

A conservative compact finite difference scheme for the KdV equation

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Received October 3, 2011, Accepted January 10, 2012

Abstract

We propose a new structure-preserving integrator for the Korteweg-de Vries (KdV) equation. In this integrator, two independent structure-preserving techniques are newly combined; the “discrete variational derivative method” for constructing invariants-preserving integrator, and the “compact finite difference method” which is widely used in the area of numerical fluid dynamics for resolving wave propagation phenomena. Numerical experiments show that the new integrator is in fact advantageous than the existing integrators.

Keywords discrete variational derivative method, compact finite difference method, conservative scheme

Research Activity Group Scientific Computation and Numerical Analysis

1. Introduction

In this report, we consider the numerical integration of the Korteweg-de Vries (KdV) equation

$$\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} + \frac{\partial^3 u}{\partial x^3} = 0 \quad (1)$$

on the torus of length L (i.e. we assume the periodic boundary condition). It is an integrable soliton equation describing shallow water waves.

For such an integrable equation, certain structure-preserving numerical methods, for example the “discrete variational derivative method” (DVDM) [1], are generally advantageous. In fact, Furihata [2] constructed a conservative scheme for KdV using DVDM, and confirmed that it gave stable and qualitatively better numerical solutions.

On the other hand, in the field of numerical fluid dynamics, it is a common practice to use the so-called “compact finite difference method” for wave equations, when correct wave behaviors are of importance; in the method, a numerical scheme is constructed so that it retains as correct dispersion relation as possible while the “stencil” (width of a difference operator) is kept “compact” (i.e. narrow). For KdV, a compact finite difference scheme was tested in [3] to prove that it was actually suitable for the equation.

Although the above two methodologies share the same target (wave equations) and goal (better qualitative behaviors), it seems that the challenges to combine them have not been done actively so far, except for the simple cases where only linear or quadratic invariants are of interest and thus conservation can be relatively easily accomplished without utilizing any structure-preserving methods such as DVDM: we can find a number of “conservative” compact finite difference schemes for the so-called “conservation laws” of the form $u_t + (f(u))_x = 0$

(which trivially preserve $\int u dx$); as an example of the quadratic cases, we refer to [4], where a Strang splitting compact finite difference scheme for the nonlinear Schrödinger equation preserving $\int |u|^2 dx$ was proposed. In more general cases, however, the help of the structure-preserving methods is indispensable. In this report, we show taking the KdV as our example that the above mentioned two methodologies can be in fact combined.

2. Compact finite difference operators

Below the idea of compact finite difference operator is summarized based on Lele [5]. Given a smooth function $f(x)$, we approximate it by f_i ($i = 0, \dots, N-1$) on the equispaced mesh with the mesh size $\Delta x = L/N$. Hereafter we always assume the discrete periodic boundary condition $f_{i \pm N} = f_i$, and also that the values outside $i = 0, \dots, N-1$ are periodically defined.

Typical compact finite difference operators for $\partial/\partial x$ are defined in the following form:

$$\begin{aligned} & \delta_c^{(1)} f_i + \alpha(\delta_c^{(1)} f_{i+1} + \delta_c^{(1)} f_{i-1}) + \beta(\delta_c^{(1)} f_{i+2} + \delta_c^{(1)} f_{i-2}) \\ &= a \frac{f_{i+1} - f_{i-1}}{2\Delta x} + b \frac{f_{i+2} - f_{i-2}}{4\Delta x} + c \frac{f_{i+3} - f_{i-3}}{6\Delta x}, \quad (2) \end{aligned}$$

where α, β, a, b , and c are real constants that characterize the compact finite difference operator. Note that, when $\alpha = \beta = 0$, the definition (2) simply means the standard central difference operators; for example, when

$$\alpha = \beta = 0, \quad a = \frac{3}{2}, \quad b = -\frac{3}{5}, \quad c = \frac{1}{10}, \quad (C6)$$

the sixth order (i.e. $O(\Delta x^6)$) standard central finite difference operator is recovered. Otherwise, the values of the compact-differences $\delta_c^{(1)} f_i$ are determined only implicitly; a tri- (when $\beta = 0$) or penta-diagonal (otherwise) linear system should be solved to obtain the val-

ues of $\delta_c^{(1)} f_i$ (in this sense, the operator is *global*). An example of the compact finite difference operator is

$$\alpha = \frac{1}{6}, \quad \beta = 0, \quad a = \frac{14}{9}, \quad b = \frac{1}{9}, \quad c = 0, \quad (\text{T6})$$

