A NOVEL NONLOCAL POTENTIAL SOLVER BASED ON NONUNIFORM FFT FOR EFFICIENT SIMULATION OF THE DAVEY−STEWARTSON EQUATIONS

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Abstract. We propose an efficient and accurate solver for the nonlocal potential in the Davey−Stewartson equations using nonuniform FFT (NUFFT). A discontinuity in the Fourier transform of the nonlocal potential causes "accuracy locking" if the potential is solved by standard FFT with periodic boundary conditions on a truncated domain. Using the fact that the discontinuity disappears in polar coordinates, we reformulate the potential integral and split it into high and low frequency parts. The high frequency part can be approximated by the standard FFT method, while the low frequency part is evaluated with a high order Gauss quadrature accelerated by nonuniform FFT. The NUFFT solver has $O(N \log N)$ complexity, where N is the total number of discretization points, and achieves higher accuracy than standard FFT solver, which makes its use in simulations very attractive. Extensive numerical results show the efficiency and accuracy of the proposed new method.

1. INTRODUCTION

The Davey−Stewartson (DS) equations arise as a model for free surface fluid waves subject to the effects of both gravity and capillarity [2,13]. A key feature of the DS equations is the nonlocal self-coupling potential term, which requires a suitable numerical effort. We propose in this paper a new numerical method for this nonlocal potential and show considerable improvement gained in accuracy and efficiency over standard approaches.

The DS equation reads, in dimensionless form, as follows:

$$i \, \partial_t u = -\partial_{xx} u + \alpha \, \partial_{yy} u - 2 \, \beta \, |u|^2 u - 4 \, \beta \, \Phi \, u, \quad t \geq 0, \tag{1.1}$$

$$-\Delta \Phi = \partial_{xx}(|u|^2), \quad t \geq 0, \tag{1.2}$$

$$u(x, y, t = 0) = u_0(x, y), \quad (x, y) \in \mathbb{R}^2, \tag{1.3}$$

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where α can take the values $\alpha = 1$ (Hyperbolic-Elliptic DS) or $\alpha = -1$ (Elliptic$-$Elliptic DS), and the constant β can be either positive, representing focusing interaction, or negative, for defocusing interaction. We restrict ourselves to the elliptic case of the potential coupling equation (1.2), and remark that in general, DS also allows for a hyperbolic coupling equation in place of (1.2), a case which we are not going to investigate. In the Hyperbolic-Elliptic case ($\alpha = 1$), the equation is completely integrable and called "DSII" in the literature [1]. This equation has recently been of interest in the modelling of rogue waves [20].

The nonlocal Poisson-type potential Φ in (1.2), generated by the density $\rho := |u|^2$, can be written equivalently by Fourier transform as

$$\Phi(\mathbf{x}, t) = \int_{\mathbb{R}^2} -\frac{k_x^2}{k_x^2 + k_y^2}\, \widehat{\rho}(\mathbf{k}, t)e^{2\pi i\, \mathbf{k}\cdot\mathbf{x}}d\mathbf{k}, \qquad \mathbf{x} = (x, y) \in \mathbb{R}^2, \tag{1.4}$$

where the Fourier transform is defined as follows

$$\widehat{\rho}(\mathbf{k}, t) = \int_{\mathbb{R}^2} \rho(\mathbf{x}, t)\, e^{-2\pi i\, \mathbf{k}\cdot\mathbf{x}}d\mathbf{x}, \quad \mathbf{k} \in \mathbb{R}^2. \tag{1.5}$$

In order to evaluate the nonlocal potential Φ, the usual approach is to truncate the whole space problem onto a bounded domain and to impose some appropriate boundary conditions. For example, the problem can be truncated on a rectangle with periodic boundary conditions, and then a standard Fast Fourier Transform (FFT) method can be applied in a straightforward way [12, 19]. For the simulation of the whole coupled system, also the "wave function" u, the other unknown of DS, has to be calculated on a bounded domain, and the standard method is also truncation. However, the domain of computation for the wave function is not necessarily the same as the one chosen for the computation of the nonlocal potential Φ. One might expect an accurate approximation for those Φ and u that decay sufficiently fast. However, the discontinuity of the Fourier multiplier in (1.4), *i.e.* $k_x^2/(k_x^2 + k_y^2)$, at $\mathbf{k} = \mathbf{0}$, is poorly resolved if the integral is discretized directly by trapezoidal quadrature no matter how small the spatial step is, and thus causes accuracy locking similar to the one found in [4, 24]. Since this discontinuity happens near low frequencies, a fast decay of the Fourier transform at far field is not necessarily leading to any smaller error.

