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A GENERAL FRAMEWORK FOR DERIVING INTEGRAL PRESERVING NUMERICAL METHODS FOR PDES*

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Abstract. A general procedure for constructing conservative numerical integrators for time-dependent partial differential equations is presented. In particular, linearly implicit methods preserving a time discretized version of the invariant are developed for systems of partial differential equations with polynomial nonlinearities. The framework is rather general and allows for an arbitrary number of dependent and independent variables with derivatives of any order. It is proved formally that second order convergence is obtained. The procedure is applied to a test case, and numerical experiments are provided.

Key words. finite difference methods, integral preservation, discrete variational derivatives, linearly implicit methods

AMS subject classification. 65M06

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1. Introduction.

Schemes that conserve geometric structure have been shown to be useful when studying the long time behavior of dynamical systems. Such schemes are sometimes called geometric or structure preserving integrators [18, 19]. In this paper we shall mostly be concerned with the conservation of first integrals.

Even if a presumption in this work is that the development of new and better integral preserving schemes is useful, we would still like to mention some situations where schemes with such properties are of importance. In the literature one finds several examples where stability of a numerical method is proved by directly using its conservative property; one example is the scheme developed for the cubic Schrödinger equation in [11]. Another application in which the exact preservation of first integrals plays an important role is the study of orbital stability of soliton solutions to certain Hamiltonian partial differential equations (PDEs) as discussed by Benjamin, Bona, and Mahony [1, 2].

For ordinary differential equations (ODEs) it is common to devise relatively general frameworks for structure preservation. This is somewhat to the contrary of the usual practice with PDEs, where each equation under consideration normally requires a dedicated scheme. But there exist certain fairly general methodologies that can be used for developing geometric schemes also for PDEs. For example, through space discretization of a Hamiltonian PDE one may obtain a system of Hamiltonian ODEs to which a geometric integrator may be applied. Another approach is to formulate the PDE in multisymplectic form, and then apply a scheme which preserves a discrete version of this form; see [4] for a review of this approach.

In this paper we consider methods for PDEs that are based on the discrete gradient method for ODEs. The discrete gradient method was perhaps first treated in a systematic way by Gonzalez [16]; see also [18, 25]. For PDEs one may either derive discrete gradients for the abstract Cauchy problem, where the solution at any time

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is considered as an element of some infinite dimensional space, or semidiscretize the equations in space and then derive the corresponding discrete gradient for the resulting ODE system. This last procedure has been elegantly presented in several articles by Furihata, Matsuo, and collaborators (see, e.g., [12, 13, 14, 21, 22, 23, 24]) using the concept of discrete variational derivatives. See also the monograph [15]. The first part of this paper develops a similar framework that is rather general and allows for an arbitrary number of dependent and independent variables with derivatives of any order. The suggested approach does not require the equations to be discretized in space.

We consider a class of conservative schemes which are linearly implicit. By linearly implicit we mean schemes which require the solution of precisely one linear system of equations in each time step. This is opposed to fully implicit schemes for which one typically applies an iterative solver that may require a linear system to be solved in every iteration. For standard fully implicit schemes one would typically balance the iteration error in solving the nonlinear system with the local truncation error. However, for conservative schemes the situation is different since exact conservation of the invariant requires that the nonlinear system be solved to machine precision. This work can be seen as a generalization of ideas introduced in [22, sect. 6].

It may not, in general, be an easy task to quantify exactly how much we can expect to gain in computational cost, if any, when replacing a fully implicit scheme with a linearly implicit one. For illustration we present an example where the Kortweg–de Vries (KdV) equation

$$u_t + u_{xxx} + (u^2)_x = 0 \tag{1.1}$$

is solved on a periodic domain using a fully implicit scheme,

$$\frac{U^{n+1} - U^n}{\Delta t} + \frac{U^{n+1}_{xxx} + U^n_{xxx}}{2} + \left(\frac{(U^{n+1})^2 + U^{n+1}U^n + (U^n)^2}{3} \right)_x = 0, \tag{1.2}$$

and a linearly implicit scheme,

$$\frac{U^{n+2} - U^n}{2\Delta t} + \frac{U^{n+2}_{xxx} + U^n_{xxx}}{2} + \left(U^{n+1} \frac{U^{n+2} + U^{n+1} + U^n}{3} \right)_x = 0, \tag{1.3}$$

where $U^n(x) \approx u(x, t^n) = u(x, t^0 + n\Delta t)$.

These schemes are derived in section 6. For space discretization, centered differences are used for both schemes. Note that the linearly implicit scheme (1.3) has a multistep nature, but it should not be confused with standard linear multistep methods. Furihata and coworkers sometimes use the term "multiple point linearly implicit schemes" to emphasize this fact.

Both schemes are second order in time, but in our example the linearly implicit multistep scheme has an error constant which is about 3–4 times larger than the fully implicit one-step scheme. In Figure 1.1 we plot the global error versus the number of linear solves for the two schemes. The linearly implicit scheme solves one linear system in each time step. The fully implicit scheme, on the other hand, solves a linear system for each Newton iteration which is repeated to machine precision in each time step. For the largest time step in our experiment this amounts to 561 linear solves per time step. The linear systems in both cases have the same matrix structure and are penta-diagonal, and we therefore assume that the cost of solving the linear system is approximately the same for both methods. The x-axis in Figure 1.1 can thus be

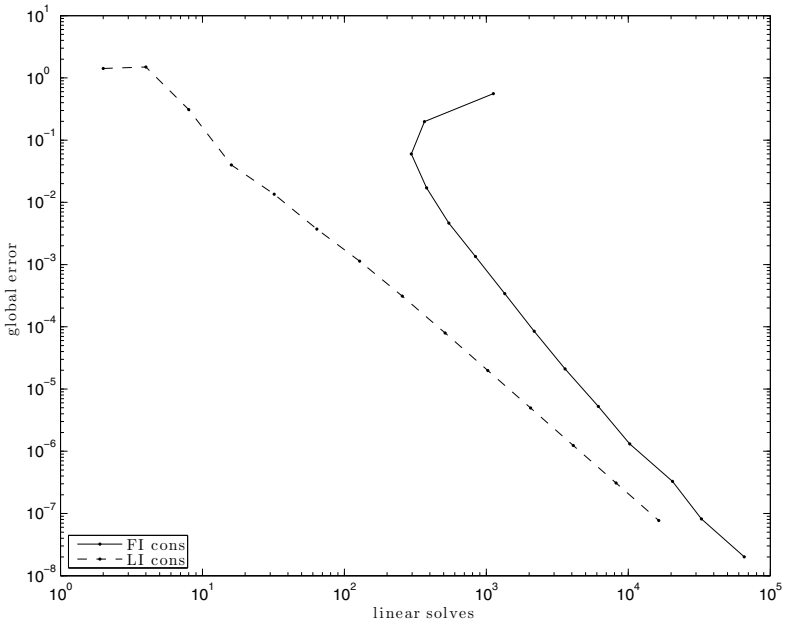

FIG. 1.1. *The global error versus the number of linear solves for the two schemes* (1.2) *(FI cons) and* (1.3) *(LI cons).*

interpreted as a measure of the computational cost in each scheme. The plot shows that for a given global error the linearly implicit scheme is computationally cheaper than the fully implicit scheme.

There are situations in which the results from this example may be less relevant. For instance, the iteration method used in fully implicit schemes may use approximate versions of the Jacobian for which faster solvers can be applied; therefore the cost of a linear solve may not be the same for the two types of schemes. For large time steps, both types of schemes are likely to encounter difficulties but for slightly different reasons. The fully implicit scheme may experience slow or no convergence, whereas the linearly implicit scheme may become unstable for time steps over a certain threshold [9]. For instance, in the case of the stiff ODE considered by Gonzales and Simo [17] one will observe that the stability properties of the linearly implicit schemes will be completely lost, whereas fully implicit conservative schemes behave remarkably well. For large-scale problems, one may have situations in which iterative linear solvers are required and where one cannot afford to solve these systems to machine accuracy; in such cases the linearly implicit schemes are less useful. In conclusion, we believe that one's choice of scheme depends on the PDE and the circumstances under which it is to be solved.

