathbb{S} = \sum_{k=0}^{n-1} \mathbb{L}(u_k, u_{k+1}; h), \quad (7)$$

subject to variations which leave the temporal endpoints u_0 and u_n fixed. The discrete variational principle $\delta\mathbb{S}(u_1, \dots, u_{n-1}) = 0$ yields the discrete Euler–Lagrange equation

$$D_1\mathbb{L}(u_k, u_{k+1}; h) + D_2\mathbb{L}(u_{k-1}, u_k; h) = 0 \quad (8)$$

for $k = 1, \dots, n-1$.

A symplectic scheme of second order for the semilinear wave equation is obtained by taking the discrete Lagrangian

$$\mathbb{L}(u_k, u_{k+1}; h) = h L\left(\frac{u_k + u_{k+1}}{2}, \frac{u_{k+1} - u_k}{h}\right). \quad (9)$$

Introducing the discrete Legendre transform [15, p. 194],

$$\begin{aligned} p_k &\equiv -D_1\mathbb{L}(u_k, u_{k+1}; h) \\ &= \frac{\delta L}{\delta \dot{u}}\left(\frac{u_k + u_{k+1}}{2}, \frac{u_{k+1} - u_k}{h}\right) - \frac{h}{2} \frac{\delta L}{\delta u}\left(\frac{u_k + u_{k+1}}{2}, \frac{u_{k+1} - u_k}{h}\right), \end{aligned} \quad (10)$$

and using the discrete Euler–Lagrange equation (8), we obtain

$$\begin{aligned} p_{k+1} &= D_2\mathbb{L}(u_k, u_{k+1}; h) \\ &= \frac{\delta L}{\delta \dot{u}}\left(\frac{u_k + u_{k+1}}{2}, \frac{u_{k+1} - u_k}{h}\right) + \frac{h}{2} \frac{\delta L}{\delta u}\left(\frac{u_k + u_{k+1}}{2}, \frac{u_{k+1} - u_k}{h}\right). \end{aligned} \quad (11)$$

The variations on the right of (10) and (11) read

$$\frac{\delta L}{\delta \dot{u}}(u, \dot{u}) = \dot{u} \quad \text{and} \quad \frac{\delta L}{\delta u}(u, \dot{u}) = \partial_{xx}u + f(u), \quad (12)$$

where we identify Q with a subspace of Q^* via the L^2 inner product. We now introduce an intermediate integration stage via

$$u_{k+1/2} = \frac{u_k + u_{k+1}}{2} \quad \text{and} \quad p_{k+1/2} = \frac{p_k + p_{k+1}}{2}. \quad (13)$$

Then, taking the sum and difference of (10) and (11), respectively, we obtain

$$u_{k+1} = u_k + h p_{k+1/2}, \quad (14a)$$

$$p_{k+1} = p_k + h \left(\partial_{xx} u_{k+1/2} + f(u_{k+1/2}) \right). \quad (14b)$$

Written in this form, the scheme is clearly recognized as the implicit midpoint rule, which is, in fact, a second order Gauss–Legendre Runge–Kutta method. To obtain a practical numerical scheme, it is better to replace the definition of the intermediate integration stage by the equivalent expressions [4]

$$u_{k+1/2} = u_k + \frac{h}{2} p_{k+1/2}, \quad (15a)$$

$$p_{k+1/2} = p_k + \frac{h}{2} \left(\partial_{xx} u_{k+1/2} + f(u_{k+1/2}) \right). \quad (15b)$$

In terms of the vector notation introduced at the end of Section 2, (15) reads

$$U_{k+1/2} = U_k + \frac{h}{2} \left(A U_{k+1/2} + B(U_{k+1/2}) \right), \quad (16)$$

or

$$U_{k+1/2} = \left(1 - \frac{h}{2} A \right)^{-1} \left(U_k + \frac{h}{2} B(U_{k+1/2}) \right). \quad (17)$$

For sufficiently small h and a suitable choice of function space, the operator on the right side of (17) is a contraction, so that the intermediate stage vector $U_{k+1/2}$ can be found iteratively.

Similarly, noting that $1 + hA \left(1 - \frac{h}{2} A \right)^{-1} = \left(1 + \frac{h}{2} A \right) \left(1 - \frac{h}{2} A \right)^{-1}$, we can write (14) in the form

$$U_{k+1} = S(hA) U_k + h \left(1 - \frac{h}{2} A \right)^{-1} B(U_{k+1/2}), \quad (18)$$

where

$$S(z) = (1 + z/2)(1 - z/2)^{-1} \quad (19)$$

is known as the *stability function* of the method. Again, equation (18) considered, for instance, in a Sobolev space $H^s(\mathbb{T})$ has only bounded operators on its right hand side, so the time- h map of the scheme does not lose derivatives. For this reason, the system (17) and (18) is the preferred form for numerical implementation of the implicit midpoint scheme.

4 Backward error analysis on the Hamiltonian side

In this section, we give an elementary derivation of the standard Hamiltonian modified equation which corresponds to the implicit midpoint rule up to terms of $O(h^4)$. The procedure is that of Hairer, Lubich, and Wanner [15, Chapter IX]; our presentation reduces the procedure to the special case at hand.

We use the following notation. Let $U: [0, T] \rightarrow Q \times Q^*$ be a curve satisfying an autonomous equation of the form

$$\dot{U} = F(U) \quad (20)$$

with $U(kh) = U_k$ for $kh \in [0, T]$. Let us fix k and Taylor expand about $t_0 = kh$. On one hand,

$$U_{k+1} = U(t_0 + h) = U_k + \dot{U}_k h + \frac{1}{2} \ddot{U}_k h^2 + \frac{1}{6} U_k^{(3)} h^3 + O(h^4), \quad (21)$$

where $\dot{U}_k \equiv U'(kh)$, $\ddot{U}_k \equiv U''(kh)$, and $U_k^{(3)} \equiv U^{(3)}(kh)$. On the other hand, U_{k+1} is determined by the implicit midpoint rule

$$\begin{aligned} U_{k+1} &= U_k + h F(U_{k+1/2}) \\ &= U_k + F(U_k) h + \frac{1}{2} F'(U_k) \dot{U}_k h^2 + \frac{1}{8} F''(U_k) (\dot{U}_k, \dot{U}_k) h^3 + \frac{1}{4} F'(U_k) \ddot{U}_k h^3 + O(h^4). \end{aligned} \quad (22)$$

