On Numerical Methods for the KdV Equation and Soliton Dynamics

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***Abstract*—We investigate explicit finite difference schemes and pseudospectral methods to numerically solve the Korteweg-de Vries (KdV) equation, as well as generalise a finite difference scheme based on the Hamiltonian formalism to higher orders which we show to be superior to a straightforward discretisation. In addition, we explore the dynamics of the soliton solutions including collisions, wave decomposition and shock waves. We manage to validate many previously found results.**

I. Introduction

Solitons have a rather peculiar origin story. In 1834, John Scott Russell was observing a wave travelling down Edinburgh's Union canal, and he was so impressed by the wave's shape preserving properties that he followed it for many miles (Its solitary shape and particle-like behaviour are the reason why we now usually refer to it as a soliton). He later would describe this day as the happiest of his life, and would conduct experiments trying to replicate the wave. He was able to empirically deduce important features of the wave, such as that the speed is correlated to the amplitude and that any initial profile will decompose into solitons [1]. Unfortunately, his enthusiasm was not shared by his contemporaries, with both Stokes and Airy doubting the existence of such as wave.

This might also be the reason why it took until 1877 for Boussinesq to discover an equation with soliton solutions [2]. The equation was later rediscovered by Korteweg and de Vries, who also found its simplest solution [3]. The form of the Korteweg-de Vries (KdV) equation that we will be interested in is

$$u_t + uu_x + u_{xxx} = 0\,, \tag{1}$$

and its solution is given by

$$u(x,t) = 12\alpha^2 \operatorname{sech}^2\left(\alpha(x - 4\alpha^2 t)\right)\,. \tag{2}$$

It was again not until some 70 years later that new progress was made. This time Zabusky and Kruskal were able to show that an initial cosine profile decomposes into solitons over time and that the KdV equation is the continuum limit of the Fermi-Pasta-Ulam-Tsingou problem (FPUT problem) [4]. The FPUT problem concerns periodic behaviours in complex systems, such as a discrete weakly-nonlinear string. More progress was made by Gardner, Greene, Kruskal and Miura who invented the method of inverse scattering transformations (IST) to solve the KdV equation analytically [5]. The IST method has since been applied to many other partial differential equations.

Nowadays, solitons and the KdV equation find application in many different fields, such as in fluid dynamics, plasmas, gauge theories and many more [6], [7].

This paper is structured as follows: Section II discusses some relevant properties of the KdV equation and its solutions. Section III gives an overview of the numerical methods used and compares them. Then, in Section IV we are investigating some dynamics of the solitons, including collisions, wave decomposition and shock waves. Finally, Section V concludes and summarises our findings.

II. Properties of the KdV Equation

Before looking at the KdV equation in more detail, it is instructive to to look at its components separately to better understand the behaviour of the whole system. We first consider equation (1) without dispersive terms,

$$u_t + uu_x = 0\,. \tag{3}$$

The resulting solution changes shape as the wave propagates and eventually becomes multi-valued. On the other hand, we can consider equation (1) without nonlinear terms,

$$u_t + u_{xxx} = 0\,. \tag{4}$$

Here the solution exhibits different phase speeds for different wave numbers, $v_p = \omega/k = 1 - k^2$, and so

disperses over time. Miraculously, combining both terms leads to their effects cancelling and results in a soliton solution which travels without disturbances to its shape. We will further investigate the effects that parts of the KdV equation have in Section IV, where we model variations to the KdV equation, such as a combination of nonlinear and dissipative terms (the Burgers' equation).

Another curious feature of the KdV equation is that it has infinitely many conservation laws. In general, one can write a conservation law as

$$\frac{\partial T}{\partial t} + \frac{\partial X}{\partial x} = 0\,, \tag{5}$$

where T and X can be functions of $x, t, u_x, u_{xx}, ...$ By integrating this with respect to x, we have

$$\frac{d}{dt}\int_{-\infty}^{\infty} T\,dx = -\left[X\right]_{-\infty}^{\infty} = 0\,, \tag{6}$$

where we have assumed that X approaches a constant value as $|x| \to \infty$. By rewriting the KdV equation in the form of equation (5), one can easily verify that we have the following conserved quantities:

$$I_1 = \int_{-\infty}^{\infty} u\,dx\,, \tag{7}$$

$$I_2 = \int_{-\infty}^{\infty} u^2\,dx\,, \tag{8}$$

$$I_3 = H = \int_{-\infty}^{\infty} \frac{1}{6}u^3 + \frac{1}{2}(u_x)^2\,dx\,. \tag{9}$$