The two schemes used in the example above have slightly different conservation properties. The first one (1.2) conserves the exact Hamiltonian

$$\mathcal{H}[U^n] = \int_\Omega \left(\frac{1}{2}(U_x^n)^2 - \frac{1}{3}(U^n)^3 \right) \mathrm{d}x,$$

whereas the second scheme (1.3) conserves what we will define as the polarized

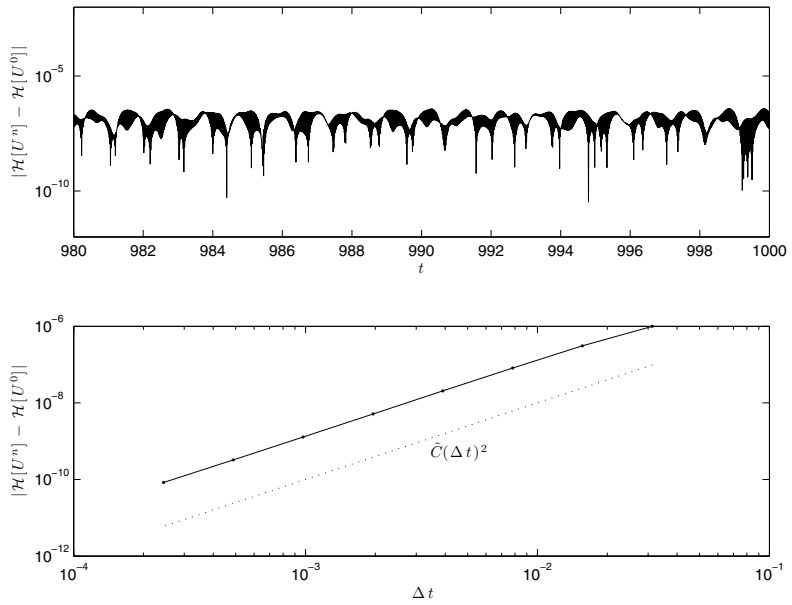

FIG. 1.2. *The error in $\mathcal{H}$ as a function of the solution obtained by the linearly implicit scheme* (1.3) *as a function of t (top) and Δt (bottom). The dotted line is a reference line $\tilde{C}(\Delta t)^2$.*

Hamiltonian

$$H[U^n, U^{n+1}] = \int_\Omega \left(\frac{1}{4} \left((U_x^n)^2 + (U_x^{n+1})^2 \right) - \frac{1}{6} \left((U^n)^2 U^{n+1} + (U^{n+1})^2 U^n \right) \right) \mathrm{d}x.$$

Both of these functions are approximations to the true Hamiltonian; the first is a spatial approximation for a fixed time, and the second also includes an averaging over time. The intention is to show that in both cases one can see the methods as exactly preserving a slightly perturbed first integral over very long times. That this seems to work for the chosen example is clearly seen in the upper plot in Figure 1.2, where we plot the error in $\mathcal{H}$ as a function of the solution obtained by the linearly implicit scheme (1.3). We integrate to $t = 1000$, and the error is plotted from $t = 980$ to $t = 1000$. Notice that in this example there is no drift in the energy error. The corresponding error plots for $\mathcal{H}$ as a function of the solution of (1.2) and H as a function of the solution of (1.3) are omitted since they are both preserved up to round-off error, and thus are not that interesting. The lower plot in Figure 1.2 shows how the error in $\mathcal{H}$ at the endpoint depends on Δt. Empirically, we have the relation

$$\mathcal{H}[U^n] = \mathcal{H}[U^0] + C(\Delta t)^2,$$

where C is a constant that depends on the solution but not on n. See section 6 for another example that tests the long time structure preserving properties of these schemes.

This and similar examples show that there are situations where linearly implicit schemes can be a better choice than their fully implicit counterparts. Figure 1.1 shows that the linearly implicit scheme is cheaper, while Figure 1.2 shows that both solutions have similar long-term behavior. Similar favorable behavior of linearly implicit schemes can be found in the literature. For the cubic Schrödinger equation, there are

such conservative schemes based on time averaged versions of the Hamiltonian by Fei, Pérez-García, and Vázquez [11] and Besse [3]. Examples of methods for other PDEs can be found in the monograph [15] and the papers [20, 29].

In the next section we define the PDE framework that we use. Then, in section 3 we consider discrete gradient methods and how they can be applied to PDEs. We study in particular the average vector field method by Quispel and McLaren [27] and the discrete variational derivative method by Furihata, Matsuo, and coauthors [12, 13, 21, 22, 23, 24]. We develop a framework that works for a rather general class of equations.

The key tools for developing linearly implicit methods for polynomial Hamiltonians are treated in section 4, which introduces the concept of polarization. There is some freedom in this procedure, and we show through a rather general example term how the choice may significantly affect the stability of the scheme.

We defer the introduction of spatial discretization until section 5. This is done mostly in order to maintain simpler notation, but also because our approach concerns conservative time discretizations and is essentially independent of the choice of spatial discretization. The last section offers additional details on the procedure for constructing schemes, and we give some indication through numerical tests on the long-term behavior of the schemes.

2. Notation and preliminaries. We consider integral preserving PDEs written in the form

$$u_t = \mathcal{D}\frac{\delta \mathcal{H}}{\delta u}, \tag{2.1}$$

where

$$\mathcal{H}[u] = \int_\Omega \mathcal{G}[u]\,\mathrm{d}x = \int_\Omega \mathcal{G}((u^\alpha_J))\,\mathrm{d}x, \quad \Omega \subseteq \mathbb{R}^d, \tag{2.2}$$

is the preserved quantity and $\mathcal{D}$ is a skew-symmetric operator that may depend on u. We write $\mathrm{d}x = \mathrm{d}x^1 \cdots \mathrm{d}x^d$. We remark in passing that the class of PDEs which can be written in the form (2.1) contains the class of Hamiltonian PDEs; however, we do not make the additional assumption that $\mathcal{D}$ satisfies the Jacobi identity [26]. By (u^α_J) we mean u itself, which may be a vector $u = (u^\alpha) \in \mathbb{R}^m$, and all its partial derivatives with respect to all independent variables, $(x^1, \ldots, x^d)$, up to and including some degree ν. Thus, J is a multi-index; we let $J = (j_1, \ldots, j_r)$, where $r = |J|$ is the number of components in J, and

$$u^\alpha_J = \frac{\partial^r u^\alpha}{\partial x^{j_1} \cdots \partial x^{j_r}}, \quad 0 \le r \le \nu.$$

As in [26], the square brackets in (2.2) are used to indicate that a function depends also on the derivatives of its arguments with respect to the independent variables. In one dimension, $d = 1$ and $m = 1$; for example, we have

$$\mathcal{G}[u] = \mathcal{G}\left((u_J)\right) = \mathcal{G}\left(u, \frac{\partial u}{\partial x}, \ldots, \frac{\partial^\nu u}{\partial x^\nu}\right).$$

The variational derivative $\frac{\delta \mathcal{H}}{\delta u}$ is an m-vector depending on u^α_J for $|J| \le \nu'$, where $\nu' \ge \nu$. It may be defined through the relation [26, p. 245]

$$\int_\Omega \frac{\delta \mathcal{H}}{\delta u} \cdot \varphi \,\mathrm{d}x = \left.\frac{\partial}{\partial \epsilon}\right|_{\epsilon=0} \mathcal{H}[u + \epsilon\varphi] \tag{2.3}$$

for any sufficiently smooth m-vector of functions $\varphi(x)$. One may calculate $\frac{\delta \mathcal{H}}{\delta u}$ by applying the Euler operator to $\mathcal{G}[u]$; the α-component is given as

$$\left(\frac{\delta \mathcal{H}}{\delta u}\right)^{\alpha} = \mathbf{E}_{\alpha}\mathcal{G}[u], \tag{2.4}$$

where

$$\mathbf{E}_{\alpha} = \sum_{|J|\leq \nu} (-1)^{|J|} D_J \frac{\partial}{\partial u_J^{\alpha}} \tag{2.5}$$

so that the sum ranges over all J corresponding to derivatives u_J^{α} featuring in $\mathcal{G}$. We have used total derivative operators,

$$D_J = D_{j_1} \dots D_{j_k}, \quad D_i = \sum_{\alpha, J} \frac{\partial u_J^{\alpha}}{\partial x^i} \frac{\partial}{\partial u_J^{\alpha}}.$$

In parts of the paper we refer to Hamiltonians as polynomial, or specifically as quadratic. By this we mean that $\mathcal{H}$ is of a form such that $\mathcal{G}$ is a multivariate polynomial in the indeterminates u_J^{α}, which in the quadratic case is of degree at most two. For example, the KdV equation (1.1) has a polynomial Hamiltonian of degree three,

$$\mathcal{H}[u] = \int_{\Omega} \left(\frac{1}{2}u_x^2 - \frac{1}{3}u^3\right) \mathrm{d}x.$$

In this case $\mathcal{G} = \mathcal{G}(u, u_x)$ and thus $m = d = \nu = 1$, and we get

$$\frac{\delta \mathcal{H}}{\delta u} = \mathbf{E}\mathcal{G}((u_J)) = \frac{\partial \mathcal{G}}{\partial u} - \frac{\partial}{\partial x}\frac{\partial \mathcal{G}}{\partial u_x} \tag{2.6}$$

$$= -u^2 - u_{xx}. \tag{2.7}$$

We always assume sufficient regularity in the solution and that the boundary conditions on Ω are such that the boundary terms vanish when doing integration by parts, for example, periodic boundary conditions. The operator $\mathcal{D}$ should be skew-symmetric with respect to the L^2 inner product

$$\int_{\Omega} (\mathcal{D}v) w \, \mathrm{d}x = -\int_{\Omega} v(\mathcal{D}w) \, \mathrm{d}x \quad \forall\, u, w. \tag{2.8}$$

For the KdV case we simply have $\mathcal{D} = \frac{\partial}{\partial x}$.