Since the implicit midpoint rule is a symmetric method, only terms at even powers of h appear in the modified equation [15]. Therefore, to determine the modified equation including terms of $O(h^2)$, we seek a vector field F_2 such that

$$\dot{U}_k = F(U_k) + F_2(U_k) h^2 + O(h^3). \quad (23)$$

We note that (23) implies the approximate identities

$$\ddot{U}_k = F'(U_k) \dot{U}_k + O(h^2), \quad (24a)$$

$$U_k^{(3)} = F''(U_k) (\dot{U}_k, \dot{U}_k) + F'(U_k) \ddot{U}_k + O(h^2). \quad (24b)$$

Then, equating (21) and (22), using (23) and (24) to eliminate all derivatives, we obtain

$$F_2(U_k) = \frac{1}{12} F'(U_k) F'(U_k) F(U_k) - \frac{1}{24} F''(U_k) (F(U_k), F(U_k)). \quad (25)$$

In the particular case of the semilinear wave equation, where

$$F(U) = AU + B(U), \quad (26)$$

we obtain by direct calculation that

$$F_2(U) = \frac{1}{12} \begin{pmatrix} \partial_{xx} p + f'(u)p \\ (\partial_{xx} + f'(u))(\partial_{xx} u + f(u)) \end{pmatrix} - \frac{1}{24} \begin{pmatrix} 0 \\ f''(u) p^2 \end{pmatrix}. \quad (27)$$

Hence, the modified equation up to terms of order $O(h^4)$ reads

$$\dot{u} = \left[1 + \frac{1}{12} h^2 (\partial_{xx} + f'(u)) \right] p, \quad (28a)$$

$$\dot{p} = \left[1 + \frac{1}{12} h^2 (\partial_{xx} + f'(u)) \right] (\partial_{xx} u + f(u)) - \frac{1}{24} h^2 f''(u) p^2. \quad (28b)$$

It is straightforward to verify that modified equations (28) define a Hamiltonian system with Hamiltonian

$$H_{\text{mod}}(p, u) = H(p, u) + \frac{1}{24} h^2 \int_{\mathbb{T}} f'(u) p^2 - (\partial_x p)^2 - (\partial_{xx} u + f(u))^2 dx. \quad (29)$$

It is generally true that symplectic Runge–Kutta schemes applied to Hamiltonian systems yield a Hamiltonian modified equation at any order [15, Section IX.3].

The difficulty with using the modified system (28) for the purpose of backward error analysis can be seen as follows. We consider, for simplicity, the linear case when $f \equiv 0$.

Writing k to denote the spatial wave number, equation (6) in the space-frequency domain reads

$$\partial_t \hat{U}_k = \left(1 - \frac{1}{12} h^2 k^2\right) \begin{pmatrix} 0 & 1 \\ -k^2 & 0 \end{pmatrix} \hat{U}_k. \quad (30)$$

We observe that the additional factor $h^2 k^2$ will introduce fast frequencies into the modified dynamics unless we restrict the admissible wave numbers and time steps. More generally, it can be shown that the modified vector field will be an asymptotic series in hk , so that the series will be properly ordered only if we restrict to a finite dimensional subspace of wave numbers—a discretization in space—and if $h = o(k_{\max}^{-1})$. This excludes the practically relevant regime of time steps as large as permitted by the CFL condition where $h \sim k_{\max}^{-1}$; see, for example, the discussion in [6].

5 Backward error analysis on the Lagrangian side

We now turn to the question of how we can derive modified equations using the variational principle which underlies the semilinear wave equation.

The notation here is analogous to the notation used in the previous section: let $u: [0, T] \mapsto Q$ be a curve in Q such that $u(kh) = u_k$ for $kh \in [0, T]$. Again, we fix k and Taylor expand u and \dot{u} about $t_0 = kh$. Then, for $|t| \leq h$,

$$u(kh + t) = u_k + \dot{u}_k t + \frac{1}{2} \ddot{u}_k t^2 + \frac{1}{6} u_k^{(3)} t^3 + O(h^4), \quad (31a)$$

$$\dot{u}(kh + t) = \dot{u}_k + \ddot{u}_k t + \frac{1}{2} u_k^{(3)} t^2 + O(h^3), \quad (31b)$$

where $\dot{u}_k \equiv \dot{u}(kh)$, $\ddot{u}_k \equiv \ddot{u}(kh)$, and $u_k^{(3)} \equiv u^{(3)}(kh)$. In particular, setting $t = h$, we have

$$u_{k+1} = u_k + \dot{u}_k h + \frac{1}{2} \ddot{u}_k h^2 + \frac{1}{6} u_k^{(3)} h^3 + O(h^4). \quad (32)$$

Substituting (32) into the discrete Lagrangian, we obtain

$$\begin{aligned} \mathbb{L}(u_k, u_{k+1}; h) &= h L(u_k + \frac{1}{2} h \dot{u}_k + \frac{1}{4} h^2 \ddot{u}_k + O(h^3), \dot{u}_k + \frac{1}{2} h \ddot{u}_k + \frac{1}{6} h^2 u_k^{(3)} + O(h^3)) \\ &= h \int_{\mathbb{T}} \frac{1}{2} (\dot{u}_k + \frac{1}{2} h \ddot{u}_k + \frac{1}{6} h^2 u_k^{(3)})^2 - \frac{1}{2} (\partial_x u_k + \frac{1}{2} h \partial_x \dot{u}_k + \frac{1}{4} h^2 \partial_x \ddot{u}_k)^2 dx \\ &\quad + h \int_{\mathbb{T}} V(u_k) + f(u_k) (\frac{1}{2} h \dot{u}_k + \frac{1}{4} h^2 \ddot{u}_k) + \frac{1}{8} h^2 f'(u_k) \dot{u}_k^2 dx + O(h^4) \\ &= h L(u_k, \dot{u}_k) + \frac{1}{2} h^2 \int_{\mathbb{T}} \ddot{u}_k \dot{u}_k - \partial_x u_k \partial_x \dot{u}_k + f(u_k) \dot{u}_k dx \\ &\quad + h^3 \int_{\mathbb{T}} \left[\frac{1}{8} \ddot{u}_k^2 + \frac{1}{6} \dot{u}_k u_k^{(3)} - \frac{1}{8} (\partial_x \dot{u}_k)^2 - \frac{1}{4} \partial_x u_k \partial_x \ddot{u}_k \right. \\ &\quad \left. + \frac{1}{4} f(u_k) \ddot{u}_k + \frac{1}{8} f'(u_k) \dot{u}_k^2 \right] dx + O(h^4). \end{aligned} \quad (33)$$