The DS equations have been studied extensively and various aspects of numerical methods have been studied, for an incomplete list, we refer to [12, 15, 18, 19]. A systematic numerical study of the DS equations on a torus in the semi-classical regime was done in [19]. As pointed out above, the standard FFT applied on a bounded domain may suffer from the discontinuity and have accuracy loss in the term Φ. Starting from the Fourier definition (1.4), we will concentrate on accurate and efficient evaluation of the nonlocal potential in which the discontinuity can be resolved accurately.

We remark that also for the wave function u, the truncation to a bounded domain, together with periodic boundary conditions, may cause non negligible errors, for example, in the case where u does not decay fast enough. Removing or suppressing these errors is an interesting problem on its own. The most accurate method for this task is the Transparent Boundary Conditions (TBC). There are successful recent works using this method for Nonlinear Schrödinger equations [3, 5, 21], however the adaptation of these methods to cases with non-local interactions like Davey$-$Stewartson is essentially an open problem. Further work in this direction surely would be very important. We mention furthermore that one could also use more flexible, but less accurate methods for reducing domain truncation errors, like *e.g.* the Absorbing potential method [22].

By adopting polar coordinates in Fourier space, the discontinuity in (1.4) disappears automatically due to the Jacobian of the coordinate change, *i.e.* from Cartesian to polar coordinates, so the use of a simple high order quadrature will be possible. Here we aim to design an accurate and efficient numerical scheme which can bypass the discontinuity. Recently, Jiang *et al.* [7, 17] proposed an accurate algorithm to efficiently evaluate a series of nonlocal convolution-type potentials whose convolution kernels (and their Fourier transforms) have singularities both in physical and Fourier space, such as Coulomb and dipolar potential in 2D and 3D, with the help of nonuniform FFT (NUFFT). Fortunately, the nonlocal potential Φ, given by (1.4), can be approximated

in a similar way. In this paper, we adapt the nonuniform FFT (NUFFT) solver to (1.4) and combine our novel NUFFT solver with the widely used *time splitting method* to study the dynamics of DS.

The paper is organized as follows. In Section 2, we present a detailed discussion of the numerical algorithm together with a brief review of nonuniform FFT fast algorithms. In Section 3, extensive numerical examples and results are shown to confirm the accuracy and efficiency of our novel NUFFT solver. Concluding remarks are drawn in Section 4.

2. Resolving discontinuities in nonlocal potential by NUFFT algorithm

In this section, we discuss the reasons for a new solver for the nonlocal term (1.4), present the basic steps of the NUFFT solver, followed by a brief review of the NUFFT fast algorithm introduced in [14, 16] and give a brief introduction of time splitting method for simulating the dynamics.

2.1. Evaluation of the nonlocal potential with resolved discontinuity

As discussed above, the Fourier multiplier in the nonlocal coupling potential (1.4) has a discontinuity at $\mathbf{k} = \mathbf{0}$, thus resolution by a uniform quadrature does not achieve good accuracy. Moreover, the discontinuity of the Fourier multiplier causes discontinuity in $\widehat{\Phi}$. To be specific, from (1.4), we have

$$\widehat{\Phi}(k_x, k_y) = -\frac{k_x^2}{(k_x^2 + k_y^2)} \, \widehat{\rho}(k_x, k_y). \tag{2.6}$$

Then we have $\widehat{\Phi}(k_x, 0) = -\widehat{\rho}(k_x, 0)$ for $k_x \neq 0$, whereas $\widehat{\Phi}(0, k_y) = 0$ for $k_y \neq 0$. So we obtain, in the whole space case,

$$\lim_{k_x \to 0} \widehat{\Phi}(k_x, 0) = -\widehat{\rho}(\mathbf{0}) \quad \text{and} \quad \lim_{k_y \to 0} \widehat{\Phi}(0, k_y) = 0. \tag{2.7}$$

Noticing that $\widehat{\rho}(\mathbf{0}) = \int_{\mathbb{R}^2} \rho(\mathbf{x}) \mathrm{d}\mathbf{x} \neq 0$, the discontinuity in $\widehat{\Phi}$ at $\mathbf{k} = \mathbf{0}$ is clear. The common strategy of forcing $\widehat{\Phi}(\mathbf{0}) = 0$ in the standard FFT solver for the bounded domain problem results in a bad resolution of the discontinuity, thus an "accuracy locking" phenomenon is observed [4, 24].