Furthermore, to be a true Hamiltonian system it should induce a Poisson bracket on the space of functionals as described, e.g., in [26, Chap. 7.1], meaning that the Jacobi identity must be satisfied. However, the approach presented here requires only that $\mathcal{D}$ be skew-symmetric so that the functional $\mathcal{H}$ is a conserved quantity. In the case that the PDE has more than one Hamiltonian formulation, we may choose which of the integrals to preserve. Our approach does not in general allow for the preservation of more than one Hamiltonian at the same time; for this see the upcoming paper [10].

PDEs such as the wave equation are typically written with u_{tt} appearing on the left-hand side; in such cases we double the dimension of u in order to apply the stated framework. For complex equations one may do something similar, either splitting the equation into a real and an imaginary part, or adding in the complex conjugate as a separate variable.

3. Discrete gradient and variational derivative methods. Discrete gradient methods for ODEs were introduced by Gonzalez [16]. See also [6, 7, 25] and [18, Chap. V.5]. Recently this idea has been applied to PDEs in the form of the average vector field (AVF) method [5] and, in a somewhat more general setting, the discrete variational derivative (DVD) method.

We recall the definition of a discrete gradient as presented for ODEs. If $H : \mathbb{R}^M \to \mathbb{R}$, a discrete gradient is a continuous map $\overline{\nabla} : \mathbb{R}^M \times \mathbb{R}^M \to \mathbb{R}^M$ such that for every $\mathbf{u}$ and $\mathbf{v}$ in $\mathbb{R}^M$,

$$H(\mathbf{u}) - H(\mathbf{v}) = \overline{\nabla} H(\mathbf{v}, \mathbf{u}) \cdot (\mathbf{u} - \mathbf{v}),$$
$$\overline{\nabla} H(\mathbf{u}, \mathbf{u}) = \nabla H(\mathbf{u}).$$

Since an ODE system preserving H can be written in the form

$$\frac{\mathrm{d}\mathbf{y}}{\mathrm{d}t} = S(\mathbf{y}) \nabla H(\mathbf{y})$$

for some skew-symmetric matrix $S(\mathbf{y})$, one obtains a conservative method simply by defining approximations $\mathbf{y}^n \approx \mathbf{y}(t^n) = \mathbf{y}(t^0 + n\Delta t)$ through the formula

$$\frac{\mathbf{y}^{n+1} - \mathbf{y}^n}{\Delta t} = \tilde{S} \overline{\nabla} H(\mathbf{y}^n, \mathbf{y}^{n+1}),$$

where $\tilde{S}$, typically allowed to depend on $\mathbf{y}^n$ and $\mathbf{y}^{n+1}$, is some skew-symmetric matrix approximating the original S.

There are many possible choices of discrete gradients for a function H; see, for instance, [18, 25]. A particular example is that used in the AVF method defined as

$$\overline{\nabla}_{\mathrm{AVF}} H(\mathbf{v}, \mathbf{u}) = \int_0^1 \nabla H(\xi \mathbf{u} + (1 - \xi)\mathbf{v}) \, \mathrm{d}\xi.$$

When applying this approach to PDEs the obvious strategy is to discretize the Hamiltonian $\mathcal{H}[u]$ in space, replacing each derivative by a suitable approximation, for example, by using finite differences, to obtain $\mathcal{H}_d(\mathbf{u})$. Similarly, the skew-symmetric operator $\mathcal{D}$ is replaced by a skew-symmetric $M \times M$-matrix $\mathcal{D}_d$ to yield the scheme

$$\frac{\mathbf{u}^{n+1} - \mathbf{u}^n}{\Delta t} = \mathcal{D}_d \overline{\nabla} \mathcal{H}_d(\mathbf{u}^n, \mathbf{u}^{n+1}) \tag{3.1}$$

for advancing the numerical solution $\mathbf{u}^n$ at time t^n to $\mathbf{u}^{n+1}$ at time t^{n+1}. Examples are worked out for several PDEs in [5].

Furihata, Matsuo, and coauthors present a whole framework for discretizing PDEs in the variational setting in a series of papers, providing a discrete analogue of the continuous calculus; see, for instance, [12]. They discretize $\mathcal{G}$ to obtain $\mathcal{G}_d$ using difference operators, and then the integral in $\mathcal{H}$ is approximated by a sum to yield $\mathcal{H}_d$. Then they derive a discrete counterpart to the variational derivative and finally state the difference scheme in a form which is a perfect analogue to the Hamiltonian PDE system (2.1), letting

$$\frac{\mathbf{u}^{n+1} - \mathbf{u}^n}{\Delta t} = \mathcal{D}_d \frac{\delta \mathcal{H}_d}{\delta(\mathbf{u}^n, \mathbf{u}^{n+1})}.$$

The use of integration by parts in deriving the Euler operator is mimicked by similar summation by parts formulas for the discrete case. Their discrete variational derivative is in fact rather similar to a discrete gradient, as it satisfies the relation

$$\mathcal{H}_d(\mathbf{u}) - \mathcal{H}_d(\mathbf{v}) = \left\langle \frac{\delta \mathcal{H}_d}{\delta(\mathbf{v},\mathbf{u})}, \mathbf{u} - \mathbf{v} \right\rangle \tag{3.2}$$

for the discrete L^2 inner product.

In the present paper, we focus on the time dimension in most of what follows; thus we shall defer the steps in which $\mathcal{H}$ and thereby $\mathcal{G}$ are discretized in space. But (3.2) makes perfect sense after removing the subscript d, replacing $\mathbf{u}$ and $\mathbf{v}$ by functions u and v, and replacing the discrete L^2 inner product by the continuous one. A DVD is here defined to be any continuous function $\frac{\delta \mathcal{H}}{\delta(v,u)}$ of $(u^{(\nu)}, v^{(\nu)})$ satisfying

$$\mathcal{H}[u] - \mathcal{H}[v] = \int_\Omega \frac{\delta \mathcal{H}}{\delta(v,u)}(u - v)\,\mathrm{d}x, \tag{3.3}$$

$$\frac{\delta \mathcal{H}}{\delta(u,u)} = \frac{\delta \mathcal{H}}{\delta u}. \tag{3.4}$$

The integrator yields a continuous function $U^n := U^n(x) \approx u(x, t^n)$ for each t^n,

$$\frac{U^{n+1} - U^n}{\Delta t} = \mathcal{D} \frac{\delta \mathcal{H}}{\delta(U^n, U^{n+1})}. \tag{3.5}$$

By combining (3.3) and (3.5) we see that the method preserves $\mathcal{H}$.

The AVF scheme can of course also be interpreted as a DVD method, where

$$\frac{\delta \mathcal{H}_{\mathrm{AVF}}}{\delta(v,u)} = \int_0^1 \frac{\delta \mathcal{H}}{\delta u}[\xi u + (1-\xi)v]\,\mathrm{d}\xi. \tag{3.6}$$

The fact that (3.6) verifies the condition (3.3) is seen from the elementary identity

$$\mathcal{H}[u] - \mathcal{H}[v] = \int_0^1 \frac{\mathrm{d}}{\mathrm{d}\xi} \mathcal{H}[\xi u + (1-\xi)v]\,\mathrm{d}\xi. \tag{3.7}$$

The derivative under the integral is written

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}\xi}\mathcal{H}[\xi u + (1-\xi)v] &= \frac{\mathrm{d}}{\mathrm{d}\varepsilon}\bigg|_{\varepsilon=0} \mathcal{H}[v + (\xi + \varepsilon)(u - v)] \\ &= \int_\Omega \frac{\delta \mathcal{H}}{\delta u}[\xi u + (1-\xi)v](u - v)\,\mathrm{d}\mathbf{x}. \end{aligned}$$

Now substitute this into (3.7) and interchange the integrals to obtain (3.3).

In most of the cited papers by Furihata, Matsuo, and coauthors, the notion of a DVD method is less general than what we just presented, in the sense that the relation (3.2) is not actually used as the defining equation for a DVD. Instead, Furihata and coauthors present a relatively general format that can be used for discretizing $\mathcal{H}$, this format is dependent on the class of PDEs under consideration, and they work out the explicit expression for a particular DVD. To give an idea of how the format may look, we briefly review some points from [12], where PDEs of the form (2.2) are considered

with $d = m = \nu = 1$ such that $\mathcal{G} = \mathcal{G}(u, u_x)$. $\mathcal{G}$ is assumed to be written as a finite sum

$$\mathcal{G}(u, u_x) = \sum_\ell \alpha_\ell f_\ell(u) g_\ell(u_x), \tag{3.8}$$

where f_ℓ and g_ℓ are differentiable functions.[1] The form (3.3) is then derived through

$$\begin{aligned} f_\ell(u)g_\ell(u_x) - f_\ell(v)g_\ell(v_x) = {} & \frac{f_\ell(u) - f_\ell(v)}{u - v} \frac{g_\ell(u_x) + g_\ell(v_x)}{2}(u - v) \\ & + \frac{g_\ell(u_x) - g_\ell(v_x)}{u_x - v_x} \frac{f_\ell(u) + f_\ell(v)}{2}(u_x - v_x) \end{aligned}$$

followed by an integration by parts on the second term. This technique can be extended in any number of ways to allow for more general classes of PDEs. For instance, one may allow for more factors in (3.8), such as

$$\mathcal{G}[u] = \sum_\ell \alpha_\ell \prod_J g_{\ell,J}(\partial_J u),$$

and repeated application of the formula $ab - cd = \frac{a+c}{2}(b - d) + \frac{b+d}{2}(a - c)$ to this equation combined with integration by parts will result in a DVD.