On the other hand, we may substitute the expansions (31) into the continuum action

functional and collect terms containing identical powers of h . We find that

$$\begin{aligned}
S &= \int_0^T L(u, \dot{u}) dt \\
&= \sum_{k=0}^{n-1} \int_0^h \int_{\mathbb{T}} \left[\frac{1}{2} (\dot{u}_k + \ddot{u}_k t + \frac{1}{2} u_k^{(3)} t^2)^2 - \frac{1}{2} (\partial_x u_k + \partial_x \dot{u}_k t + \frac{1}{2} \partial_x \ddot{u}_k t^2)^2 \right. \\
&\quad \left. + V(u_k) + f(u_k) \dot{u}_k t + \frac{1}{2} f'(u_k) \dot{u}_k^2 t^2 + \frac{1}{2} f(u_k) \ddot{u}_k t^2 \right] dx dt + O(h^3) \\
&= \sum_{k=0}^{n-1} \left[h L(u_k, \dot{u}_k) + \frac{h^2}{2} \int_{\mathbb{T}} \dot{u}_k \ddot{u}_k - \partial_x u_k \partial_x \dot{u}_k + f(u_k) \dot{u}_k dx \right. \\
&\quad \left. + \frac{h^3}{6} \int_{\mathbb{T}} \ddot{u}_k^2 + \dot{u}_k u_k^{(3)} - (\partial_x \dot{u}_k)^2 - \partial_x u_k \partial_x \ddot{u}_k + f'(u_k) \dot{u}_k^2 + f(u_k) \ddot{u}_k dx \right] + O(h^3). \tag{34}
\end{aligned}$$

Inserting the expanded discrete Lagrangian (33) into the discrete action (7) and comparing with (34), we find that

$$\begin{aligned}
\mathbb{S} &= S - \frac{h^3}{24} \sum_{k=0}^{n-1} \int_{\mathbb{T}} \ddot{u}_k^2 - (\partial_x \dot{u}_k)^2 + 2 \partial_x u_k \partial_x \ddot{u}_k + f'(u_k) \dot{u}_k^2 - 2 f(u_k) \ddot{u}_k dx + O(h^3) \\
&= S - \frac{h^2}{24} \int_0^T \int_{\mathbb{T}} \ddot{u}^2 - (\partial_x \dot{u})^2 + 2 \partial_x u \partial_x \ddot{u} + f'(u) \dot{u}^2 - 2 f(u) \ddot{u} dx dt + O(h^3). \tag{35}
\end{aligned}$$

Integrating by parts with respect to time, we obtain up to boundary terms which do not contribute to the variational principle because u and \dot{u} are held fixed at the temporal endpoints that

$$\mathbb{S} = \int_0^T \left[L(u, \dot{u}) - h^2 \int_{\mathbb{T}} \frac{1}{24} \ddot{u}^2 - \frac{1}{8} (\partial_x \dot{u})^2 + \frac{1}{8} f'(u) \dot{u}^2 dx \right] dt + O(h^3). \tag{36}$$

Thus, the discrete variational principle with Lagrangian \mathbb{L} is equivalent up to terms of $O(h^3)$ to the continuous variational principle for the modified Lagrangian

$$L_{\text{mod}}(u, \dot{u}, \ddot{u}; h) = L(u, \dot{u}) - h^2 \int_{\mathbb{T}} \frac{1}{24} \ddot{u}^2 - \frac{1}{8} (\partial_x \dot{u})^2 + \frac{1}{8} f'(u) \dot{u}^2 dx. \tag{37}$$

We now seek stationary points of the modified action with respect to variation where u and \dot{u} are held fixed at $t = 0$ and $t = T$. The resulting Euler–Lagrange equations read, abstractly,

$$\frac{d^2}{dt^2} \frac{\delta L_{\text{mod}}}{\delta \ddot{u}} - \frac{d}{dt} \frac{\delta L_{\text{mod}}}{\delta \dot{u}} + \frac{\delta L_{\text{mod}}}{\delta u} = 0. \tag{38}$$

This expression evaluates to

$$\ddot{u} - \partial_{xx} u - f(u) + h^2 \left[\frac{1}{12} u^{(4)} - \frac{1}{4} \partial_{xx} \ddot{u} - \frac{1}{8} f''(u) \dot{u}^2 - \frac{1}{4} f'(u) \ddot{u} \right] = 0. \tag{39}$$

We note that this equation is of higher order with respect to time compared to the original semilinear wave equation, i.e., it has the form of a singular perturbation problem in a

bigger phase space. As this is undesirable, we seek to restrict the modified dynamics to the phase space of the original equation.

In this simple example, this could be done *ad hoc* by using the second time derivative of the semilinear wave equation to eliminate the fourth time derivative from the modified equation—an approximation which gives a formally correct result. In this case, the resulting equation would only contain frequencies on the order of those already present in the original problem and, although non-variational, approximately preserve energy over long times. However, our main point is that there is a systematic way to address the problem of the blown-up phase space which leads, by construction, to a variational system. This shall be explained in the next section.

