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Here the operators S_m and S_n are used to write the concise expressions of the discrete counterparts of the total derivatives in x and t, namely, the forward difference operators

$$D_m^+ = \frac{S_m - I}{\Delta x}, \qquad D_n^+ = \frac{S_n - I}{\Delta t},$$

where I is the identity operator.

The approach we consider in this paper relies on the fact that conservation laws are in the kernel of the Euler operator. This provides a system of equations that must be satisfied by the components of a conservation law. We will solve such equations in order to get the searched methods.

We recall the main result for the continuous case below (see [13, 14, 15] for details and proofs). We begin by introducing the Euler operator.

Definition 1. *The Euler operator is the vector $\mathbf{E} = (E^1, \dots, E^N)$, whose components are the operators*

$$E^\alpha = \sum_{j} (-D)_J \frac{\partial}{\partial u_J^\alpha}, \qquad \alpha = 1, \dots, N.$$

The following theorem holds.

Theorem 1. *A function $f(x, [u])$ is a divergence, i.e., $f = \text{Div}\,\mathbf{F}$, if and only if $\mathbf{E}(f) = 0$.*

Analogous results hold in the discrete setting. We introduce the discrete Euler operator below.

Definition 2. *The discrete Euler operator is the vector $\mathbf{E} = (\mathsf{E}^1, \dots, \mathsf{E}^N)$, whose components are the operators*

$$\mathsf{E}^\alpha = \sum_{i,j} S_m^{-i} S_n^{-j} \frac{\partial}{\partial u_{i,j}^\alpha}, \qquad \alpha = 1, \dots, N.$$

The discrete version of Theorem 1 is the following.

Theorem 2. *A function $f(\mathbf{n}, [u])$ is a discrete divergence, i.e., $f = \text{Div}\,\mathbf{F}$, if and only if $\mathbf{E}(f) = 0$.*

In the following, we apply the described procedure to the mKdV equation.

THE MODIFIED KdV EQUATION

The mKdV equation
$$u_t + \alpha u^2 u_x + u_{xxx} = 0, \tag{3}$$
arises in several physical applications.

Denoting with I the identity operator, the forward difference, D_m, D_n, and the forward average, μ_m, μ_n, are defined by

$$D_m = \tfrac{1}{\Delta x}(S_m - I), \quad D_n = \tfrac{1}{\Delta t}(S_n - I), \quad \mu_m = \tfrac{1}{2}(S_m + I), \quad \mu_n = \tfrac{1}{2}(S_n + I).$$

Approximating the derivatives in (1) by means of suitable finite differences, yields a partial difference equation (PΔE),

$$\widetilde{\mathcal{A}}(x_i, t_j, u_{i,j}) = 0. \tag{3}$$

Here and henceforth, tildes represent discretizations of the corresponding continuous terms. We seek schemes having the following discrete analogue of each conservation law:

$$\mathrm{Div}\,\widetilde{\mathbf{F}} \equiv D_m\{\widetilde{F}(x_i, t_j, u_{i,j})\} + D_n\{\widetilde{G}(x_i, t_j, u_{i,j})\}, \tag{4}$$

which is zero on all solutions of (3). The functions $\widetilde{F}$ and $\widetilde{G}$ are respectively the flux and the density of the conservation law (4). A conservation law (4) is in characteristic form if

$$\mathrm{Div}\,\widetilde{\mathbf{F}} = \widetilde{\mathcal{Q}}\widetilde{\mathcal{A}},$$

where the multiplier function $\widetilde{\mathcal{Q}}(x_i, t_j, u_{i,j})$ is called the *characteristic* [13].