Following a similar procedure introduced for the evaluation of nonlocal potentials in [7, 17], we first split (1.4) into two parts as follows:

$$\Phi(\mathbf{x}) = \int_{\mathbb{R}^2} -\frac{k_x^2}{k_x^2 + k_y^2} \widehat{\rho}(\mathbf{k}) \mathrm{e}^{2\pi i \, \mathbf{k} \cdot \mathbf{x}} \mathrm{d}\mathbf{k} \tag{2.8}$$

$$= \int_{\mathbb{R}^2} \frac{-k_x^2}{k_x^2 + k_y^2} \widehat{\rho}(\mathbf{k}) \, (1 - p(\mathbf{k})) \, \mathrm{e}^{2\pi i \, \mathbf{k} \cdot \mathbf{x}} \mathrm{d}\mathbf{k} \tag{2.9}$$

$$+ \int_{\mathbb{R}^2} \frac{-k_x^2}{k_x^2 + k_y^2} \widehat{\rho}(\mathbf{k}) \, p(\mathbf{k}) \, \mathrm{e}^{2\pi i \, \mathbf{k} \cdot \mathbf{x}} \mathrm{d}\mathbf{k} \tag{2.10}$$

$$:= I_1(\mathbf{x}) + I_2(\mathbf{x}),$$

where $p(\mathbf{k})$ is a partition function used to separate high and low frequency parts of the integrand. The function $p(\mathbf{k})$ is chosen such that it satisfies two properties. First, it has to be $C^\infty(\mathbb{R}^2)$ and to decay fast enough at far field. Second, $(1 - p(\mathbf{k}))/|\mathbf{k}|^2$ has to be continuous at $\mathbf{k} = \mathbf{0}$. The choice of $p(\mathbf{k})$ is of course not unique, for more details we refer to [17]. In this case, we choose $p(\mathbf{k}) = \mathrm{e}^{-|\mathbf{k}|^2/\sigma^2}$ where σ is a tunable positive number to be specified later. Taking this $p(\mathbf{k})$, the integrand of I_1 is continuous in Cartesian coordinates, and the integrand of I_2 is continuous in polar coordinates, therefore the discontinuity difficulty is resolved.

Since the integrand of I_1 is continuous and equals to zero at the origin, we can easily apply a standard FFT method. The commonly-used technique of setting $\widehat{\rho}(\mathbf{0}) = 0$ does not have any discontinuity difficulty in the

Fourier space. To approximate $I_1(\mathbf{x})$ within some prescribed accuracy ε, we can truncate the whole Fourier space into a square, *i.e.* $B_f := [-F, F]^2$ with $F = O(\varepsilon^{-1/(n-2)})$. As is known from standard Fourier analysis, $\widehat{\rho}(\mathbf{k}) = O(|\mathbf{k}|^{-n})$ as $|\mathbf{k}| \to \infty$ if $\rho \in C^n(\mathbb{R}^2)$ for positive integer n. In computation, the density is truncated on a bounded square, *i.e.* $B_p := [-P, P]^2$, and is discretized on a uniform mesh grid $\mathbf{x_n} = (x_{n_1}, y_{n_2})$ with $x_{n_1} = -P + n_1 h_x, n_1 = 0, \ldots, N_x, y_{n_2} = -P + n_2 h_y, n_2 = 0, \ldots, N_y$ and $h_x = \frac{2P}{N_x}, h_y = \frac{2P}{N_y}$. The Fourier transform $\widehat{\rho}(\mathbf{k})$ is also discretized on a uniform Fourier grid, *i.e.* $\mathbf{k_m} = (k_{m_1}, k_{m_2})$ with $k_{m_1} = \pi m_1/P, k_{m_2} = \pi m_2/P, m_1 = -N_x/2, \ldots, N_x/2+1, m_2 = -N_y/2, \ldots, N_y/2+1$. The Fourier transforms $\widehat{\rho}(\mathbf{k_m})$ are approximated by applying the trapezoidal rule to (1.5) on B_p, and the summation is accelerated by Fast Fourier transform (FFT) within $O(N \log N)$ arithmetic operations (where N is the total number of grid points). In implementation, we extend the density, which is originally given on B_p, to a larger square $B_{\widetilde{p}} = [-\widetilde{P}, \widetilde{P}]^2$ with $\widetilde{P} = \kappa P, \kappa \geq 2$ by zero-padding, so as to achieve better accuracy in I_1 by decreasing the frequency step, *i.e.* $|\Delta \mathbf{k}| = O(P^{-1})$.