6 Method of degenerate variational asymptotics

We introduce a near identity configuration space transformation of the general form

$$u_h = u + h^2 w, \quad (40)$$

where u_h denotes the solution curve in old physical configuration space coordinates and u denotes the solution in a new coordinate system in which the modified equation will be computed. The field w can be seen as the leading order generator of the transformation. It will be chosen *a posteriori* in such a way that the transformed modified Lagrangian (37), when truncated to $O(h^2)$, will not depend on time derivatives of order two and higher. We compute

$$\begin{aligned} L_{\text{mod}}(u, \dot{u}, \ddot{u}; h) &= \int_{\mathbb{T}} \frac{1}{2} (\dot{u} + h^2 \dot{w})^2 - \frac{1}{2} (\partial_x u + h^2 \partial_x w)^2 + V(u + h^2 w) \, dx \\ &\quad - h^2 \int_{\mathbb{T}} \frac{1}{24} \ddot{u}^2 - \frac{1}{8} (\partial_x \dot{u})^2 + \frac{1}{8} f'(u) \dot{u}^2 \, dx + O(h^3) \\ &= L(u, \dot{u}) - h^2 \int_{\mathbb{T}} \ddot{u} w + \partial_x u \partial_x w - f(u) w \, dx + h^2 \frac{d}{dt} \int_{\mathbb{T}} \dot{u} w \, dx \\ &\quad - h^2 \int_{\mathbb{T}} \frac{1}{24} \ddot{u}^2 - \frac{1}{8} (\partial_x \dot{u})^2 + \frac{1}{8} f'(u) \dot{u}^2 \, dx + O(h^3). \end{aligned} \quad (41)$$

We now observe that choosing $w = -\frac{1}{24} \ddot{u} + G(u)$, where G is some functional acting on $u(\cdot, t)$ for t fixed, we formally eliminate the excess time derivatives from the $O(h^2)$ terms in (41). The choice of G is determined by dimensional consistency and introduces some freedom in choosing a coordinate system for the Lagrangian modified system. We will restrict our attention to transformations of the form

$$w = -\frac{1}{24} \ddot{u} - a \partial_{xx} u - b f(u), \quad (42)$$

where $a, b \in \mathbb{R}$ are arbitrary free parameters. We note that, in particular, if $a = b = -\frac{1}{24}$, then w formally vanishes up to terms of $O(h^2)$.

Inserting (42) into (41), integrating by parts, discarding all perfect time derivatives,

and truncating to $O(h^2)$, we obtain the family of modified Lagrangians

$$L_{\text{mod}}(u, \dot{u}; h) = L(u, \dot{u}) + h^2 \int_{\mathbb{T}} \left[\left(\frac{1}{12} + a \right) (\partial_x \dot{u})^2 - \left(\frac{1}{12} + b \right) f'(u) \dot{u}^2 + (a + b) f'(u) (\partial_x u)^2 - a (\partial_{xx} u)^2 - b f^2(u) \right] dx. \quad (43)$$

We compute

$$\frac{\delta L_{\text{mod}}}{\delta \dot{u}} = \left(1 - h^2 \left(\frac{1}{6} + 2b \right) f'(u) - h^2 \left(\frac{1}{6} + 2a \right) \partial_{xx} \right) \dot{u} \quad (44a)$$

and

$$\begin{aligned} \frac{\delta L_{\text{mod}}}{\delta u} &= \left(1 - h^2 2(a + b) f'(u) \right) \partial_{xx} u + f(u) \\ &\quad - h^2 \left[\left(\frac{1}{12} + b \right) f''(u) \dot{u}^2 + (a + b) f''(u) (\partial_x u)^2 + 2a \partial_x^4 u + 2b f(u) f'(u) \right]. \end{aligned} \quad (44b)$$

Hence, the transformed modified Euler–Lagrange equations read

$$\begin{aligned} &\left(1 - h^2 \left(\frac{1}{6} + 2b \right) f'(u) - h^2 \left(\frac{1}{6} + 2a \right) \partial_{xx} \right) \ddot{u} - \left(1 - h^2 2(a + b) f'(u) \right) \partial_{xx} u - f(u) \\ &\quad - h^2 \left[\left(\frac{1}{12} + b \right) f''(u) \dot{u}^2 - (a + b) f''(u) (\partial_x u)^2 - 2a \partial_x^4 u - 2b f(u) f'(u) \right] = 0. \end{aligned} \quad (45)$$

The equations of motion conserve the energy

$$\begin{aligned} H_{\text{mod}} &= \left\langle \frac{\delta L_{\text{mod}}}{\delta \dot{u}}, \dot{u} \right\rangle - L_{\text{mod}} \\ &= H + h^2 \int_{\mathbb{T}} \left[\left(\frac{1}{12} + a \right) (\partial_x \dot{u})^2 - \left(\frac{1}{12} + b \right) f'(u) \dot{u}^2 \right. \\ &\quad \left. - (a + b) f'(u) (\partial_x u)^2 + a (\partial_{xx} u)^2 + b f^2(u) \right] dx, \end{aligned} \quad (46)$$

where $\langle \cdot, \cdot \rangle$ denotes the L^2 -pairing between Q and Q^* .

We close this derivation with two remarks. First, note that when $a = b = -\frac{1}{24}$, i.e., when the change of coordinates is the identity transformation up to terms of $O(h^4)$, we once again obtain the high frequencies which appear in the Hamiltonian modified equations in Section 4, so the construction would not yield anything new. For this reason, we do not consider this case further.

Second, the transformation we use as well as the resulting Hamiltonian are different from classic Hamiltonian normal form theory (see, e.g., [1] for a general exposition and [7] for an application of normal form theory to a fast-slow system with gyroscopic forcing for which the method of degenerate variational asymptotics was originally developed). To see this, one can write the modified Hamiltonian (46) in canonical variables u and $p = \delta L / \delta \dot{u}$, expand in powers of h so that $H_{\text{mod}} = H_0 + h^2 H_2 + O(h^4)$ and verify that the Poisson bracket $\{H_0, H_2\}$ does not vanish. The construction principles behind the two approaches are also markedly different: our transformation (42) depends implicitly on the dynamics of the resulting equations of motion up the order of truncation, whereas in the traditional normal form approach, the transformation itself is constructed in an explicit iterative procedure without reference to the equations of motion.

7 Initialization

A variational derivation of the modified equation will naturally yield a second order system which may be cast into a system of first order equations in several equivalent ways. Hence, care must be taken in matching of the initial and final time data of the Lagrangian modified equation with that of the implicit midpoint numerical scheme.