A crucial result for our purposes is due to Kuperschmidt [15] and states that the set of all discrete divergence expressions (4) is the kernel of the difference Euler operator,

$$\mathbf{E} = \sum_{i,j} S_m^{-i} S_n^{-j} \frac{\partial}{\partial u_{i,j}},$$

(see also [14] for the generalisation of this result). Consequently, if $\widetilde{\mathcal{Q}} \approx \mathcal{Q}$ is such that $\mathbf{E}(\widetilde{\mathcal{Q}}\widetilde{\mathcal{A}}) = 0$, there exists $\widetilde{\mathbf{F}} \approx \mathbf{F}$ such that $\widetilde{\mathcal{Q}}\widetilde{\mathcal{A}} = \mathrm{Div}\,\widetilde{\mathbf{F}}$, corresponding to a conservation law of which $\widetilde{\mathcal{Q}}$ is the characteristic.

The approach in [10, 11, 12] to find schemes that preserve conservation laws is straightforward. Choose a stencil of points and consider the most general discretizations $\widetilde{\mathcal{A}}$ of the PDE and $\widetilde{\mathcal{Q}}$ of the characteristic of the desired conservation law. These discretizations depend on a number of free parameters. In order to preserve the conservation law, set the parameters in such a way to satisfy the constraints given by the algebraic condition $\mathbf{E}(\widetilde{\mathcal{Q}}\widetilde{\mathcal{A}}) = 0$. If not all the free parameters have been set, this procedure can be iterated for multiple characteristic $\widetilde{\mathcal{Q}}_\ell$, to obtain the preservation of all the corresponding conservation laws, provided that the system of algebraic equations obtained can be solved. Finally, consistency conditions are applied to ensure that $\widetilde{\mathcal{A}}$ converges to $\mathcal{A}$ and each $\widetilde{\mathcal{Q}}_\ell$ converges to $\mathcal{Q}_\ell$ as the stepsizes tend to zero, giving further constraints on the free parameters.

A crucial step of this procedure is to solve, for each characteristic $\widetilde{\mathcal{Q}}_\ell$, the condition

$$\mathbf{E}(\widetilde{\mathcal{Q}}_\ell \widetilde{\mathcal{A}}) = 0. \tag{5}$$

This has to be done symbolically and it is not easy in general. In particular, if the non-linearity in $\mathcal{A}$ and $\mathcal{Q}_\ell$ is of polynomial type, (5) amounts to a large system of polynomial equations. This, in principle, can be solved by finding a Groebner basis, but the calculation may take a huge amount of memory and a very long computation time even when the nonlinearity is only quadratic and using a compact stencil.

Nevertheless, the complexity of the symbolic calculations may be reduced by restricting the dependence of few key quantities in $\widetilde{\mathcal{A}}$ and $\widetilde{\mathcal{Q}}_\ell$, on only points of the most compact sub-stencil that allows the desired order of accuracy. In particular, approximating nonlinear terms using as few points as possible, may be effective to the point of being able to solve (5) with a fast symbolic computation that does not need a Groebner basis (see [10]).

In the next section we use the procedure described above to find bespoke finite difference schemes preserving two conservation laws of a Hamiltonian PDE presenting a cubic nonlinearity.

MODIFIED KDV EQUATION

In this section we use the procedure described above to develop conservative finite difference schemes for the modified Korteweg-de Vries (mKdV) equation

$$\mathcal{A} \equiv u_t + u^2 u_x + u_{xxx} = 0, \quad (x,t) \in \Omega \equiv [a,b] \times [0,\infty). \tag{6}$$
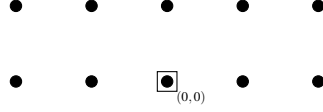
FIGURE 1. 10-point rectangular stencil.