For I_2, the discontinuity of the integrand is removed by the transformation to polar coordinates:

$$I_2(\mathbf{x_n}) = -\int_0^\infty k \, \mathrm{d}k \int_0^{2\pi} \cos^2(\theta) \widehat{\rho}(\mathbf{k}) \, p(\mathbf{k}) \, \mathrm{e}^{2\pi i \, \mathbf{k} \cdot \mathbf{x_n}} \, \mathrm{d}\theta, \quad \mathbf{x_n} \in B_p. \tag{2.11}$$

Similarly to the calculation of I_1, I_2 is approximated on the bounded disk $D_c = \{|\mathbf{k}| \leq c, c > 0\}$, where c is a multiple of the parameter σ in the auxiliary function $p(\mathbf{k})$. We apply a high order Gauss–Jacobi quadrature in the radial direction with nodes and weights $\{(r_{j_1}, \omega_{j_1}^r)\}_{j_1=1}^{N_r}$, and the trapezoidal rule in the azimuthal direction with nodes and weights $\{(\theta_{j_2}, \omega_{j_2}^\theta)\}_{j_2=1}^{N_\theta}$. Define $\mathbf{j} = (j_1, j_2)$, $\omega_\mathbf{j} = \omega_{j_1}^r \omega_{j_2}^\theta$ and $\mathbf{k_j} = r_{j_1}(\cos \theta_{j_2}, \sin \theta_{j_2})$, we have

$$I_2(\mathbf{x_n}) \approx -\sum_{j_1=1}^{N_r} \sum_{j_2=1}^{N_\theta} \omega_\mathbf{j} (\cos \theta_{j_2})^2 \, \widehat{\rho}(\mathbf{k_j}) \, p(\mathbf{k_j}) \mathrm{e}^{2\pi i \, \mathbf{k_j} \cdot \mathbf{x_n}}, \quad \mathbf{x_n} \in B_p. \tag{2.12}$$

Note that $\mathbf{k_j}$ are non-uniform grid points, therefore standard FFT can not be applied to accelerate either the computation of $\widehat{\rho}(\mathbf{k_j})$ or $I_2(\mathbf{x_n})$. Direct computation of $\widehat{\rho}(\mathbf{k_j})$ or (2.12) requires $O(NN_rN_\theta)$ operations, which is a much higher cost than a uniform FFT method requires. Fortunately, the nonuniform FFT "fast algorithm" [14, 16] reduces the computational cost to $O(N \log N)$, where N is the total number of grid points in both physical and Fourier space, within any prescribed approximation accuracy. The NUFFT algorithm has been developed a lot since Dutt and Rokhlin constructed the first NUFFT algorithm with full control of precision in [14]. Here we apply an optimized NUFFT proposed by Greengard and Lee in [16], which utilizes Gaussians as interpolation or 'gridding' schemes to accelerate the algorithm by a significant factor, particularly in 2D and 3D. We shall not elaborate on this topic in detail, instead we refer the readers to [16,17] for a detailed discussion. In the section below, we shall give a really brief review of NUFFT.

It still remains to decide how to choose the cutoff parameter σ for the separation of high and low frequency regime. On one hand, one would need fewer points in the irregular, low-frequency regime I_2 if σ is small, which helps reduce the computational cost of I_2. On the other hand, in this case the integrand of I_1 will be sharply peaked, so to achieve high accuracy a small grid step in the uniform grid in I_1 would be necessary, which would increase cost. Following a dimensional analysis argument, the parameter σ is chosen to optimize the total computation cost as follows:

$$\sigma = O(\min(\Delta k_x, \Delta k_y)) = O(P^{-1}).$$

Complete details of the optimal choice are discussed and presented in [17].