A straightforward Taylor expansion of the discrete Legendre transform (10) shows that

$$\begin{aligned} p_k &= \dot{u}_k + \frac{h}{2} (\ddot{u}_k - \partial_{xx} u_k - f(u_k)) + h^2 \left(\frac{1}{6} u_k^{(3)} - \frac{1}{4} \partial_{xx} \dot{u}_k - \frac{1}{4} f'(u_k) \dot{u}_k \right) + O(h^3) \\ &= \dot{u}_k - \frac{h^2}{12} (\partial_{xx} \dot{u}_k + f'(u_k) \dot{u}_k) + O(h^3). \end{aligned} \quad (47)$$

This relation directly implies that

$$\dot{u}_k = p_k + \frac{h^2}{12} (\partial_{xx} p_k + f'(u_k) p_k) + O(h^3). \quad (48)$$

Note that this expression coincides with the first equation (28a) of the Hamiltonian modified system. It implies that the initial data for p cannot be identified with the initial data for \dot{u} to the order that the modified equation is valid. Rather, if p denotes the initial data for the implicit midpoint rule, then the initialization of \dot{u} for the modified equation needs to receive data which is related to p via (48). Vice versa, the final time data for \dot{u} of the modified equation needs to be expressed in terms of the implicit midpoint p via (47) before the two can be consistently compared.

We remark that this relation must be used when consistently comparing any modified equation which is second order in time, variational or not, to the implicit midpoint rule. The change of coordinates which appears in our method of degenerate variational asymptotics appears additionally when investigating the variational modified equations numerically, as explained next.

8 Numerical Experiments

In the following, we focus on the modified equations derived in Section 6 in the special case $a = b = 0$ when (45) takes the relatively simple form

$$K(u)\ddot{u} - \partial_{xx} u - f(u) - \frac{h^2}{12} f''(u) \dot{u}^2 = 0 \quad (49)$$

with

$$K(u)v = \left(1 - \frac{h^2}{6} f'(u) - \frac{h^2}{6} \partial_{xx}\right)v. \quad (50)$$

We choose $p = \dot{u}$ as for the original semilinear wave equation. (We could equally well choose $p = \delta L_{\text{mod}}/\delta \dot{u} = K(u)\dot{u}$ in which case the initialization described in Section 7 has to be consistently adapted.) Then the corresponding first order system reads

$$\dot{U} \equiv \begin{pmatrix} \dot{u} \\ \dot{p} \end{pmatrix} = \begin{pmatrix} p \\ K^{-1}(\partial_{xx} u + f(u) + \frac{h^2}{12} f''(u) p^2) \end{pmatrix}, \quad (51)$$

where the solution of operator equation $K(u)v = z$ is computed as the fixed point of the contraction mapping

$$v = (1 - \frac{h^2}{6} \partial_{xx})^{-1} (z + \frac{h^2}{6} f'(u) v). \quad (52)$$

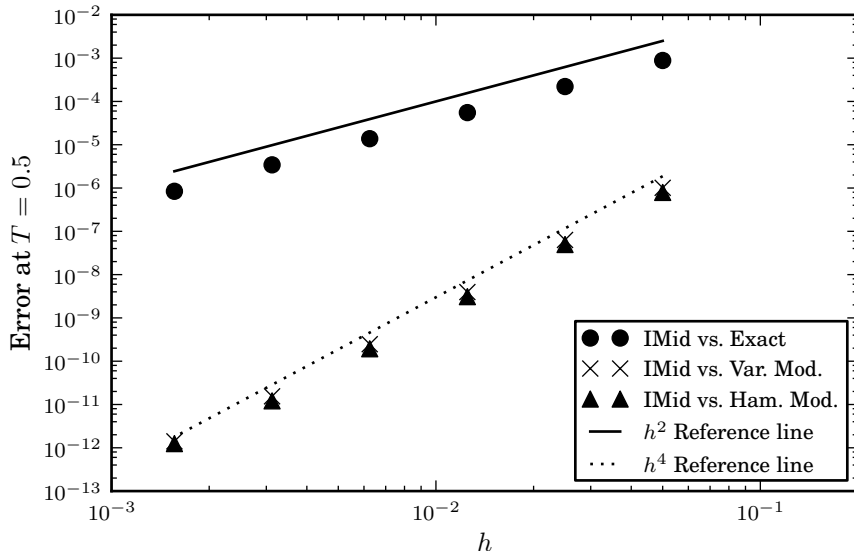


Figure 1: Scaling of the error at final time $T = 0.5$.

We note that the linear modified dynamics has Fourier representation

$$\partial_t \hat{U}_k = \begin{pmatrix} 0 & 1 \\ \frac{-k^2}{1 + \frac{1}{6} h^2 k^2} & 0 \end{pmatrix} \hat{U}_k. \quad (53)$$

Clearly, the highest frequencies are $O(h^{-1})$ without restrictions on the spatial wave numbers, which is markedly different from the classic linear modified equations (30).

When initializing the modified equation, we must invert the transformation (42), which now takes the form

$$U_h = U - \frac{1}{24} h^2 \ddot{U}. \quad (54)$$

This relation can also be cast into fixed point form as follows. Differentiating (49) in time, we find

$$Ku^{(3)} - \partial_{xx} \dot{u} - f'(u) \dot{u} - \frac{h^2}{12} f'''(u) \dot{u}^3 - \frac{h^2}{3} f''(u) \dot{u} \ddot{u} = 0. \quad (55)$$

Then, for a given vector U_h , (54) can be solved for U via the contraction mapping

$$U = U_h + \frac{1}{24} h^2 \ddot{U}, \quad (56a)$$

$$\ddot{U} = (1 - \frac{h^2}{6} \partial_{xx})^{-1} G(U, \ddot{U}), \quad (56b)$$

with

$$G(U, \ddot{U}) = \begin{pmatrix} \frac{h^2}{6} f'(u) \ddot{u} + \partial_{xx} u + f(u) + \frac{h^2}{12} f''(u) p^2 \\ \frac{h^2}{6} f'(u) \ddot{p} + \partial_{xx} p + f'(u) p + \frac{h^2}{12} f'''(u) p^3 + \frac{h^2}{3} f''(u) p \ddot{u} \end{pmatrix}. \quad (57)$$

In our numerical example, we take the nonlinearity $V(u) = -\frac{1}{10} u^4$. Figure 1 shows that both the Hamiltonian and the variational modified system show the expected $O(h^4)$ scaling when compared to the solution of the implicit midpoint rule. (Due to the symmetry of the method only even powers of h appear in the modified equations at any order.)