Equation (6) has infinitely many conservation laws. The first three are

$$D_t(G_1) + D_x(F_1) \equiv D_t(u) + D_x\left(\tfrac{1}{3}u^3 + u_{xx}\right) = 0, \tag{7}$$

$$D_t(G_2) + D_x(F_2) \equiv D_t(\tfrac{1}{2}u^2) + D_x\left(\tfrac{1}{4}u^4 + uu_{xx} - \tfrac{1}{2}u_x^2\right) = 0, \tag{8}$$

$$D_t(G_3) + D_x(F_3) \equiv D_t(\tfrac{1}{12}u^4 + \tfrac{1}{2}uu_{xx}) + D_x\left(\tfrac{1}{2}\left(\tfrac{1}{3}u^3 + u_{xx}\right)^2 + u_x u_t - uu_{xt}\right) = 0. \tag{9}$$

These are known as the local conservation laws of mass, momentum and energy, respectively and, assuming conservative boundary conditions, integration in space yields the conservation of three global invariants. The conservation laws (7)–(9) can be written in characteristic form with characteristics, respectively,

$$\mathcal{Q}_1 = 1, \quad \mathcal{Q}_2 = u, \quad \mathcal{Q}_3 = \tfrac{1}{3}u^3 + u_{xx}.$$

Our purpose here is to find second-order accurate finite difference schemes defined on the 10-point stencil in Figure 1 that preserve both the conservation laws (7) and (9). Henceforth grid points are labelled with respect to the lattice point denoted with a square in Figure 1. Setting $\widetilde{\mathcal{Q}}_1 = 1$, the second-order approximations of the conservation laws (7) and (9) are taken to be of the form

$$\widetilde{\mathcal{A}} = D_m(\widetilde{F}_1) + D_n(\widetilde{G}_1) = 0, \qquad \widetilde{\mathcal{Q}}_3\widetilde{\mathcal{A}} = 0.$$

Since $\widetilde{\mathcal{A}}$ is defined to be a discrete conservation law, $\mathbf{E}(\widetilde{\mathcal{Q}}_1\widetilde{\mathcal{A}}) = \mathbf{E}(\widetilde{\mathcal{A}}) = 0$, for any discretizations $\widetilde{F}_1$ and $\widetilde{G}_1$. Nevertheless, as both $\widetilde{\mathcal{A}}$ and $\widetilde{\mathcal{Q}}_3$ include a cubic nonlinearity, the solution of $\mathbf{E}(\widetilde{\mathcal{Q}}_3\widetilde{\mathcal{A}}) = 0$ cannot be easily tackled without introducing some simplifying assumption on the approximations (see [10]). Approximating both G_1 and the cubic term in $\mathcal{Q}_3$ on compact sub-stencils makes the symbolic computations fast. Taking into account that the approximations have to be second-order, this implies that $\widetilde{G}_1$ depends only on the grid point $(0,0)$ and the approximation of the cubic term in $\mathcal{Q}_3$ depends only on the two lattice points $(0,0)$ and $(0,1)$. Hence we consider here discretizations of $\mathcal{Q}_3, G_1$ and F_1 of the form

$$\widetilde{\mathcal{Q}}_3 = \alpha_1 u_{0,0}^3 + \alpha_2 u_{0,1}u_{0,0}^2 + \alpha_3 u_{0,0}u_{0,1}^2 + \alpha_4 u_{0,1}^3 + \frac{1}{\Delta x^2}\sum_{i=-2}^{2}\sum_{j=0}^{1}\beta_{i,j}u_{i,j}, \qquad \widetilde{G}_1 = u_{0,0},$$

$$\widetilde{F}_1 = \sum_{i=-2}^{1}\left(\sum_{k=i}^{1}\sum_{r=k}^{1}\sum_{j=0}^{1}\gamma_{i,j,k,j,r,j}u_{i,j}u_{k,j}u_{r,j} + \sum_{k=-2}^{1}\sum_{r=k}^{1}\left(\gamma_{i,1,k,0,r,0}u_{i,1}u_{k,0}u_{r,0} + \gamma_{i,0,k,1,r,1}u_{i,0}u_{k,1}u_{r,1}\right) + \frac{1}{\Delta x^2}\sum_{j=0}^{1}\xi_{i,j}u_{i,j}\right).$$