These are called mass, momentum and energy, respectively. A more complete discussion of conservation laws can be found in [8]. Particular attention should be drawn to the energy, as it is a Hamiltonian of the KdV equation (hence the name energy). And we may write the KdV equation as

$$u_t = -\frac{\partial}{\partial x}\frac{\delta \mathcal{H}}{\delta u}\,, \tag{10}$$

where

$$\frac{\delta \mathcal{H}}{\delta u} = \frac{1}{2}u^2 + u_{xx} \tag{11}$$

is the variational derivative of the Hamiltonian density, $\mathcal{H}$, i.e. the integrand of equation (9).

We also note a few basic properties of the soliton solution that will become relevant in Section IV when we investigate the dynamics. We can read off the amplitude and the speed of the soliton form equation (2), they are given by $h = 12\alpha^2$ and $v = 4\alpha^2$, respectively. So combining them we get a relation between height and speed, $v = \frac{h}{3}$.

III. Numerical Methods

In this section, we will discuss two different types methods for numerically solving the KdV equation. In particular, an explicit finite difference scheme, using a straightforward discretisation and one based on the Hamiltonian formalism, as well as a pseudospectral method. We will compare their results to the exact solution as well as investigate how well they conserve the conservation laws in section II.

A. Explicit Finite Difference Schemes

The idea of finite difference schemes (FDS) is to approximate derivatives at some point, say x_i, by using other points surrounding it, such as $x_{i\pm1}$. We want to discretise a function $u(x,t)$ into an equispaced rectangular grid and introduce the following notation $u(x_i, t_n) = u_i^n$ where $x_i = i\Delta x$ and $t_n = n\Delta t$ with $i, n \in \mathbb{Z}$ and $\Delta x, \Delta t$ referring to the spatial and time separation between two points. For example, we can write the nearest-neighbours of u_i^n in space and time as $u_{i+1}^n, u_{i-1}^n, u_i^{n+1}$ and u_i^{n-1}. We also want to rewrite the KdV equation as

$$\frac{\partial u}{\partial t} = f(u, u_x, u_{xxx}) \equiv f\,, \tag{12}$$

where $f = -uu_x - u_{xxx}$.

Typically one may then apply the Euler method for the time step, i.e. the left-hand side of equation (12), but here this does not work since the amplification factor is $g = 1 - 2\alpha\tanh\left(\alpha(x - 4\alpha^2 t)\right)\Delta t$ which is not less or equal to 1 for relevant configurations of x, α and t. Instead we will use a Runge-Kutta method of 2nd-order (RK2) and of 4th-order (RK4), which are more stable and accurate. They approximate the next value in time by first estimating the slope of $u(x,t)$ a number of times inside the interval to the next value. The order of the method refers to the number of slope estimates per time step and it also gives the global error of the method. For example, RK4 is of order $\mathcal{O}\left((\Delta t)^4\right)$. It is hence clear that higher accuracy comes at the price of computation time. One can also make a couple basic experimental observations about Δx, Δt and α in regards to stability: The higher α is, the larger we can make Δt but the smaller Δx has to be, and vice versa. This indicates that Δt and Δx are inversely related. In practice, one usually determines an appropriate Δx such that a particular

TABLE I: Relevant weights for central difference schemes, where we have omitted a factor of $\frac{1}{\Delta x}$, $\frac{1}{(\Delta x)^2}$ and $\frac{1}{(\Delta x)^3}$ for the first, second and third order derivatives, respectively. An extended version can be found in [9].