For the low-frequency part, we choose an irregular (polar) 60×60 grid in the Fourier domain, independently from the grid spacing in real space. This choice guarantees 12 digits of accuracy (by NUFFT) in the calculation I_2, a level of accuracy which is high enough (*i.e.* higher than error terms incurred from other parts of the algorithm) in the whole range of test cases which we will consider. The choice of the non-uniform grid step and the related accuracy were studied in [17], and our choice follows recommendations given there.

2.2. Brief introduction of NUFFT

As is well known, standard FFT accelerates the following summations

$$F(k) = \sum_{j=0}^{N-1} f(j) e^{-2\pi ikj/N}, \quad k = 0, \ldots, N-1, \tag{2.13}$$

$$f(j) = \frac{1}{N} \sum_{k=0}^{N-1} F(k) e^{2\pi ikj/N}, \; j = 0, \ldots, N-1, \tag{2.14}$$

down to $O(N \log N)$ operations on uniform mesh grids in both physical domain ($\mathbf{x}$) and frequency domain $\mathbf{k}$. For values defined on nonuniform mesh grids, either in physical or frequency or even in both domains, standard FFT can not be applied due to the loss of the algebraic structure in the discrete transform matrix. NUFFT is then proposed to remove this restriction, while maintaining a computational complexity of $O(N \log N)$, where N denotes the total number of points in both the physical and Fourier domains. There are three kinds of NUFFTs, namely, type 1 (from nonuniform grids to uniform grids in dual domain), type 2 (uniform to nonuniform) and type 3 (nonuniform to nonuniform).

To be more specific, the type 1 NUFFT evaluates sums of the form

$$f(\mathbf{x}_j) = \sum_{n=0}^{N-1} F_n e^{i\mathbf{k}_n \cdot \mathbf{x}_j}, \tag{2.15}$$

for "targets" $\mathbf{x}_j$ on a uniform grid in $\mathbb{R}$, given F_n at nonuniform $\mathbf{k}_n$ in the dual space. The type 2 NUFFT evaluates sums of the form

$$F(\mathbf{k}_n) = \sum_{j=1}^{N} f(\mathbf{x}_j) e^{-i\mathbf{k}_n \cdot \mathbf{x}_j}, \tag{2.16}$$

where the "targets" $\mathbf{k}_n$ are nonuniform points in $\mathbb{R}$, and $f(\mathbf{x}_j)$ are given on uniform grid points in the dual space. The type-3 NUFFT evaluates the sum of values defined on nonuniform grids at nonuniform grids in dual space and will not be listed here. Note that NUFFTs can be extended to higher dimensions.

The NUFFT is essentially an approximation algorithm, which means the summations are accelerated within a controlled accuracy, and in this point it differs from standard FFT, where efficiency is achieved by exploring the algebraic structure of the transform matrix without accuracy loss. The discussion of details regarding the relation of accuracy control to the algorithm parameters of NUFFT is beyond the scope of this work, and we refer to the work of Greengard *et al.* [16].

Remark 2.1. The above algorithm can actually be applied to various nonlocal potentials once their Fourier transforms are given analytically or can be evaluated numerically. This includes *e.g.* those which exist in Kadomtsev–Petviashvili equations [19]. For an application to various nonlocal potentials used in BEC simulations, we refer to [7,11].

2.3. Time splitting method

For computing the dynamics, we adapt the *time-splitting spectral method* (TSSP) which has been widely and successfully used for the nonlinear Schrödinger equation (NLSE) and DS system [12] with many applications [8–10,24]. We shall briefly introduce the *time splitting method* for DS equations to make the following sections reasonably self-contained.

To advance the evolution from $t = t_n$ to $t = t_{n+1}$, we first truncate the problem (1.1) on a square B_p with periodic boundary conditions for the wave function u and then solve it in two steps. First we solve the linear

equation,

$$i\,\partial_t v(\mathbf{x},t) = (-\partial_{xx} + \alpha\,\partial_{yy})v(\mathbf{x},t), \qquad \mathbf{x} \in B_p, \qquad t_n \le t \le t_{n+1} \tag{2.17}$$

$$v(\mathbf{x},t_n) = u^n(\mathbf{x}), \tag{2.18}$$

for a time step τ, and then we solve the nonlinear equation $t_n \le t \le t_{n+1}$

$$i\,\partial_t w(\mathbf{x},t) = \left(-2\,\beta\,|w|^2 - 4\,\beta\,\Phi\right)w(\mathbf{x},t), \qquad \mathbf{x} \in B_p, \tag{2.19}$$