Schemes which are built on this particular type of DVD will be called Furihata methods in what follows since they were first introduced in [12]. Matsuo and Furihata extend the method to complex equations in [22], while [13, 21] derive methods for equations with second order time derivatives. Other papers using the DVD approach include [14, 24, 30].

The lack of a general formalism in the papers just mentioned makes it somewhat difficult to compare the approach to the AVF method and to characterize in which cases they lead to the same scheme. Taking for instance the KdV equation (1.1), one easily finds that both approaches lead to the scheme (1.2); however, considering for instance the Hamiltonian

$$\mathcal{H}[u] = \int_\Omega u u_x^2 \,\mathrm{d}x,$$

one would obtain two different types of DVD in the Furihata method and the AVF method; that is, $\frac{\delta \mathcal{H}_F}{\delta(v,u)} \neq \frac{\delta \mathcal{H}_{\mathrm{AVF}}}{\delta(v,u)}$. In some important cases, the Furihata method and the AVF method lead to the same scheme.

THEOREM 3.1. *Suppose that the Hamiltonian $\mathcal{H}[u]$ is a linear combination of terms of either of the types*

1. $\int_\Omega \partial_J u \cdot \partial_K u \,\mathrm{d}x$ *for multi-indices J and K, or*
2. $\int_\Omega g(\partial_J u) \,\mathrm{d}x$ *for differentiable $g : \mathbb{R} \to \mathbb{R}$.*

Then the AVF and Furihata methods yield the same scheme.

Proof. It suffices to check one general term of each type.

1. We find the variational derivative using (2.3),

$$\frac{\delta \mathcal{H}}{\delta u} = \left((-1)^{|J|} + (-1)^{|K|}\right) \partial_{J+K} u.$$

[1] In [12] the expression is discretized in space, and $g_\ell(u_x)$ is replaced by a product $g_\ell^+(\delta_k^+ U_k) g_\ell^-(\delta_k^- U_k)$, where δ_k^+ and δ_k^- are forward and backward divided differences, respectively.

Inserting the variational derivative into (3.6) gives

$$\frac{\delta \mathcal{H}_{\text{AVF}}}{\delta(v,u)} = \left((-1)^{|J|} + (-1)^{|K|}\right) \partial_{J+K} \left(\frac{u+v}{2}\right).$$

To find the DVD of the Furihata method we compute

$$\begin{aligned}\mathcal{H}[u] - \mathcal{H}[v] &= \int_\Omega \partial_J u \cdot \partial_K u - \partial_J v \cdot \partial_K v \,\mathrm{d}x \\ &= \frac{1}{2}\int_\Omega (\partial_J u - \partial_J v)\cdot(\partial_K u + \partial_K v) + (\partial_J u + \partial_J v)\cdot(\partial_K u - \partial_K v)\,\mathrm{d}x.\end{aligned}$$

After integration by parts we get

$$\frac{\delta \mathcal{H}_F}{\delta(v,u)} = \left((-1)^{|J|} + (-1)^{|K|}\right) \partial_{J+K} \left(\frac{u+v}{2}\right),$$

and we see that

$$\frac{\delta \mathcal{H}_{\text{AVF}}}{\delta(v,u)} = \frac{\delta \mathcal{H}_F}{\delta(v,u)}.$$

2. In this case we get

$$\frac{\delta \mathcal{H}}{\delta u} = (-1)^{|J|} \partial_J g'(\partial_J u),$$

so that

$$\begin{aligned}\frac{\delta \mathcal{H}_{\text{AVF}}}{\delta(v,u)} &= (-1)^{|J|}\int_0^1 \partial_J g'(\partial_J(\xi u + (1-\xi)v))\,\mathrm{d}\xi \\ &= (-1)^{|J|}\partial_J\left(\frac{g(\partial_J u) - g(\partial_J v)}{\partial_J u - \partial_J v}\right).\end{aligned}$$

For the Furihata method one would here just compute

$$H[u] - H[v] = \int_\Omega \frac{g(\partial_J u) - g(\partial_J v)}{\partial_J u - \partial_J v}\,(\partial_J u - \partial_J v)\,\mathrm{d}x,$$

and integration by parts yields

$$\frac{\delta \mathcal{H}_F}{\delta(v,u)} = \frac{\delta \mathcal{H}_{\text{AVF}}}{\delta(v,u)}. \qquad \square$$

4. Linearly implicit difference schemes.

4.1. Polarization. The key to constructing conservative linearly implicit schemes will be to portion out the nonlinearity over consecutive time steps. In effect, this means that we replace the original Hamiltonian $\mathcal{H}$ with an approximate one H. We shall call H a polarization of $\mathcal{H}$ since its definition resembles the way an inner product is derived from a quadratic form. We shall see that the difference scheme resulting from such a polarized Hamiltonian will be a multistep method. This method will now preserve exactly H, as opposed to $\mathcal{H}$ for the methods in the previous section. The requirements on H are given in the following definition.

DEFINITION 4.1 (the polarized Hamiltonian). *Given a Hamiltonian $\mathcal{H}[u]$, the polarized Hamiltonian H depends on k arguments and is*

- *consistent:*

$$H[u,u,\dots,u] = \mathcal{H}[u]; \tag{4.1}$$

- *invariant under any cyclic permutation of the arguments*

$$H[w_1,w_2,\dots,w_k] = H[w_2,\dots,w_k,w_1]. \tag{4.2}$$

Polarizations exist for any Hamiltonian; this is asserted by the example

$$H[w_1,w_2,\dots,w_k] = \frac{1}{k}\left(\mathcal{H}[w_1] + \mathcal{H}[w_2] + \cdots + \mathcal{H}[w_k]\right).$$

We may impose the polarization directly on the density $\mathcal{G}((u_J^\alpha))$, letting

$$H[w_1,w_2,\dots,w_k] = \int_\Omega G[w_1,w_2,\dots,w_k]\,\mathrm{d}x.$$

The conditions (4.1), (4.2) are then inherited as

$$G(u,u,\dots,u) = \mathcal{G}(u), \qquad G[w_1,w_2,\dots,w_k] = G[w_2,\dots,w_k,w_1].$$

In section 4.2 we will discuss local order of consistency; it will then be convenient to make the stronger assumption that $\mathcal{H}$ and H are at least twice Fréchet differentiable. To distinguish from the weaker notion of the variational (Gâteaux) derivative, we replace δ by ∂, noting that the first derivative in the two definitions is the same when both definitions exist. We then find from (4.1) and (4.2) that the Fréchet derivatives satisfy the relation

$$\frac{\partial \mathcal{H}}{\partial u}[u] = k\,\frac{\partial H}{\partial w_1}[u,\dots,u]. \tag{4.3}$$

For the second derivatives, we find the identity

$$\frac{\partial^2 H}{\partial w_1 \partial w_j}[u,\dots,u] = \frac{\partial^2 H}{\partial w_1 \partial w_{k+2-j}}[u,\dots,u], \quad j = 2,\dots,\lfloor k/2\rfloor + 1, \tag{4.4}$$

which is used to compute

$$\frac{\partial^2 \mathcal{H}}{\partial u^2}[u] = \begin{cases} k\left(\dfrac{\partial^2 H}{\partial w_1^2} + 2\displaystyle\sum_{\ell=2}^{\frac{k+1}{2}} \frac{\partial^2 H}{\partial w_1 \partial w_\ell}\right), & k \text{ odd}, \\ k\left(\dfrac{\partial^2 H}{\partial w_1^2} + 2\displaystyle\sum_{\ell=2}^{\frac{k}{2}} \frac{\partial^2 H}{\partial w_1 \partial w_\ell} + \frac{\partial^2 H}{\partial w_1 \partial w_{\frac{k}{2}+1}}\right), & k \text{ even}, \end{cases} \tag{4.5}$$

with all second derivatives on the right being evaluated at $[u,\dots,u]$.