Order of Derivative	Order of Accuracy	u_{i-4}	u_{i-3}	u_{i-2}	u_{i-1}	u_i	u_{i+1}	u_{i+2}	u_{i+3}	u_{i+4}
1	2				-1/2	0	1/2			
	4			1/12	-2/3	0	2/3	-1/12		
	6		-1/60	3/20	-3/4	0	3/4	-3/20	1/60	
2	2				1	-2	1			
	4			-1/12	4/3	-5/2	4/3	-1/12		
	6		1/90	-3/20	3/2	-49/18	3/2	-3/20	1/90	
3	2			-1/2	1	0	-1	1/2		
	4		1/8	-1	13/8	0	-13/8	1	-1/8	
	6	-7/240	3/10	-169/120	61/30	0	-61/30	169/120	-3/10	7/240

spatial resolution is achieved (this is often set by the problem at hand), and then tries to optimise the time step appropriately.

To discretise f we can consult [9] to find the relevant central difference schemes for u_x and u_{xxx}. Here we consider the schemes of orders $2, 4$ and 6, which we have summarised in table I. These can be combined appropriately to give discretisations of f. So, for example, the 2nd-order discretisation would be

$$f_i = -\frac{1}{2\Delta x} u_i \left(u_{i+1} - u_{i-1}\right) - \frac{1}{2(\Delta x)^3}\left(2u_{i-1} - 2u_{i+1} + u_{i+2} - u_{i-2}\right) . \quad (13)$$

As we will see later on, these methods already give very accurate results, yet they can be improved to not only be more accurate but also conserve the conservation laws better by using the Hamiltonian form of the KdV equation (10). We follow the principles in [10], and generalise the method to higher orders. To derive the Hamiltonian discretisation, we simply need to apply the relevant central difference scheme from the ones we have already met in table I to the operator $\frac{\partial}{\partial x}$ in equation (10) and u_{xx} in equation (11), and hence arrive at a new discretisation of f. Our 2nd-order discretisation in equation (13) now becomes

$$f_i = -\frac{1}{4\Delta x}(u_{i+1}^2 - u_{i-1}^2) - \frac{1}{2(\Delta x)^3}(u_{i+2} - 2u_{i+1} + 2u_{i-1} - u_{i-2}) . \quad (14)$$

At first sight this may appear counter-intuitive as we are loosing the benefit of knowing u_i and seemingly are just replacing it with an average over its neighbouring points. But, as it turns, out the Hamiltonian scheme is performing significantly better.

B. Pseudospectral Method

Fornberg and Whitham [11] suggested a method where $u(x,t)$ is transformed into Fourier-space via a discrete fast Fourier transform (DFFT) with respect to x. We define the transform and its inverse as

$$\mathcal{F}[u] = \hat{u} = \sum_{m=0}^{N-1} u(m\Delta y, t) e^{-2\pi i \frac{mn}{N}} , \quad (15)$$

$$\mathcal{F}^{-1}[\hat{u}] = \frac{1}{N}\sum_{n=0}^{N-1} \hat{u}(n\Delta k, t) e^{2\pi i \frac{mn}{N}} , \quad (16)$$

where N is the number of x points. We have also, for convenience, mapped our x domain to $y \in [0, 2\pi]$. Now we can write the spatial derivatives as

$$\frac{\partial^n}{\partial x^n} u = \mathcal{F}^{-1}\left[(2\pi i k)^n \mathcal{F}[u]\right] . \quad (17)$$

To improve the performance of the DFFT we may also choose the number of points, N, to be a power of two. We arrive at a final expression

$$f = -\frac{i\pi}{2}\mathcal{F}^{-1}[k\mathcal{F}[u^2]] + i\pi^3 \mathcal{F}^{-1}[k^3 \mathcal{F}[u]] . \quad (18)$$

Having discretised f we can again use RK2 or RK4 for the time step.

C. Comparison

To test how well different methods perform, we setup up an initial soliton wave with $\alpha = 4$ and $x_0 = 2$ and we want our methods to propagate the soliton to $x = 8$ with the lowest possible error and the least amount of steps i.e. in the shortest time. There are multiple things to consider when defining the error, we can on the one hand look at the absolute difference between the numerical solution and the exact solution from equation (2), or we can look at how well different quantities are