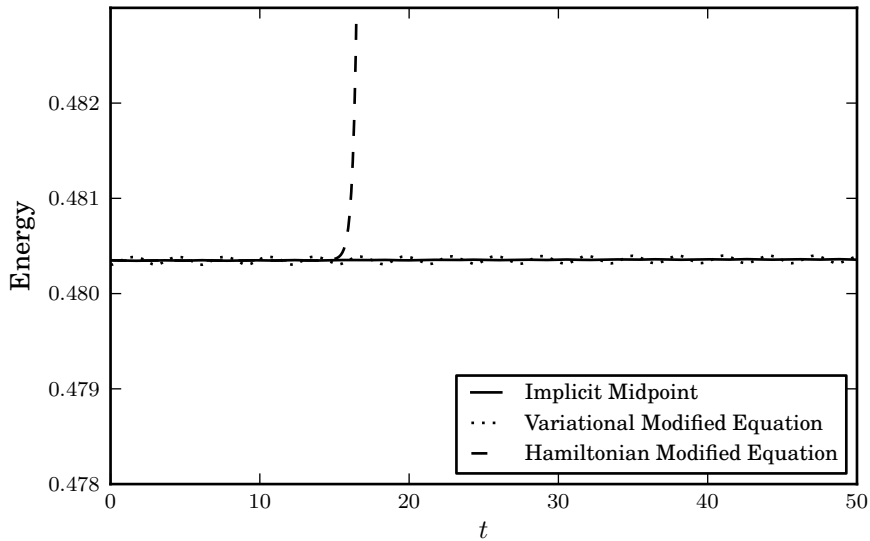


Figure 2: Approximate energy preservation of the implicit midpoint rule and modified equations. The Hamiltonian modified equation has a numerical blowup due to a CFL violation while the variational modified equations is stably solved under identical conditions using a fourth order explicit Runge–Kutta scheme with a fixed step size $\Delta t = 0.025 < h = 0.037$.

The modified equations were solved with a highly resolved standard fourth order explicit Runge–Kutta method.

Figure 2 shows the approximate preservation of energy of the implicit midpoint rule and of the two modified systems. The occurrence of high frequencies in the Hamiltonian construction leads to numerical blowup, unless the stepsize used in the explicit Runge–Kutta scheme is adjusted to fit a stricter CFL bound. The graphs display the semilinear wave energy; the respective modified energies would be exactly preserved by the true solutions to the modified equations.

9 Well-posedness of the new modified system

In the following we provide a functional framework which shows that, in the limit of vanishing stepsize h , the variational modified system with the choice of parameters as in Section 8 behaves analytically like the original semilinear wave equation. We begin by proving a statement on the operator K defined in (50). For convenience, we write $K(u) = L + M(u)$ with

$$Lv = \left(1 - \frac{h^2}{6} \partial_{xx}\right)v \quad (58)$$

and

$$M(u)v = -\frac{h^2}{6} f'(u) v. \quad (59)$$

Let $L^2(\mathbb{T})$ denote the Lebesgue space of square integrable functions on the circle, which we endow with norm

$$\|v\|_{L^2} = \sum_{k \in \mathbb{Z}} |v_k|^2, \quad (60)$$

$L^\infty(\mathbb{T})$ the space of essentially bounded functions endowed with the usual essential sup-norm, and $H^s(\mathbb{T})$ the Sobolev space of functions whose generalized derivative of order s belongs to $L^2(\mathbb{T})$, endowed with norm

$$\|v\|_{H^s} = \sum_{k \in \mathbb{Z}} (1 + |k|^{2s}) |v_k|^2. \quad (61)$$

Lemma 1. *For every $C > 0$ there exists $h_* > 0$ such that for every $h \in (0, h_*]$, $u \in H^1(\mathbb{T})$ with $\|u\|_{H^1} \leq C$, and $z \in L^2(\mathbb{T})$, the equation $K(u)v = z$ has a unique solution $v \in H^2(\mathbb{T})$ and there exists a constant $c = c(C) > 0$ such that*

$$\|v\|_{L^2} \leq \frac{1}{1 - ch^2} \|z\|_{L^2}, \quad (62)$$

and

$$\|v\|_{H^2} \leq 6 \left(\frac{1}{h^2} + \frac{c}{1 - ch^2} \right) \|z\|_{L^2}. \quad (63)$$

Moreover, for fixed $z \in L^2(\mathbb{T})$ and under the above bounds on u and h , the mapping $u \mapsto K(u)^{-1}z$ is uniformly Lipschitz continuous as a map from H^1 to H^2 .

Proof. As in (52), we write $Kv = z$ in fixed point form as

$$v = F(v) \equiv L^{-1}(z - M(u)v). \quad (64)$$

Since L^{-1} , the inverse Helmholtz operator, has norm 1 as an operator from H^s to H^s , there exists a constant $c > 0$ such that

$$\|F(v_1) - F(v_2)\|_{L^2} \leq c \frac{h^2}{6} \|f'(u)\|_{H^1} \|v_1 - v_2\|_{L^2}. \quad (65)$$

Hence, there exists $h_* > 0$ such that for all $h \in [0, h_*]$ the map F is a contraction, hence has a unique fixed point v by the contraction mapping theorem.

Taking the L^2 -norm of (64), we obtain

$$\|v\|_{L^2}^2 \leq \|z\|_{L^2} + \frac{h^2}{6} \|f'(u)\|_{L^\infty} \|v\|_{L^2}, \quad (66)$$

which implies (62). Taking the H^2 -norm of (64) and noting that L^{-1} has norm $6/h^2$ as an operator from L^2 into H^2 , we find

$$\|v\|_{H^2}^2 \leq \frac{6}{h^2} \|z\|_{L^2} + \|f'(u)\|_{L^\infty} \|v\|_{L^2} \quad (67)$$

which together with (62) implies (63).