which attains the same order of accuracy as (C6) (i.e. $O(\Delta x^6)$), while referring to only three grid points ($i, i \pm 1$). This is contrastive to (C6) which requires five points for the accuracy. The name “compact” finite difference comes from this property. Another interesting choice of the parameters is (in double precision)

$$\begin{aligned} \alpha &= 0.5381301488732363, & \beta &= 0.066633190123881123, \\ a &= 1.367577724399269, & b &= 0.8234281701082790, \\ c &= 0.018520783486686603, \end{aligned} \quad (\text{S6})$$

which also attains $O(\Delta x^6)$. Since (S6) refers to five points, it apparently does not seem “compact” in the present context. Still it is called so, due to the following reason. (S6) refers to five grid points, both in the left and right hand side of (2). In this setting, the best attainable order of accuracy is $O(\Delta x^{10})$. The choice (S6), however, stays only at $O(\Delta x^6)$, and instead uses the remaining degrees of freedom of the coefficients in order to replicate the dispersion relation of waves as good as possible, practically at quite close level to the so-called spectral difference operator, which is purely a global operator involving FFT (recall that (S6) only involves penta-diagonal linear system). Due to this, (S6) is called “spectral-like” (sixth order) compact finite difference operator (see [6, 7] for the detail).

Next, let us consider the skew-symmetry of the difference operators, which plays a crucial role in the subsequent section. As is well-known, the standard central difference operator (C6) is skew symmetric: for any N -periodic sequences $\{f_i\}, \{g_i\}$,

$$\sum_{i=0}^{N-1} f_i \delta_c^{(1)} g_i \Delta x = - \sum_{i=0}^{N-1} (\delta_c^{(1)} f_i) g_i \Delta x \quad (3)$$

(see [8] for a proof). (T6) and (S6) also enjoy this property.

Lemma 1 *The compact finite difference operators characterized by (T6) and (S6) are also skew symmetric.*

Proof Let us write $\mathbf{f} = (f_0, \dots, f_{N-1})^\top$ and $\delta_c^{(1)} \mathbf{f} = (\delta_c^{(1)} f_0, \dots, \delta_c^{(1)} f_{N-1})^\top$, and rewrite (2) in matrix-vector form: $T \delta_c^{(1)} \mathbf{f} = S \mathbf{f} / \Delta x$, where T and S are the coefficient matrices determined by (2). The matrix T is invertible in (T6) and (S6). T and S are circulant matrices which means they are commutative. Furthermore, T is obviously symmetric ($T^\top = T$), and S skew symmetric ($S^\top = -S$). Gathering these facts, we conclude $(T^{-1} S)^\top = S^\top T^{-\top} = T^{-\top} S^\top = -T^{-1} S$, which is the desired skew symmetry.

(QED)

3. A conservative compact finite difference scheme for the KdV equation

Now we are in a position to demonstrate how we can construct a conservative scheme using the compact finite difference operators. Let us consider KdV (1) as

our example. In what follows, we basically follow the procedure of the discrete variational derivative method (DVDM) [1]. In this case, KdV (1) should be first rewritten into the variational form

$$\frac{\partial u}{\partial t} = \frac{\partial}{\partial x} \left(-\frac{u^2}{2} - \frac{\partial^2 u}{\partial x^2} \right) = \frac{\partial}{\partial x} \frac{\delta G}{\delta u}, \quad G = -\frac{u^3}{6} + \frac{u_x^2}{2},$$

where G is the energy density function. Then it is straightforward to show that KdV is conservative in the following sense.

$$\frac{d}{dt} \int_0^L G dx = \int_0^L \frac{\delta G}{\delta u} u_t dx = \int_0^L \frac{\delta G}{\delta u} \left(\frac{\partial}{\partial x} \frac{\delta G}{\delta u} \right) dx = 0. \quad (4)$$

In the DVDM, we try to mimic the variational form in discrete setting. Let us denote the approximate solution by $U_i^m \simeq u(i\Delta x, m\Delta t)$ (Δt is the size of the time mesh). We also write $\mathbf{U}^m = (U_0^m, \dots, U_{N-1}^m)^\top$ to save space. We then commence by defining a discrete energy function with $\delta_c^{(1)}$:

$$(G_d(\mathbf{U}^m))_i = -\frac{1}{6}(U_i^m)^3 + \frac{1}{2}(\delta_c^{(1)} U_i^m)^2.$$