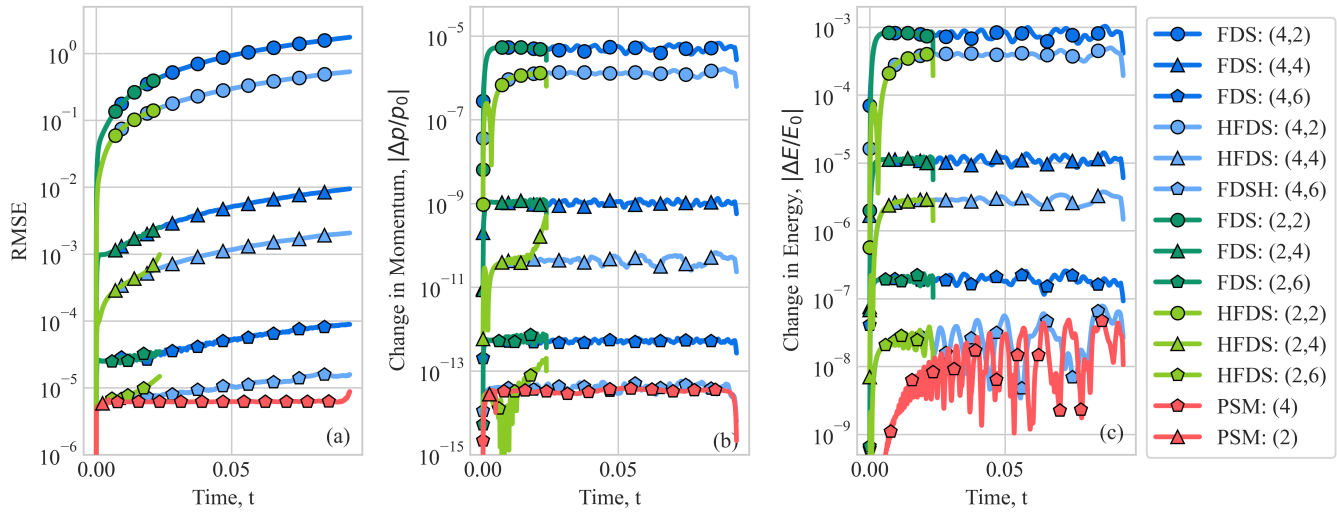

Fig. 1: Comparison of different methods, where we used the following shortcuts for different methods: 'FDS' - Finite Difference Scheme (dark blue - RK4, dark green - RK2), 'HFDS' - Hamiltonian Finite Difference Scheme (light blue - RK4, light green - RK2), 'PSM' - Pseudospectral Method (red). For FDS and HFDS, the bracket refers to the order of (Runge-Kutta, Discretisation). For PSM, it refers to the order of the Runge-Kutta method used only. (a) The root-mean-square error against time. The PSM (4) performs best, followed closely by HFDS (4,6). (b) Change in momentum, as fraction of initial momentum. Similar result to RMSE, but trends are flatter. (c) Change in energy, as a fraction of initial energy.

conserved. Here, we will be looking at the root-mean-square error to the exact solution and the change in momentum/energy as a fraction of the initial momentum/energy over time, see Fig. 1.

We find that the PSM-4 (Pseudospectral Method using RK4) performs best over all three categories, with the HFDS-46 (Hamiltonian Finite Difference Scheme using RK4 and a 6th order discretisation) nearly matching it. But the PSM-4 method used a step size about 3-4 times smaller due to stabiltiy reasons, which therefore naturally makes the error smaller.

In general, RK2 methods used 4-8 times smaller Δt steps and still became unstable sooner in time. But for the short times that they were stable, they managed to replicate the result of the corresponding RK4 method very well.

The Hamiltonian schemes consistently performed about 1 order of magnitude better than the non-Hamiltonian FDSs. Demonstrating the significant impact different discretisations can have.

Time-wise, the FDSs (RK4 only) were ahead. Due to being more stable, they managed a larger Δt and hence they only took between 5-10s to run, whereas the PSM-4 with step size 3-4 times smaller needed just over 40s.

Another interesting feature of the different methods (FDS and PSM) is the way the error develops. In Fig. 2, we can see that the FDS develops the largest deviations to the exact solution in regions where the soliton is, whereas the PSM seems to distribute the error throughout the domain. This is in agreement with what one might expect, as the FDS is approximating derivatives, it should be making more mistakes in areas where the derivatives change. The PSM, on the other hand, only introduces errors from transforming in and out of k-space, and hence develops the errors in the whole domain.