Now suppose that $K(u_1)v_1 = z$ and $K(u_2)v_2 = z$. Then

$$v_1 - v_2 = -L^{-1}(M(u_1)(v_1 - v_2) + (M(u_1) - M(u_2))v_2). \quad (68)$$

Taking the L^2 -norm on both sides, we find that

$$\|v_1 - v_2\|_{L^2} \leq \frac{h^2}{6} \|f'(u_1)\|_{L^\infty} \|v_1 - v_2\|_{L^2} + \frac{h^2}{6} \|f'(u_1) - f'(u_2)\|_{L^\infty} \|v_2\|_{L^2}, \quad (69)$$

so that, for some $\tilde{c} = \tilde{c}(C)$,

$$\|v_1 - v_2\|_{L^2} \leq \frac{\tilde{c}h^2}{1 - ch^2} \|v_2\|_{L^2} \|u_1 - u_2\|_{H^1}. \quad (70)$$

Due to (62), this estimate implies uniform Lipschitz continuity of $u \mapsto K(u)^{-1}z$ as a map from H^1 into L^2 . Then, taking the H^2 -norm of (68) and using the operator norm of L^{-1} as a map from L^2 to H^2 implies uniform Lipschitz continuity into H^2 as well. \square

To proceed, we write $H_h^1(\mathbb{T})$ to denote the space $H^1(\mathbb{T})$ endowed with the nonuniform norm

$$\|v\|_{H_h^1}^2 = \sum_{k \in \mathbb{Z}} (1 + \frac{h^2}{6} |k|^2) |v_k|^2. \quad (71)$$

Note that the space $H^1 \times H_h^1$ is the ‘‘energy space’’ which corresponds to the modified Hamiltonian (46) with $a = b = 0$. We therefore seek local well-posedness in this space.

Theorem 2. *For every $C > 0$ there exists $T = T(C) > 0$ and $h_* = h_*(C) > 0$ such that for every $U_0 \in H^1(\mathbb{T}) \times H_h^1(\mathbb{T})$ with $\|U_0\|_{H^1 \times H_h^1} \leq C$ and every $h \in (0, h_*]$ there exists a unique mild solution $U \in C([0, T]; H^1(\mathbb{T}) \times H_h^1(\mathbb{T}))$ to the new modified equation (6) with bounds which remain uniform in h .*

Proof. We first observe, as can be checked by direct computation, that

$$K^{-1} - L^{-1} = -K^{-1}ML^{-1}, \quad (72)$$

so that the new modified system (51) can be written as a semilinear evolution equation of the form (6) with

$$A = \begin{pmatrix} 0 & 1 \\ L^{-1}\partial_{xx} & 0 \end{pmatrix} \quad (73)$$

and

$$B(U) \equiv \begin{pmatrix} 0 \\ b(U) \end{pmatrix} = \begin{pmatrix} 0 \\ K^{-1}(-ML^{-1}\partial_{xx}u + f(u) + \frac{h^2}{12}f''(u)p^2) \end{pmatrix}. \quad (74)$$

The crucial observation is that A generates a unitary group $\exp(tA)$ on the quotient $H^1 \times H_h^1/\mathbb{R}^2$ endowed with norm

$$\|U\|_{H^1 \times H_h^1/\mathbb{R}^2}^2 = \|\partial_x u\|_{L^2}^2 + \|p\|_{H_h^1}^2. \quad (75)$$

Moreover,

$$\begin{aligned} b(U_1) - b(U_2) &= (K(u_1)^{-1} - K(u_2)^{-1}) (-M(u_1)L^{-1}\partial_{xx}u_1 + f(u_1) + \frac{h^2}{12}f''(u_1)p_1^2) \\ &\quad - K(u_2)^{-1} (M(u_1) - M(u_2))L^{-1}\partial_{xx}u_1 \\ &\quad + K(u_2)^{-1} [-M(u_2)L^{-1}\partial_{xx}(u_1 - u_2) + f(u_1) - f(u_2) \\ &\quad + \frac{h^2}{12}((f''(u_1) - f''(u_2))p_1^2 + f''(u_2)(p_1 + p_2)(p_1 - p_2))] \end{aligned} \quad (76)$$

Taking the L^2 -norm of this expression, using the uniform Lipschitz continuity of K^{-1} and estimate (62) as asserted by Lemma 1, and supposing that U has an $H^1 \times H_h^1$ bound of $2C$, say, we find that there exists $h_* > 0$ such that for all $h \in (0, h_*]$,

$$\begin{aligned} \|b(U_1) - b(U_2)\|_{L^2} &\leq c_1 \|u_1 - u_2\|_{H^1} \\ &\quad \cdot (\|M(u_1)L^{-1}\partial_{xx}u_1\|_{L^2} + \|f(u_1)\|_{L^2} + h^2 \|f''(u_1)p_1^2\|_{L^2}) \\ &\quad + c_2 h^2 \|f'(u_1) - f'(u_2)\|_{L^\infty} \|L^{-1}\partial_{xx}u_1\|_{L^2} \\ &\quad + c_3 [\|M(u_2)L^{-1}\partial_{xx}(u_1 - u_2)\|_{L^2} + \|f(u_1) - f(u_2)\|_{L^2} + h^2 (\|p_1\|_{L^\infty} + \|p_2\|_{L^\infty}) \\ &\quad \cdot (\|f''(u_1) - f''(u_2)\|_{L^\infty} \|p_1\|_{L^2} + \|f''(u_2)\|_{L^\infty} \|p_1 - p_2\|_{L^2})] \end{aligned} \quad (77)$$

Noting that

$$h^2 \|L^{-1} \partial_{xx} v\|_{L^2} \leq c_3 \|v\|_{L^2} \quad (78)$$

and

$$\|p\|_{L^\infty} \leq c_4 h^{-2} \|p\|_{H_h^1} \quad (79)$$

uniformly under the assumed bounds on h and U , we find that

$$\|b(U_1) - b(U_2)\|_{L^2} \leq c_5 \|U_1 - U_2\|_{H^1 \times H_h^1}. \quad (80)$$

A similar argument, now taking the H^1 -norm of (76) and using (63) rather than (62) shows that

$$\|b(U_1) - b(U_2)\|_{H^1} \leq c_6 h^{-2} \|U_1 - U_2\|_{H^1 \times H_h^1}. \quad (81)$$

This proves uniform Lipschitz continuity of B in $H^1 \times H_h^1$.

Altogether, we find that the above formulation of the new modified equation fits into the standard framework for mild solutions of semilinear evolution equations [16, 28], from which the conclusion ensues. \square

This theorem shows that the new modified equation is well posed in a space which limits to the standard setting $H^1 \times L^2$ for the original semilinear wave equation as $h \rightarrow 0$. We note that the theorem and proof easily translates up the scale of standard Sobolev spaces.