4.1.1. Polynomial Hamiltonians. The polarization of polynomial Hamiltonians will be key to constructing linearly implicit schemes. We will now explain in detail how to do this, and we begin with an example term in the integrand $\mathcal{G}[u] = \mathcal{G}(\partial_J^\alpha u)$ depending on just one scalar indeterminate, namely $\mathcal{G}(z) = z^p$, where $z = \partial_J u^\alpha$ for some (J,α) and where $p \le 4$. This example is important not only because it is a simple illustration of the procedure, but also because terms of this type are common

in many of the Hamiltonians found in physics. As we will see in the next section, it will be natural to use two arguments, $k = 2$, in the polarized Hamiltonian. In fact, we need to restrict our attention to cases with polynomial Hamiltonians for our technique to yield linearly implicit schemes. Then, by using $k \geq \lceil p/2 \rceil$, we can obtain polarized Hamiltonians which are at most quadratic in each argument. We call these quadratic polarizations. We see that if $k = 2$, then cyclic is the same as symmetric $G(u, v) = G(v, u)$, and the possible quadratic polarizations for $p = 2, 3, 4$ are, respectively,

$$p = 2: \qquad G(u,v) = \theta \frac{u^2 + v^2}{2} + (1-\theta)uv\,, \quad \theta \in [0,1], \tag{4.6}$$

$$p = 3: \qquad G(u,v) = uv\frac{u+v}{2}, \tag{4.7}$$

$$p = 4: \qquad G(u,v) = u^2v^2. \tag{4.8}$$

Note that for these monomials both the third and fourth degree cases are uniquely given, but the second degree case is not. In section 4.3 we will consider how the choice of θ influences the stability of the scheme for a term which appears frequently in PDEs.

We now consider the general case when $\mathcal{G}[u]$ is a multivariate polynomial in N_ν variables of degree p. It suffices in fact to let $\mathcal{G}((u_J^\alpha))$ be a monomial since each term can be treated separately for $u \in \mathbb{R}^{N_\nu}$. For a convenient notation, we rename the vector of indeterminates (u_J^α) by using a single index, i.e., $u = (u_1, \ldots, u_{N_\nu})$, and write

$$\mathcal{G}(u) = u_{i_1} u_{i_2} \ldots u_{i_p}. \tag{4.9}$$

One may use the following procedure for obtaining a quadratic polarization from (4.9):

1. Group the factors of the right-hand side of (4.9) into pairs $z_r = u_{i_{2r-1}} u_{i_{2r}}$, and if p is odd, $z_k = u_{i_p}$. Set

$$K(z_1, \ldots, z_k) = z_1 \cdots z_k.$$

   Note that there are potentially many ways of ordering the factors in (4.9) which give rise to different polarizations.
2. Symmetrize K with respect to the cyclic subgroup of permutations. Letting the left shift permutation σ be defined through $\sigma K(z_1, \ldots, z_k) = K(z_2, \ldots, z_k, z_1)$, we set

$$G(z_1, \ldots, z_k) = \frac{1}{k} \sum_{k=1}^{k} \sigma^{k-1} K(z_1, \ldots, z_k).$$

   The resulting G is now both consistent (4.1) and cyclic (4.2).

4.2. Linearly implicit methods. We may now define the DVD for this polarized Hamiltonian as a generalization of (3.3) and (3.4). We let

$$\frac{\delta H}{\delta(w_1, \ldots, w_{k+1})}$$

be a continuous function of $k + 1$ arguments, satisfying

$$H[w_2, \ldots, w_{k+1}] - H[w_1, \ldots, w_k] = \int_\Omega \frac{\delta H}{\delta(w_1, \ldots, w_{k+1})}(w_{k+1} - w_1)\,\mathrm{d}x, \tag{4.10}$$

$$k\,\frac{\delta H}{\delta(u,\dots,u)} = \frac{\delta \mathcal{H}}{\delta u}. \tag{4.11}$$

Our standard example will be a generalization of the AVF DVD, which we define as

$$\frac{\delta H_{\mathrm{AVF}}}{\delta(w_1,\dots,w_{k+1})} = \int_0^1 \frac{\delta H}{\delta w_1}[\xi w_{k+1} + (1-\xi)w_1, w_2, \dots, w_k]\,\mathrm{d}\xi. \tag{4.12}$$

Here the variational derivative on the right-hand side, $\frac{\delta H}{\delta w_1}$, is defined as before, considering H as a function of its first argument only, leaving the others fixed. Similar DVDs could be derived in a number of different ways. In particular, one finds that when the function H is quadratic in all of its arguments, the approach used in deriving the Furihata methods would lead to a discrete variational derivative which is identical to that of the AVF method.

Now we define the polarized DVD scheme and prove that, under some assumptions, this scheme is conservative and linearly implicit and has formal order of consistency two.

DEFINITION 4.2. *For a Hamiltonian PDE of the form* (2.1)*, let H be a polarized Hamiltonian of k arguments, satisfying* (4.1) *and* (4.2)*, and suppose that approximations U^j to $u(j\Delta t,\cdot)$ are given for $j = 0,\dots,k-1$.*

- *The polarized DVD (PDVD) scheme is given as*

$$\frac{U^{n+k} - U^n}{k\Delta t} = kD\frac{\delta H}{\delta(U^n,\dots,U^{n+k})}, \quad n \geq 0. \tag{4.13}$$

- *D is a skew-symmetric operator approximating $\mathcal{D}$. In* (4.13)*, D may depend on U^{n+j}, $1 \leq j \leq k-1$,*[2] *and be consistent,*

$$D[u,\dots,u] = \mathcal{D}[u]. \tag{4.14}$$

D is called cyclic if

$$D[w_1, w_2, \dots, w_{k-1}] = D[w_2, \dots, w_{k-1}, w_1]. \tag{4.15}$$

- *If the DVD is given by* (4.12)*, then the scheme is called the polarized AVF (PAVF) scheme.*

THEOREM 4.3. *The scheme* (4.13) *is conservative in the sense that*

$$H[U^{n+1},\dots,U^{n+k}] = H[U^0,\dots,U^k] \quad \forall n \geq 1$$

for any polarized Hamiltonian function H.

Proof. By induction, this is an immediate consequence of (4.10) ∎

In a framework as general as that presented here, it is not possible to present a general analysis for convergence or the order of the truncation error. However, it seems plausible that a necessary condition to obtain a prescribed order of convergence can be derived through a formal Taylor expansion of the local truncation error; we denote this *the formal order of consistency*.

THEOREM 4.4.

- *The PAVF scheme defined by* (4.12) *and* (4.13) *has formal order of consistency one.*

[2] D should not depend on U^{n+k} since otherwise the method would no longer be linearly implicit.

- *If in addition* (4.15) *is satisfied, the scheme has formal order of consistency two.*

Proof. We show that when the exact solution is substituted into (4.13), where the DVD is given by (4.12), the residual is $\mathcal{O}(\Delta t^2)$. Throughout the proof we assume the existence of Fréchet derivatives. Writing, for any j, $u^j = u(\cdot, t^j)$ for the exact local solution at $t = t^j$, we get for the left-hand side

$$\frac{u^{n+k} - u^n}{k\Delta t} = \partial_t u^n + \frac{k\,\Delta t}{2}\partial_t^2 u^n + \mathcal{O}(\Delta t^2) = \mathcal{D}\frac{\partial \mathcal{H}}{\partial u}\bigg|_{u^n} + \frac{k\Delta t}{2}\left(\frac{\partial \mathcal{D}}{\partial u}(\partial_t u^n)\frac{\partial \mathcal{H}}{\partial u} + \mathcal{D}\frac{\partial^2 \mathcal{H}}{\partial u^2}(\cdot, \partial_t u^n)\right)\bigg|_{u^n} + \mathcal{O}(\Delta t^2). \tag{4.16}$$

Next we expand (4.12) to get

$$\begin{aligned}\frac{\delta H_{\text{AVF}}}{\delta(u^n, \dots, u^{n+k})} &= \int_0^1 \frac{\delta H}{\delta w_1}(\xi u^{n+k} + (1-\xi)u^n, u^{n+1}, \dots, u^{n+k-1})\,\mathrm{d}\xi \\ &= \frac{\partial H}{\partial w_1}\bigg|_{\mathbf{u}} + \left(\frac{k}{2}\,\frac{\partial^2 H}{\partial w_1^2}\bigg|_{\mathbf{u}} + \Delta t \sum_{j=2}^{k}(j-1)\,\frac{\partial^2 H}{\partial w_1 \partial w_j}\bigg|_{\mathbf{u}}\right)(\cdot, \partial_t u^n) + \mathcal{O}(\Delta t^2),\end{aligned}$$

where $\mathbf{u} = (u^n, \dots, u^n)$. Using first (4.4) and then (4.3), (4.5), we find

$$\frac{\delta H_{\text{AVF}}}{\delta(u^n, \dots, u^{n+k})} = \frac{1}{k}\,\frac{\partial \mathcal{H}}{\partial u}\bigg|_{u^n} + \frac{\Delta t}{2}\,\frac{\partial^2 \mathcal{H}}{\partial u^2}\bigg|_{u^n}(\cdot, \partial_t u^n) + \mathcal{O}(\Delta t^2). \tag{4.17}$$

Expanding D, we get

$$D[u^{n+1}, \dots, u^{n+k-1}] = \mathcal{D}[u^n] + \Delta t \sum_{j=1}^{k-1} j\,\frac{\partial D}{\partial w_j}\bigg|_{\mathbf{u}}(\partial_t u^n) + \mathcal{O}(\Delta t^2). \tag{4.18}$$