IV. Soliton Dynamics

As established in Section II, solitons of different heights have different speeds. So naturally one might be curious as to what happens when a faster soltion catches up to another and they collide. Since the KdV equaion is nonlinear, we can already rule out that the two solitons superpose. If we give our numerical methods an initial profile of two solitons with different α values and propagate them through time, we find the following: During the collision, the larger soliton's height decreases whereas the smaller soliton's height increases. This process continues until the smaller one grows to the size of the larger and the larger shrinks to the size of the smaller. The total effect being that the large soliton overtook the

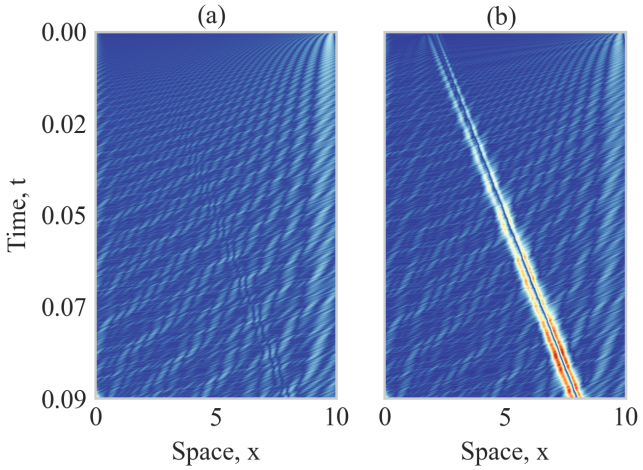

Fig. 2: Absolute difference between exact solution and numerical solution over space and time. (a) PSM-4: error is distributed throughout space. (b) FDS-46: error develops in region of soliton.

smaller one, with both solitons shifting a little bit in their x position, see Fig. 3. From an analytic solution for 2 solitons, one can derive the shifts to be

$$\Delta x_1 = \frac{1}{\alpha_1} \ln\left(\frac{\alpha_1 + \alpha_2}{\alpha_1 - \alpha_2}\right) > 0\,, \tag{19}$$

$$\Delta x_2 = \frac{1}{\alpha_2} \ln\left(\frac{\alpha_1 - \alpha_2}{\alpha_1 + \alpha_2}\right) < 0\,, \tag{20}$$

where $\alpha_1 > \alpha_2$. The analytical value for the shift agrees with the simulation.

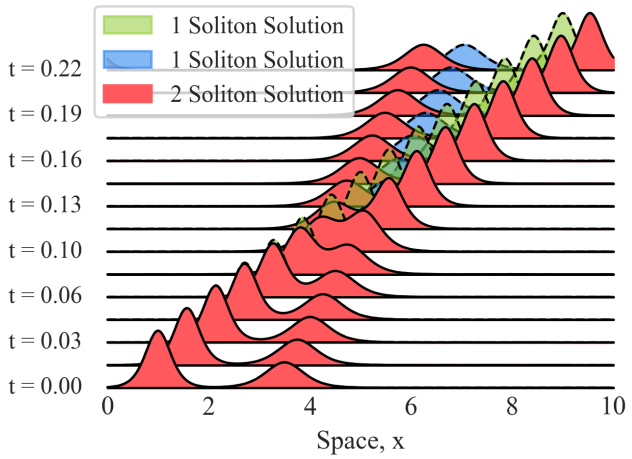

Fig. 3: Collision of two solitons. Blue and green profiles show how a single soliton would propagate, red shows how the combination of both propagates.

Initially observed by Zabusky and Kruskal [4], a sine wave shape will decompose into separate solitons at about the time that the nonlinear equation without the dispersion term (3) would "tumble over" and become multi-valued. They also showed that the heights of the train of solitons follows a linear relationship, we replicate this result in Fig. 4 for a sine wave shape, but also show that the same is true for other shapes, such as a triangular shape.