10 Higher order variational backward error analysis

Let us now consider how the procedure set up in Sections 5 and 6 might allow us to construct constructing modified equations that are valid up to an arbitrary but fixed order.

Let us first consider the linear wave equation where $f = 0$. In the linear case, it is possible to give a complete explicit answer. We shall only indicate the main features of the construction without stating details which are technical, but ultimately straightforward.

First, by performing all steps laid out in Section 5 consistently up to $O(h^{2m})$, we find that the general modified Lagrangian for the implicit midpoint rule applied to the linear wave equation reads

$$L_{\text{mod}}(u, \dot{u}, \dots, u^{(m+1)}) = \sum_{i=0}^m (-1)^i h^{2i} \int_{\mathbb{T}} a_i (u^{(i+1)})^2 - b_i (\partial_x u^{(i)})^2 dx \quad (82)$$

where $a_0 = b_0 = 1/2$ and, for $i \geq 1$,

$$a_i = \frac{1}{(2i+2)!} \quad \text{and} \quad b_i = \frac{1}{4(2i)!}. \quad (83)$$

The corresponding Euler–Lagrange equations arise as stationary point of the associated action with respect to variations where $u, \dot{u}, \dots, u^{(m)}$ are held fixed at the temporal endpoints. In the derivation of (82), these endpoint conditions ensure that we can always replace equidistant Riemann summations by time integrals via the Euler–Maclaurin summation formula up to terms of $o(h^{2m})$.

Since the modified variational principle yields Euler–Lagrange equations of order $2(m + 1)$ in ∂_t , we generalize the transformational approach of Section 6 to this case. In effect, we need to set up the transformation which trades time derivatives for space derivatives in the modified Lagrangian. The general transformation in the linear case reads

$$u_h = u + \sum_{i=1}^m h^{2i} w_i \quad (84)$$

where

$$w_i = \sum_{\alpha+\beta=i} c_\alpha^i \partial_t^{2\alpha} \partial_x^{2\beta} u. \quad (85)$$

Now the task is to insert the transformation into (82) and determine the coefficients c_α^i by requiring that the resulting Euler–Lagrange equation become second order in time. This can be done by an inductive construction in i . Let us fix i and suppose that c_α^k are already known for all $k \leq i - 1$ and $\alpha \leq k$. Then c_α^i is uniquely determined by the condition that the contribution to the resulting Lagrangian at order h^{2i} does not contain time derivatives of order $2(i + 1)$. From there, c_{i-1}^i is uniquely determined by the absence of time derivatives of order $2i$, and so on down to c_1^i which is uniquely determined by the absence of time derivatives of order 4. Now the only remaining time derivatives in the Lagrangian at order h^{2i} are of the form $(\partial_x^i u)^2$ and the sign of its coefficient can be controlled by the choice of c_0^i , which is the only remaining free parameter.

We conclude that in the linear case, the construction of the new modified equations is fully transparent. Moreover, the free parameters controlling the transformation reduce to choices of the c_0^i , which control the sign of the higher order terms in the generalized version of the operator K . A choice ensuring that K is invertible is always possible. This construction will result in a finite highest temporal frequency independent of the spacial wave number k at every order in the construction.

When restoring the nonlinearity, the expressions get combinatorially much more complicated, as the expansion of the transformed Lagrangian involves the Faà di Bruno formula. It is nonetheless possible to follow the same elimination scheme by adding to (85) another series of multilinear expressions in the various time derivatives of u ordered in with decreasing order of the total number of time derivatives. We now observe that that the nonlinear terms which come in at order h^{2i} contain at most $2i$ derivatives in time or space before the transformation. Thus, after the transformation, the leading order contributions to the general nonlinear operator K always come from the linear theory while the nonlinear contributions come in as small perturbations which can be treated via contraction mapping argument such as those employed in Section 9. An explicit implementation of this scheme to any order is difficult because of the complexity of the expressions which arise and is subject to ongoing research. However, there is no principle obstacle to this construction.

11 Conclusions

Modified equations for backward error analysis of variational integrators can be systematically constructed using a formal Taylor expansion of the action integral. However, a straightforward variational construction necessitates the use of an extended phase space.

We have demonstrated for the model case of the implicit midpoint rule applied to the semilinear wave equation that a carefully chosen configuration space transformation allows us to eliminate the dependence of the modified Lagrangian on higher order time derivatives, thus reducing the phase space, and refitting the modified equations into the standard framework of Lagrangian mechanics. Furthermore, such construction yields modified equations whose dynamics lives on timescales that coincide with the timescales of the unmodified partial differential equation. This is clearly not the case for the modified equations derived on the Hamiltonian side using the traditional method as can already be seen for the linear dynamics.

While our proof-of-concept was done only on the next-order correction corresponding to the implicit midpoint scheme, we have shown that the construction naturally generalizes to any order. We also expect that the computations shown here generalize in a straightforward way to semilinear Hamiltonian evolution equations when the unbounded linear operator is self-adjoint and provided there is a regular Legendre transform.

Our approach was initially developed in the context of Hamiltonian systems with strong gyroscopic forces [13, 24]; the present work demonstrates that the strategy is more widely applicable and might point toward an abstract theory of degenerate variational asymptotics. We also note that the flexibility of the approach comes from the fact that the variational construction modifies the symplectic structure and the Hamiltonian simultaneously. In contrast, the traditional construction keeps a canonical symplectic structure and only modifies the Hamiltonian.

Two major questions remain open. First, is it possible to show, using the new variational modified equation, that the implicit midpoint rule preserves the energy to fourth order without assuming that $h = o(k^{-1})$? Note that for the new modified equations, the truncation remainder is $O(1)$ for h fixed and $k \rightarrow \infty$, while it is unbounded in the traditional setting. Therefore, we expect that we still need some assumptions on the regularity of the solution—even though numerical simulations indicate that energy preservation of the implicit midpoint rule is very good even for non-smooth data—but the regularity conditions are possibly less stringent than those needed in [32]. Second, is it possible to achieve exponential asymptotics as in the standard backward error analysis for ODEs? To answer this question, it is necessary to describe the combinatorics of the new asymptotic series, which should be possible, but is more complicated than the conventional construction.

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