There is a degree of freedom in this definition, but in this short report, we only consider this simplest case (see also the concluding remark below). Next, we define a discrete version of the variational derivative by

$$\begin{aligned} \frac{\delta G_d}{\delta(\mathbf{U}^{m+1}, \mathbf{U}^m)_i} &= -\frac{(U_i^{m+1})^2 + U_i^{m+1} U_i^m + (U_i^m)^2}{6} \\ &\quad - (\delta_c^{(1)})^2 \left(\frac{U_i^{m+1} + U_i^m}{2} \right), \end{aligned} \quad (5)$$

which is obviously an approximation to the true variational derivative. It is an easy exercise to show the discrete derivative (5) satisfies

$$\begin{aligned} \sum_{i=0}^{N-1} (G_d(\mathbf{U}^{m+1})_i - G_d(\mathbf{U}^m)_i) \Delta x \\ = \sum_{i=0}^{N-1} \frac{\delta G_d}{\delta(\mathbf{U}^{m+1}, \mathbf{U}^m)_i} (U_i^{m+1} - U_i^m) \Delta x. \end{aligned} \quad (6)$$

Finally, we define a scheme as follows: for $m = 0, 1, 2, \dots$,

$$\frac{U_i^{m+1} - U_i^m}{\Delta t} = \delta_c^{(1)} \frac{\delta G_d}{\delta(\mathbf{U}^{m+1}, \mathbf{U}^m)_i} \quad (i = 0, \dots, N-1). \quad (7)$$

The scheme is conservative in the following sense, which corresponds to (4).

Theorem 1 *The solutions of the scheme (7) enjoy*

$$\begin{aligned} \sum_{i=0}^{N-1} G_d(\mathbf{U}^{m+1})_i \Delta x &= \sum_{i=0}^{N-1} G_d(\mathbf{U}^m)_i \Delta x \\ (m &= 0, 1, 2, \dots). \end{aligned}$$

Proof From (6) and (7), we see

$$\frac{1}{\Delta t} \sum_{i=0}^{N-1} (G_d(\mathbf{U}^{m+1})_i - G_d(\mathbf{U}^m)_i) \Delta x$$

$$\begin{aligned}
&= \sum_{i=0}^{N-1} \frac{\delta G_d}{\delta(\mathbf{U}^{m+1}, \mathbf{U}^m)_i} \left(\frac{U_i^{m+1} - U_i^m}{\Delta t} \right) \Delta x \\
&= \sum_{i=0}^{N-1} \frac{\delta G_d}{\delta(\mathbf{U}^{m+1}, \mathbf{U}^m)_i} \delta_c^{(1)} \frac{\delta G_d}{\delta(\mathbf{U}^{m+1}, \mathbf{U}^m)_i} \Delta x \\
&= 0.
\end{aligned} \tag{8}$$

The last equality follows from the skew symmetry of $\delta_c^{(1)}$ (Lemma 1). (QED)

We show a numerical example. We take $L = 50$, and employ the initial condition $u(x, 0) = 3 \operatorname{sech}^2(0.5x)$ (strictly speaking, we truncate and place it on the torus at $x = 0$). Other parameters are set to $\Delta x = 0.5$ (i.e. $N = 100$), $\Delta t = 1/50$. Then scheme (7) is tested with (C6) and (S6) as $\delta_c^{(1)}$. Note that, as mentioned above, (C6) is just a standard central difference operator, and in this case the conservation has been already proved in [8]. Since the scheme (7) is $O(\Delta t^2)$, we also try the Heun method as the time stepping applied to an ordinary differential equation

$$\frac{d\mathbf{U}}{dt} = -\mathbf{U} * \delta_c^{(1)} \mathbf{U} - \delta_c^{(1)} \delta_c^{(2)} \mathbf{U}, \tag{9}$$

where $\mathbf{U}(t) = (u_0(t), \dots, u_{N-1}(t))^T$ is the semi-discretization of $u(x, t)$, and the symbol $*$ represents the Hadamard product (the elementwise product). $\delta_c^{(2)}$ is the difference operator for $\partial^2/\partial x^2$, which is chosen to the standard sixth order central difference operator when $\delta_c^{(1)}$ is approximated by (C6), and to the sixth order spectral-like compact finite difference operator when $\delta_c^{(1)}$ is taken to (S6) (see [7] for the definition; we omit its description here due to the restriction of space. See also the concluding remark below). In summary, we test the following four schemes:

- Heun method applied to (9) with (C6) as $\delta_c^{(1)}$,
- Heun method applied to (9) with (S6),
- Scheme (7) with (C6),
- Scheme (7) with (S6).

Only the last two are conservative.