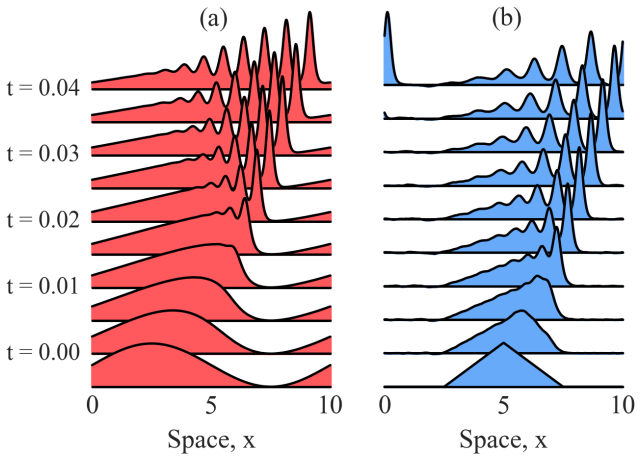

Fig. 4: Different initial wave forms decomposing into solitons. (a) Sine wave. (b) Triangular wave.

To investigate the effects that different parts of the KdV equations have, we will model

$$u_t + uu_x = \nu u_{xx}\,, \tag{21}$$

where ν is some parameter. Equation (21) is usually known as the viscous Burgers' equation, and if $\nu = 0$ it is called the inviscid Burgers' equation. They find application in fluid dynamics, nonlinear acoustics and traffic flow. We know from the discussion on the KdV equation in Section II that the inviscid equation will eventually become multi-valued since it is not linear. A possible way to circumvent this would be to introduce a discontinuity in such a way that it preserves the area. Strictly speaking, this shock wave is not a solution of the inviscid Burgers' equation, but it is an allowed solution of an integral conservation equation from which the inviscid Burgers' equation could have been derived from. In Fig. 5, we consider the inviscid equation up to the point where it breaks down. We also see that the viscous Burgers' equation escapes becoming multi-valued by diffusing away.

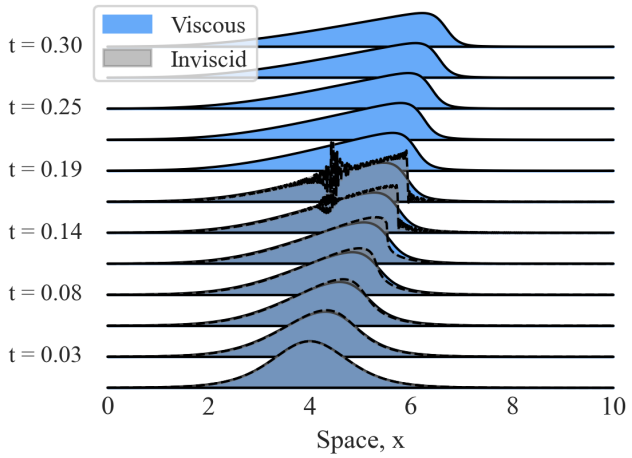

Fig. 5: Comparison between inviscid and viscous Burgers' equation. The inviscid equation becomes multivalued and unstable, whereas the viscous one diffuses and escapes any instabilities.

V. Conclusion

We studied explicit finite difference schemes of orders $\mathcal{O}((\Delta x)^2)$, $\mathcal{O}((\Delta x)^4)$ and $\mathcal{O}((\Delta x)^6)$ together with Runge-Kutta 2 and 4 methods, both using a straightforward discretisation as well as a discretisation based on the Hamiltonian formalism. We also investigated a pseudospectral method, again using Runge-Kutta 2 and 4. We conclude that the Hamiltonian scheme for the $\mathcal{O}((\Delta x)^6)$ discretisation is overall the best method, it approximately matches the performance of the pseudospectral method with RK4, but is more stable and quicker. In general, we found the Hamiltonian discretisations to be about one order of magnitude more accurate than its counterparts.

Additionally, we looked at various dynamical properties of solitons. We found that the shift in the x position of two solitons after a collision that can be derived analytically agrees with our simulations. We also replicated results from Zabusky and Kruskal [4] that showed that an intial sine wave profile will break up into a train of solitons, we additionally simulated this for a triangular profile. Finally, we looked at two variations of the KdV equation: without dispersion term and replacing the dispersion term with a diffusive term. These gave inside into how shock waves form and how diffusion stops the wave from becoming multi-valued.

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