If the cyclicity condition (4.15) holds for D, we can simplify (4.18) to obtain

$$\begin{aligned}D[u^{n+1}, \dots, u^{n+k-1}] &= \mathcal{D}[u^n] + \frac{k(k-1)\Delta t}{2}\,\frac{\partial D}{\partial w_1}\bigg|_{\mathbf{u}}(\partial_t u^n) + \mathcal{O}(\Delta t^2) \\ &= \mathcal{D}[u^n] + \frac{k\Delta t}{2}\,\frac{\partial \mathcal{D}}{\partial u}\bigg|_{u^n}(\partial_t u_n) + \mathcal{O}(\Delta t^2).\end{aligned} \tag{4.19}$$

By substituting into (4.13) the expressions (4.16), (4.17), and (4.19), all terms of zeroth and first order cancel, and we are left with $\mathcal{O}\left((\Delta t^2)\right)$. ∎

THEOREM 4.5. *Suppose that the polarized Hamiltonian H is a quadratic polynomial in each of its arguments; then the PAVF scheme is linearly implicit*

Proof. Since H is at most quadratic in the first argument, it follows from (2.5) that $\frac{\delta H}{\delta w_1}$ is of degree at most one in its first argument, and so we see from (4.12) that

$$\frac{\delta H}{\delta(U^n, \dots, U^{n+k})}$$

is linear in U^{n+k}. Since D does not depend on U^{n+k}, we conclude that the scheme (4.13) is linearly implicit. ∎

In some cases one wishes to have time-symmetric numerical schemes; see, for example, [18]. The numerical scheme (4.13) will in general not be symmetric; however, it is not hard to modify the procedure to yield symmetric schemes. One needs to polarize $\mathcal{H}$ such that H is invariant also when the order of its arguments is reversed; it turns out that this can be achieved by symmetrizing over the dihedral group rather than just the cyclic group. A similar adjustment must be made for D.

We remark that one can construct explicit schemes by using p time steps (as opposed to k) in H such that H becomes p-linear (as opposed to k-quadratic). The rest of the procedure for the explicit case is the same as that for the linearly implicit case. Clearly, one expects that explicit schemes will have more severe stability restrictions than the linearly implicit ones.

Since these multistep schemes need the k previous values, they are not self-starting. We have to provide the starting values $U^1, \dots, U^k$ in addition to the initial value U^0. Usually these are computed using another sufficiently accurate conservative scheme such as, for example, the AVF scheme. Another possibility is to use any integrator and integrate to machine precision.

4.3. Stability. In [9] we studied linearly implicit schemes for the cubic Schrödinger equation and found that two-step schemes can develop a two-periodic instability in time. We also saw that this can be remedied by choosing a different polarization of the Hamiltonian.

As it turns out, a common case is when the Hamiltonian is a univariate polynomial of degree four or less. If we polarize this Hamiltonian using two time steps, we get three linearly independent H's, corresponding to (4.6), (4.7), and (4.8). The third and fourth degree Hamiltonians are uniquely given. However, in the second degree case we can choose $\theta \in [0, 1]$ such that the scheme becomes unstable. Since Hamiltonians of the type (4.6) appear in many important PDEs, it may be useful to determine which $\theta \in [0, 1]$ lead to unstable schemes.

We choose to study the test equation with Hamiltonian

$$\mathcal{H}[u] = \frac{1}{2} \int_\Omega u_x^2 \, \mathrm{d}x$$

and a skew-symmetric operator $\mathcal{D}$, which satisfies the eigenvalue equation

$$\mathcal{D} \mathrm{e}^{\mathrm{i}kx} = \mathrm{i}\lambda_k \mathrm{e}^{\mathrm{i}kx}, \quad \lambda_k \in \mathbb{R},$$

for all integers k. The Airy equation

$$u_t + u_{xxx} = 0$$

is of this type with $\mathcal{D} = -\partial_x$ and $\lambda_k = -k$. Other equations which have such terms in the Hamiltonian include the nonlinear Schrödinger equation, the linear wave equation, the KdV equation, and the Kadomtsev–Petviashvili equation.

Rewriting (4.6) gives

$$H[v, u] = \frac{1}{2} \int \left(\theta \frac{u_x^2 + v_x^2}{2} + (1 - \theta) u_x v_x \right) \mathrm{d}x,$$

and the numerical scheme is

$$\frac{U^{n+2} - U^n}{2\Delta t} = -\mathcal{D} \left(\theta \frac{U_{xx}^{n+2} + U_{xx}^n}{2} + (1 - \theta) U_{xx}^{n+1} \right). \tag{4.20}$$

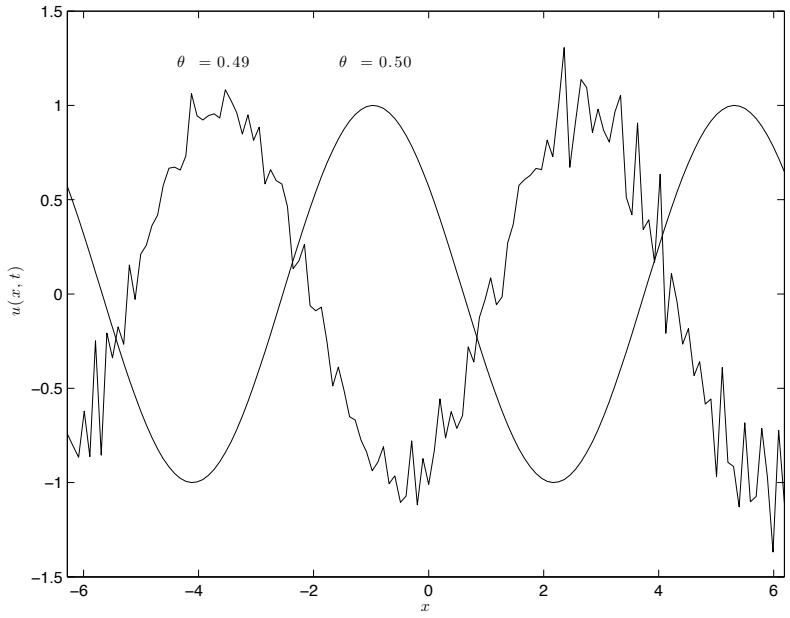

FIG. 4.1. *The numerical solution of the Airy equation with two different values of θ. The two solutions are shown after $n = 10^6$ time steps ($\theta = 0.5$) and $n = 115$ time steps ($\theta = 0.49$).*

Since this is a linear equation, we can use von Neumann stability analysis [8]. We insert the ansatz

$$U^n(x) = \zeta^n \mathrm{e}^{\mathrm{i}kx}$$

to obtain the quadratic equation

$$(1 - \theta\tau\mathrm{i})\zeta^2 - 2(1-\theta)\tau\mathrm{i}\zeta - (1 + \theta\tau\mathrm{i}) = 0, \quad \tau = \lambda_k \Delta t k^2. \tag{4.21}$$

A necessary condition for stability is $|\zeta| \leq 1$ which implies

$$\theta \geq \frac{1}{2} - \frac{1}{2\tau^2}.$$

Assuming that $\{\lambda_k k^2\}_{k\in\mathbb{Z}}$ is unbounded, we must require that θ is chosen greater than or equal to $\frac{1}{2}$. This is exactly the condition found in [9] for the cubic Schrödinger equation. When $\theta \geq \frac{1}{2}$, the roots of (4.21) satisfy $|\zeta_1| = |\zeta_2| = 1$.

In Figure 4.1 we solve the Airy equation with the scheme (4.20) using $\theta = 0.5$ and $\theta = 0.49$. We use the initial value $u(x, 0) = \sin(x)$, which, in the exact case, yields the traveling wave solution $u(x, t) = \sin(x + t)$. The $\theta = 0.49$ solution blows up in few time steps, while the $\theta = 0.50$ solution shows no signs of instability. Doing a discrete Fourier transform of the unstable solution, we see that the instability starts at high frequencies, that is, large k, which corresponds to the results shown above.

There might be cases where the schemes develop instabilities due to spurious modes no matter what polarization one chooses. A full stability analysis of either the fully or linearly implicit schemes has not, to our knowledge, been done. Standard linearization techniques will usually lead to the conclusion that the schemes are neutrally stable. The nonlinear effects, however small, may still cause the scheme to be

unstable. The tests we have done on a wide range of PDEs seem to indicate that the stability usually is very good; future work may shed a light on this issue.

5. Space discretization. Until now we have mostly considered the situation where the PDE is discretized in time while remaining continuous in space. The methodology developed in the previous sections applies equally well to systems of ODEs. Arguably, the most straightforward approach is simply to discretize the space derivatives in the Hamiltonian, for instance, by finite differences. This leads to

$$\mathcal{H}(u) \longrightarrow \mathcal{H}_d(\mathbf{u}).$$

One also needs to replace the skew-symmetric operator $\mathcal{D}$ by a skew-symmetric matrix $\mathcal{D}_d$. The fully implicit method reviewed in section 3 is then just the discrete gradient method (3.1), which conserves the discretized Hamiltonian $\mathcal{H}_d(\mathbf{u})$ in every time step.