Fig. 1 shows the evolution of numerical solutions. The results by the Heun method (the top two graphs) are catastrophic. They obviously need much finer time mesh for stable computation. This instability can be also understood from Fig. 2, which shows the energy evolutions; in the Heun schemes, the energies rapidly diverge, which agrees with the severe instability. On the other hand, the results by the scheme (7) successfully preserve the energy as planned (Fig. 2), and capture the soliton propagation at satisfactory level in both cases of $\delta_c^{(1)}$ ((C6) and (S6), the bottom two graphs in Fig. 1). This means that the special structure-preserving time stepping of scheme (7) is in fact advantageous than the generic Heun method.

Next, let us have a closer look at the difference between (C6) and (S6) to see if the compact finite difference operator (S6) is in fact advantageous than (C6). In order to see this, we try a coarser space mesh: the parameters are set to $L = 90$, $\Delta x = 0.9$ (i.e. $N = 100$),

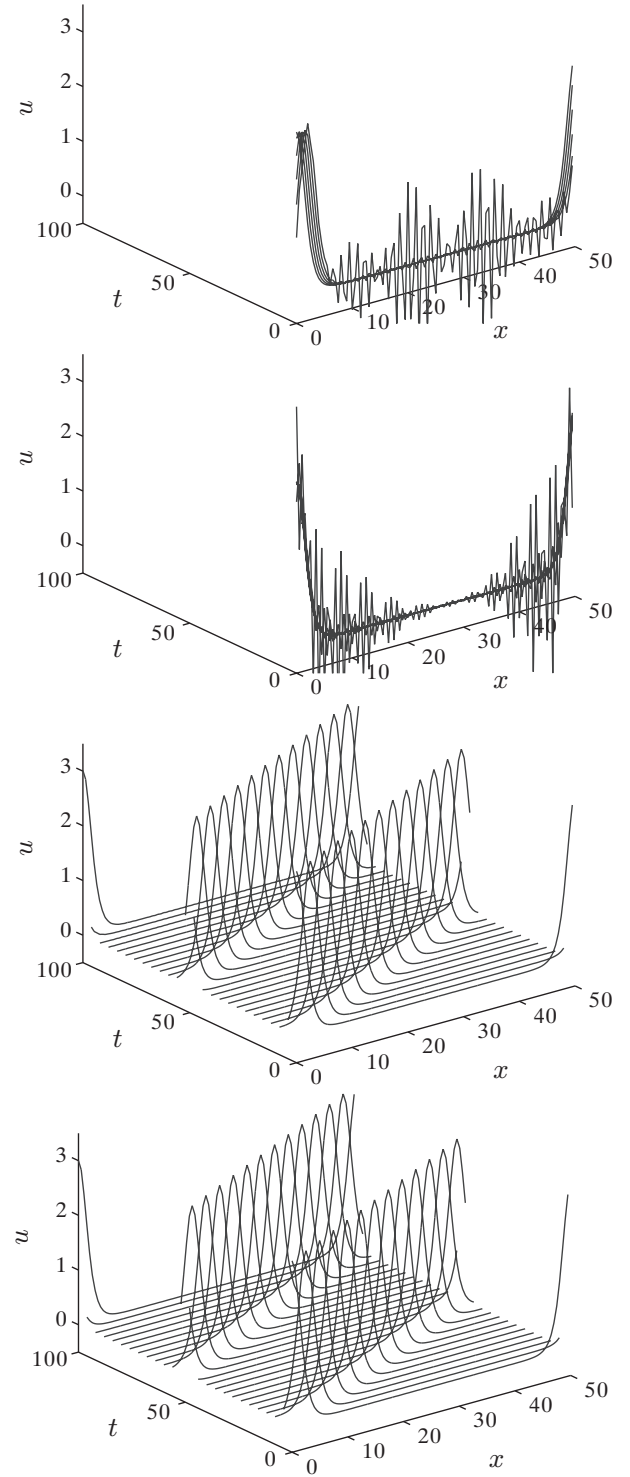


Fig. 1. Evolution of the soliton solution: (top) Heun+(9)+(C6), (2nd) Heun+(9)+(S6), (3rd) scheme (7)+(C6), (bottom) scheme (7)+(S6).