We find the undetermined coefficients α, β, γ, and ξ by symbolically solving $\mathbf{E}(\widetilde{\mathcal{Q}}_3\widetilde{\mathcal{A}}) = 0$ and imposing the consistency conditions giving second-order accuracy. This yields a one-parameter family of second-order schemes,

$$\text{EC}(\lambda) \equiv D_m(\widetilde{F}_1) + D_n(\widetilde{G}_1) = 0, \qquad \widetilde{F}_1 = \mu_m\varphi_{-1,0}, \qquad \widetilde{G}_1 = u_{0,0},$$

$$\varphi_{-1,0} = \tfrac{1}{3}(\mu_n u_{-1,0}^2)(\mu_n u_{-1,0}) + \mu_n D_m^2 u_{-2,0} + \lambda\Delta x^2 D_m D_n \mu_m u_{-2,0}.$$

Clearly, each of these schemes preserves the local conservation law of the mass. The numerical solution also satisfies the following discrete energy conservation law

$$\widetilde{\mathcal{Q}}_3\widetilde{\mathcal{A}} = D_m(\widetilde{F}_3) + D_n(\widetilde{G}_3) = 0, \qquad \widetilde{\mathcal{Q}}_3 = \varphi_{0,0}, \qquad \widetilde{G}_3 = \tfrac{1}{12}u_{0,0}^4 + \tfrac{1}{2}u_{0,0}(D_m^2 u_{-1,0})$$

$$\widetilde{F}_3 = \tfrac{1}{2}\left(\varphi_{-1,0}\varphi_{0,0} + (D_m\mu_n u_{-1,0})(D_n\mu_m u_{-1,0}) - (\mu_m\mu_n u_{-1,0})(D_m D_n u_{-1,0}) + \lambda\Delta x^2(D_n u_{0,0})(D_n u_{-1,0})\right),$$

where $\widetilde{F}_3$ and $\widetilde{G}_3$ have been reconstructed from the characteristic (see [13]). As the free parameter λ appears as a factor of a second order perturbation in each scheme, one may be able to find an optimal value that reduces the local truncation error. However, this depends on the particular problem and no choice of λ gives a higher order method.

TABLE 1. Maximum value of the absolute error in global invariants at every step and relative error in the solution at the final time.

Method	Err_1	Err_2	Err_3	Error in solution
EC(0.023)	1.69e-14	1.41e-04	1.24e-13	0.0036
EC(-0.07)	1.78e-14	9.50e-05	1.88e-13	0.0587
Multisymplectic	3.73e-14	6.56e-04	0.7423	0.3225
Narrow box	2.22e-14	0.0013	0.7836	0.1443

NUMERICAL TEST

In this section we present a numerical test that shows the effectiveness of the schemes developed in the previous section compared with two well-known methods both satisfying only a discrete local conservation law of the mass. These are the multisymplectic and the narrow box schemes proposed in [3] and inspired to the analogous methods developed by Ascher and McLachlan in [1, 2] for the KdV equation. These schemes are both implicit and defined on an 8-point stencil, which is the most compact for discretizing the mKdV equation. We consider equation (6) setting periodic boundary conditions over $[-20,20]$ for $t \in [0,2]$ and initial condition given by the single-soliton solution on $\mathbb{R}$,

$$u(x,t) = \sqrt{30}\,\mathrm{sech}\left(\sqrt{5}x - 5\sqrt{5}(t-1)\right).$$

Each scheme is solved with stepsizes $\Delta x = 0.1$ and $\Delta t = 0.01$. In Table 1, we compare the relative error in the solution at the final time, and the error in the conservation laws (7)-(9) measured by the maximum value of the absolute error in the global invariants at every iteration step. These are denoted by Err_1, Err_2 and Err_3, respectively. We show the results for two particular EC(λ) schemes corresponding to the values of the parameter $\lambda = 0.023$ and $\lambda = -0.07$ minimizing the error in the solution and in the global momentum, respectively. EC(0.023) is by far the most accurate scheme. Nevertheless, choosing the free parameter to minimize the non-preserved conservation law, yields a solution error about 2.5 and 5.5 times smaller than the narrow box and the multisymplectic scheme, respectively.

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