We consider now finite difference approximations. The function space to which the solution u belongs is replaced by a finite dimensional space with functions on a grid indexed by $I_g \subset \mathbb{Z}^d$. We use boldface symbols for these functions. Let there be N_r grid points in the space direction r so that $\mathbf{N} = N_1 \cdots N_d$ is the total number of grid points. We denote by $\mathbf{u}^\alpha$ the approximation to u^α on such a grid, and denote by $\mathbf{u}$ the vector consisting of $(\mathbf{u}^1, \ldots, \mathbf{u}^m)$. We will replace each derivative u^α_J by a finite difference approximation $\delta_J \mathbf{u}^\alpha$ and replace the integral by a quadrature rule. We then let

$$\mathcal{H}_d(\mathbf{u}) = \sum_{\mathbf{i} \in I_g} b_{\mathbf{i}} (\mathcal{G}_d((\delta_J \mathbf{u})))_{\mathbf{i}} \, \Delta x. \tag{5.1}$$

Here Δx is the volume (length, area) of a grid cell and $\mathbf{b} = (b_{\mathbf{i}})_{\mathbf{i} \in I_g}$ are the weights in the quadrature rule. The discretized $\mathcal{G}_d$ has the same number of arguments as $\mathcal{G}$, and each input argument, as well as the output, is a vector in $\mathbb{R}^N$. We have here approximated the function u^α_J by a difference approximation $\delta_J \mathbf{u}^\alpha$, where $\delta_J : \mathbb{R}^{\mathbf{N}} \to \mathbb{R}^{\mathbf{N}}$ is a linear map. As in the continuous case, we use square brackets, say $F[\mathbf{u}]$, as shorthand for a list of arguments involving difference operators $F[\mathbf{u}] = F(\mathbf{u}, \delta_{J_1}\mathbf{u}, \ldots, \delta_{J_q}\mathbf{u})$. We compute

$$\begin{aligned} \mathcal{H}_d[\mathbf{u}] - \mathcal{H}_d[\mathbf{v}] &= \sum_{\mathbf{i} \in I_g} b_{\mathbf{i}} \sum_{J,\alpha} \int_0^1 \left(\frac{\partial \mathcal{G}_d}{\partial \delta_J \mathbf{u}^\alpha} \right)_{\mathbf{i}} [\xi \mathbf{u} + (1-\xi)\mathbf{v}] \mathrm{d}\xi (\delta_J(\mathbf{u}^\alpha - \mathbf{v}^\alpha)) \, \Delta x \\ &= \left\langle \frac{\delta \mathcal{H}_d}{\delta(\mathbf{v}, \mathbf{u})}, \mathbf{u} - \mathbf{v} \right\rangle, \end{aligned} \tag{5.2}$$

where

$$\frac{\delta \mathcal{H}_d}{\delta(\mathbf{v}, \mathbf{u})} = \sum_{J,\alpha} \delta_J^T \, B \left(\int_0^1 \frac{\partial \mathcal{G}_d}{\partial \mathbf{u}_J} [\xi \mathbf{u}^\alpha + (1-\xi)\mathbf{v}^\alpha] \, \mathrm{d}\xi \right),$$

B is the diagonal linear map $B = \mathrm{diag}(b_{\mathbf{i}})$, $\mathbf{i} \in I_g$, and the discrete inner product used in (5.2) is

$$\langle \mathbf{u}, \mathbf{v} \rangle = \sum_{\alpha, \mathbf{i} \in I_g} \mathbf{u}^\alpha_{\mathbf{i}} \mathbf{v}^\alpha_{\mathbf{i}}.$$

Notice the resemblance between the operator acting on $\mathcal{G}_d$ in (5.2) and the continuous Euler operator in (2.5). Alternatively, suppose the following:

1. The spatially continuous method (3.5) (using (3.6)) is discretized in space, using a skew-symmetric $\mathcal{D}_d$ and a selected set of difference quotients δ_J for each derivative ∂_J.
2. Considering (2.4) and (2.5), the choice of discretization operators δ_J used in $\partial\mathcal{G}/\partial u^\alpha_J[u]$ is arbitrary, but the corresponding D_J is replaced by the transpose δ_J^T.

In this case, using the same $\mathcal{D}_d$, an identical set of difference operators in discretizing $\mathcal{H}$ (5.1), and choosing all the quadrature weights $b_{\mathbf{i}} = 1$, the resulting scheme would be the same as that given by the procedure outlined in the two points above. That is, one can get the same scheme by either discretizing the Hamiltonian in space first (and then deriving the scheme) or discretizing the scheme in space first (and then deriving the conserved Hamiltonian).

Letting the rth canonical unit vector in $\mathbb{R}^d$ be denoted $\mathbf{e}_r$, we define the most used first order difference operators:

$$(\delta_r^+ \mathbf{u})_{\mathbf{i}} = \frac{\mathbf{u}_{\mathbf{i}+\mathbf{e}_r} - \mathbf{u}_{\mathbf{i}}}{\Delta x_r},$$
$$(\delta_r^- \mathbf{u})_{\mathbf{i}} = \frac{\mathbf{u}_{\mathbf{i}} - \mathbf{u}_{\mathbf{i}-\mathbf{e}_r}}{\Delta x_r},$$
$$(\delta_r^{\langle 1\rangle} \mathbf{u})_{\mathbf{i}} = \frac{\mathbf{u}_{\mathbf{i}+\mathbf{e}_r} - \mathbf{u}_{\mathbf{i}-\mathbf{e}_r}}{2\Delta x_r}.$$

These difference operators are all commuting, but only the last is skew-symmetric. However, the first two have the useful identities

$$(\delta_r^+)^T = -\delta_r^-, \qquad (\delta_r^-)^T = -\delta_r^+.$$

Higher order difference operators δ_J can generally be defined by taking compositions of these operators; in particular, we shall consider examples in the next section using the second and third derivative approximations

$$\delta_r^{\langle 2\rangle} = \delta_r^+ \circ \delta_r^-, \quad \delta^{\langle 3\rangle} = \delta^{\langle 1\rangle} \circ \delta^{\langle 2\rangle}.$$

We may now introduce numerical approximations $\mathbf{U}^n$ representing the fully discretized system; the scheme is

$$\frac{\mathbf{U}^{n+1} - \mathbf{U}^n}{\Delta t} = \mathcal{D}_d \frac{\delta \mathcal{H}_d}{\delta(\mathbf{U}^n, \mathbf{U}^{n+1})}.$$

The conservative schemes based on polarization are adapted in a straightforward manner, introducing a function $H_d[\mathbf{w_1}, \ldots, \mathbf{w_k}]$, which is consistent and cyclic as in (4.1), (4.2), and a skew-symmetric map D_d depending on at most $k-1$ arguments. The scheme is then

$$\frac{\mathbf{U}^{n+k} - \mathbf{U}^n}{k\Delta t} = k D_d \frac{\delta H_d}{\delta(\mathbf{U}^n, \ldots, \mathbf{U}^{n+k})}. \tag{5.3}$$

This scheme conserves the function H_d in the sense that

$$H_d[\mathbf{U}^{n+1}, \ldots, \mathbf{U}^{n+k}] = H_d[\mathbf{U}^0, \ldots, \mathbf{U}^{k-1}], \quad n \geq 0.$$

6. Examples. To illustrate the procedures for constructing conservative schemes presented in this paper, we consider as an example the generalized Korteweg–de Vries (gKdV) equation

$$u_t + u_{xxx} + (u^{p-1})_x = 0$$

for an integer $p \geq 3$; see, for example, [28]. The case $p = 3$ is the KdV equation (1.1), the case $p = 4$ is known as the modified KdV equation, and $p = 6$ is sometimes referred to as the mass critical gKdV equation. The gKdV can be written as (2.1) with

$$\mathcal{H}[u] = \int_\Omega \left(\frac{1}{2} u_x^2 - \frac{1}{p} u^p \right) \mathrm{d}x, \quad \mathcal{D} = \frac{\partial}{\partial x}.$$

The AVF DVD (3.6) gives rise to the fully implicit scheme (3.5),

$$\frac{U^{n+1} - U^n}{\Delta t} + \frac{U_{xxx}^{n+1} + U_{xxx}^n}{2} + \frac{1}{p} \left(\sum_{i=0}^{p-1} (U^{n+1})^{p-1-i} (U^n)^i \right)_x = 0. \tag{6.1}$$

After applying the polarizing procedure of section 4.1 to $\mathcal{H} = \int_\Omega \mathcal{G}\, \mathrm{d}x$, we get $H = \int_\Omega G\, \mathrm{d}x$, which depends on $k = \lceil p/2 \rceil$ arguments

$$G[w_1, \ldots, w_k] = \frac{1}{2k} \sum_{i=1}^k (w_i)_x^2 - \begin{cases} \frac{1}{pk} \left(\prod_{j=1}^k w_j^2 \right) \left(\sum_{i=1}^k \frac{1}{w_i} \right), & p \text{ odd}, \\ \frac{1}{p} \prod_{j=1}^k w_j^2, & p \text{ even}. \end{cases}$$

After finding the AVF DVD from (4.12), we get the linearly implicit PAVF scheme (4.13),

$$\begin{aligned} &\frac{U^{n+k} - U^n}{k\Delta t} + \frac{U_{xxx}^{n+k} + U_{xxx}^n}{2} \\ &\qquad + \begin{cases} \frac{1}{p} \left[\left(\prod_{j=1}^{k-1} (U^{n+j})^2 \right) \left(\sum_{i=1}^{k-1} \frac{U^{n+k} + U^n}{U^{n+i}} + 1 \right) \right]_x = 0, & p \text{ odd}, \\ \frac{1}{2} \left[\left(\prod_{j=1}^{k-1} (U^{n+j})^2 \right) \left(U^{n+k} + U^n \right) \right]_x = 0, & p \text{ even}. \end{cases} \end{aligned} \tag{6.2}$$

Notice that U^{n+k} are indeed appearing only as linear terms in this scheme. The schemes (1.2) and (1.3) are found by setting $p = 3$ ($k = 2$) in (6.1) and (6.2), respectively. Following the procedure of section 5, one can get a fully discretized scheme by replacing U by $\mathbf{U}$ and replacing the first and third derivative operators by $\delta^{\langle 1 \rangle}$ and $\delta^{\langle 3 \rangle}$, respectively.