$\Delta t = 1/40$. The initial data is chosen to the same one as before. Fig. 3 is the magnified detail of the soliton profiles by scheme (7) with (C6) (shown in red) and (S6) (in blue), around $u = 0$ at $t = 10$. In the figure, it can be clearly observed that the result by (C6) exhibits undesirable small oscillations in the right half of the space interval, i.e., at the tail of the moving soliton. It should be attributed to the fact that the standard central finite difference operator (C6) does not preserve correct

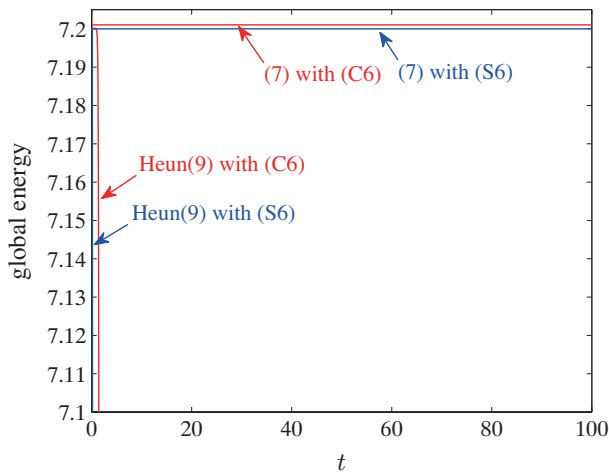
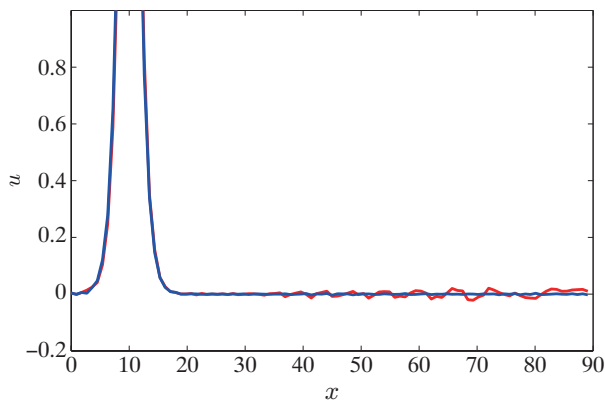


Fig. 2. Evolution of the discrete energies.

Fig. 3. Soliton profile detail around $u = 0$ at $t = 10$; (red) detail by (C6), (blue) by (S6).

dispersion relation. The result by (S6) gives a far better result, from which we conclude that the compact finite difference method is really suitable for wave propagation phenomena.

Wrapping up the above observations, we conclude that the combination of the structure-preserving method (DVDM) and the compact finite difference method is a strong new integrator for KdV. It is expected that the combination is also useful for other wave equations.

4. Further discussions

In this report, we showed that the so-called compact finite difference method can be incorporated into the discrete variational derivative method (DVDM) to construct conservative numerical scheme which well replicates the wave behaviors. The key was the skew symmetry of the compact finite difference operators. Although this can be easily understood, as was shown in Lemma 1, the authors do not know any reference in which this fact was explicitly written. We also showed several numerical examples, which confirmed the effectiveness of the conservative compact finite difference scheme for KdV.

We would like to make several remarks on this work. Firstly, although in this report we concentrated mainly on the compact finite difference operator (S6), the story can be easily extended to other compact finite difference operators of the form (2) (and further general forms with

wider stencils).

Secondly, notice that in the scheme (7) (with the discrete variational derivative (5)), $\partial^3/\partial x^3$ in KdV was approximated by $(\delta_c^{(1)})^3$. This is, however, obviously not optimal. To understand this, let us first consider the operator $\partial^2/\partial x^2$. Usually, when the approximation is done by the standard finite differences (i.e. not by the compact finite differences), the operator is approximated by $\delta^{(2)}f_i = (f_{i+1} - 2f_i + f_{i-1})/\Delta x^2$, instead of using the product of the first order difference operator $\delta^{(1)}f_i = (f_{i+1} - f_{i-1})/(2\Delta x)$. This is absolutely the preferable choice, because the first one has narrower and thus better stencil than the latter. Similarly, the operator $\partial^3/\partial x^3$ is usually approximated by $\delta^{(3)} = \delta^{(1)}\delta^{(2)}$, instead of $(\delta^{(1)})^3$. In fact, in Furihata [2], $\delta^{(1)}\delta^{(2)}$ was employed in the conservative scheme for KdV. Getting back to the compact finite difference case, we know there are also compact finite difference operators for $\partial^2/\partial x^2$, noted by $\delta_c^{(2)}$ here, which are generally preferable than $(\delta_c^{(1)})^2$. Accordingly, $\partial^3/\partial x^3$ in KdV should be $\delta_c^{(1)}\delta_c^{(2)}$, instead of $(\delta_c^{(1)})^3$ in the scheme (7). This, however, seriously complicates the situation, where we would need to reconstruct the system of the compact finite difference operators so that it fits more to DVDM.

The above points will be discussed in detail in our forthcoming paper [9] (see also [10]).

Acknowledgments

This work was partly supported by Grant-in-Aid for Scientific Research (C) and for Young Scientists (B).

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