In Figures 6.1 and 6.2 we compare the conservative methods (1.2) and (1.3) with the fully implicit midpoint method

$$\frac{U^{n+1} - U^n}{\Delta t} + \frac{U_{xxx}^{n+1} + U_{xxx}^n}{2} + \left(\left(\frac{U^{n+1} + U^n}{2} \right)^2 \right)_x = 0 \tag{6.3}$$

and a naive linearly implicit method

$$\frac{U^{n+1} - U^n}{\Delta t} + \frac{U_{xxx}^{n+1} + U_{xxx}^n}{2} + \left(U^n U^{n+1} \right)_x = 0. \tag{6.4}$$

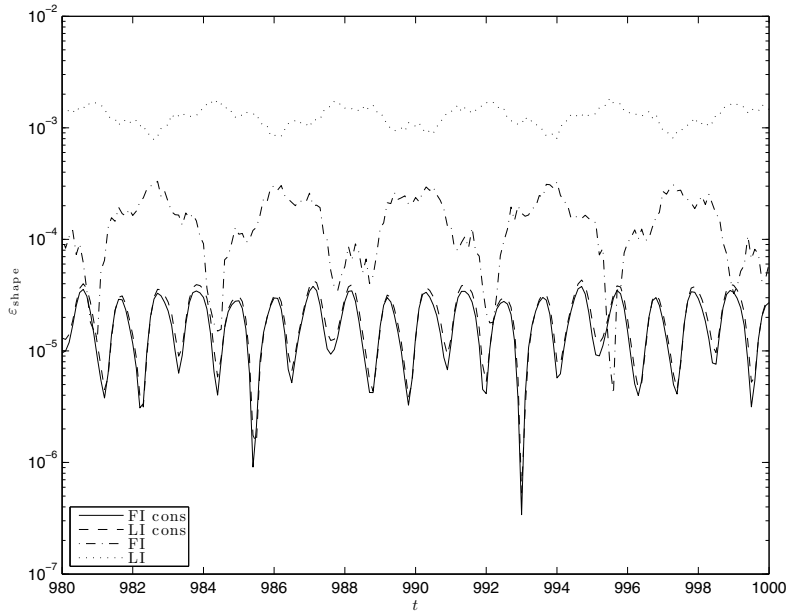

FIG. 6.1. *The shape error* $\varepsilon_{\text{shape}}$ (6.5) *for the schemes* (1.2) *(FI cons),* (1.3) *(LI cons),* (6.3) *(FI), and* (6.4) *(LI). Only the largest times are shown; the plot is similar for smaller* t.

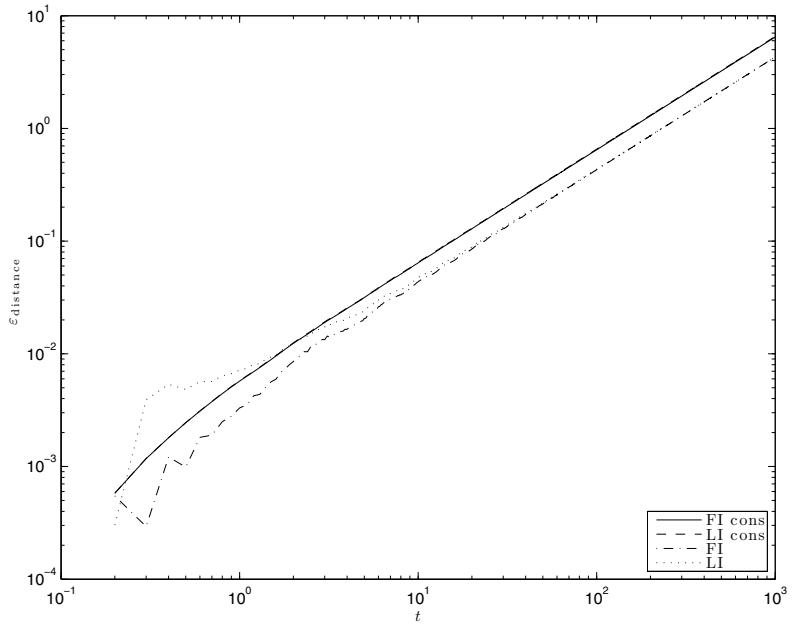

FIG. 6.2. *The distance error* $\varepsilon_{\text{distance}}$ (6.6) *for the schemes* (1.2) *(FI cons),* (1.3) *(LI cons),* (6.3) *(FI), and* (6.4) *(LI). FI cons and FI are almost indistinguishable in this plot.*

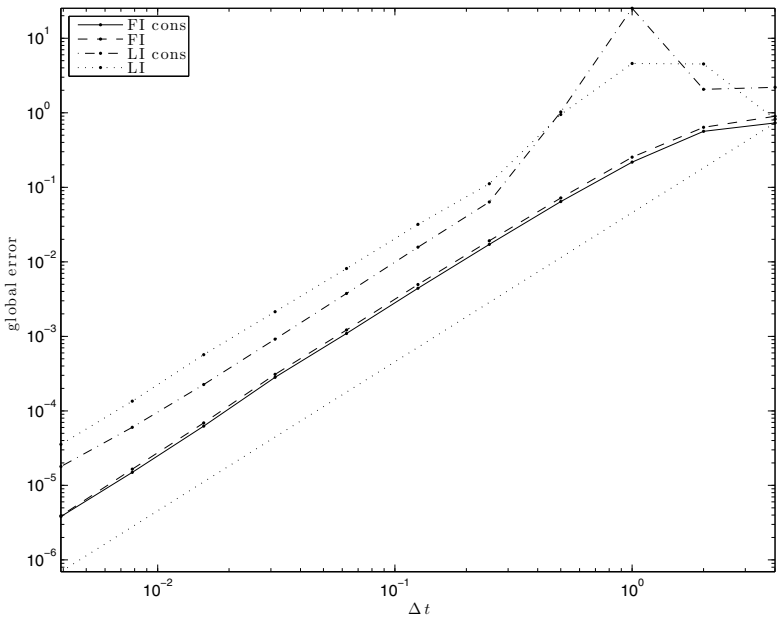

FIG. 6.3. *The global error at $t = 8$ for the schemes* (1.2) *(FI cons),* (1.3) *(LI cons),* (6.3) *(FI), and* (6.4) *(LI). The dotted line is a second order reference line.*

We test the four methods on a traveling wave solution

$$\Phi(x - ct) = \frac{3c}{2}\operatorname{sech}^2\left(\frac{3\sqrt{c}}{2}(x - ct)\right), \quad c > 0,$$

using the parameters $c = 1$, $x = (-5, 5)$, $\Delta x = \frac{10}{32}$, and $\Delta t = 0.1$. As an indication of the long time behavior of the presented schemes, we consider the extent to which the methods are able to preserve the shape and propagation speed of a traveling wave solution. We define the two quantities

$$\varepsilon_{\text{shape}} = \min_{\tau} \|U^n - \Phi(\cdot - \tau)\|_2^2 \tag{6.5}$$

and

$$\varepsilon_{\text{distance}} = |\operatorname{argmin}_{\tau} \|U^n - \Phi(\cdot - \tau)\|_2^2 - ct^n|. \tag{6.6}$$

Thus $\varepsilon_{\text{shape}}$ measures the shape error of the numerical solution, and $\varepsilon_{\text{distance}}$ measures the error in the travelled distance of the numerical solution.

We see in Figure 6.1 that the fully implicit schemes preserve the shape better than the linearly implicit ones, and that the conservative schemes perform better than the nonconservative ones. In Figure 6.2 we see that the linearly implicit schemes have a more accurate phase speed than the fully implicit ones. Figure 6.3 shows the global error as a function of the time step. As expected, the plot shows that the four methods are second order and that the linearly implicit schemes are inaccurate for large Δt. In conclusion we see that the linearly implicit conservative scheme (1.3) performs comparably to the fully implicit conservative scheme (1.2) (seen in Figures 6.1 and 6.2) while being more efficient (seen in Figure 1.1).

An interesting topic for future studies would be devising linearly implicit schemes for nonpolynomial systems.

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