$$w(\mathbf{x},t_n) = v(\mathbf{x},t_{n+1}), \tag{2.20}$$

for the same step τ, and then set $u^{n+1}(\mathbf{x}) = w(\mathbf{x},t_{n+1})$. The wave function is discretized by the Fourier spectral method, and equation (2.17)−(2.18) can be integrated exactly in Fourier space. Notice that density ρ is left unchanged in (2.19), therefore the nonlinear PDE is reduced to ODEs, pointwise in $\mathbf{x}$, and can be integrated analytically. The nonlocal potential $\Phi(\mathbf{x},t) \equiv \Phi(\mathbf{x},t_n)$ can be evaluated by the NUFFT scheme proposed in Section 2.1. The above time splitting scheme is the known Lie–Trotter splitting scheme. Higher order splitting methods are obtained by suitable compositions of (2.17)−(2.18) and (2.19)−(2.20).

Denote the solution to linear equation as $v^* := \mathrm{e}^{\mathcal{A}\,\tau}u^n$ and the solution to the nonlinear equation as $u^{n+1} := \mathrm{e}^{\mathcal{B}\tau}v^*$, where $\mathcal{A}$ and $\mathcal{B}$ are the corresponding operators. In this article, we use a fourth order time splitting method, also named Yoshida splitting method, [19,23] to make the temporal errors negligible compared to the spatial errors, therefore we shall focus on the spatial discretization hereafter. To be more precise, the Yoshida splitting reads as follows

$$u^{n+1} = \mathrm{e}^{\mathcal{A}\,a_1\tau}\mathrm{e}^{\mathcal{B}\,b_1\tau}\mathrm{e}^{\mathcal{A}\,a_2\tau}\mathrm{e}^{\mathcal{B}\,b_2\tau}\mathrm{e}^{\mathcal{A}\,a_3\tau}\mathrm{e}^{\mathcal{B}\,b_3\tau}\mathrm{e}^{\mathcal{A}\,a_4\tau}\,u^n, \tag{2.21}$$

with the coefficients

$$b_3 = \frac{1}{2-\sqrt[3]{2}} = b_1, \; b_2 = -\sqrt[3]{2}\,b_3, \;\; a_4 = \frac{1}{2}b_3 = a_1, \, a_3 = \frac{1}{2}(b_3+b_2) = a_2.$$

3. Numerical results

In this section, we shall present numerical results concerning the accuracy and efficiency of our novel NUFFT solver. We apply the pseudo-spectral Fourier method on the rectangle $[-L_x, L_x] \times [-L_y, L_y]$ with periodic boundary conditions. We denote the mesh step by $h_x = 2L_x/N_x, h_y = 2L_y/N_y$ and the mesh grid by $(x_j, y_k) := (-L_x + jh_x, -L_y + kh_y),\; j = 0,1,\ldots,N_x,\; k = 0,1,\ldots,N_y$ with N_x, N_y being positive even integers. For the sake of simplicity, we choose $L_x = L_y$, $h_x = h_y$ and denote them by L and h respectively.

3.1. Comparison for nonlocal potential evaluation

In this subsection, we shall present accuracy and efficiency results of both standard FFT and NUFFT solver for two different examples of calculation of Φ for a given ρ. In the tables of this subsection, we use the relative discrete l^∞ norm as error measure, *i.e.* $\|\Phi_{L,h} - \Phi\|_{l^\infty}/\|\Phi\|_{l^\infty}$.

Example 3.1. Gaussian density.

We choose $\rho(x,y) = \pi\,\mathrm{e}^{-\pi^2(x^2+y^2)}$, and the potential is given explicitly, in polar coordinates, as

$$\Phi(r,\theta) = -\left(\frac{\pi}{2}\,\mathrm{e}^{-\pi^2 r^2} + \cos(2\theta)\,\mathrm{e}^{-\pi^2 r^2}(2\pi r^2)^{-1}(1 + \pi^2 r^2 - \mathrm{e}^{\pi^2 r^2})\right). \tag{3.22}$$

First, we present the accuracy results of FFT and NUFFT. Table 1 presents the errors of the potential obtained by the standard FFT solver on $[-L, L]^2$ with different mesh sizes h and errors with the same mesh $h = 1/16$ on different domains. Table 2 shows errors of the potential obtained by the NUFFT solver on $[-L, L]^2$ with different mesh size h.

TABLE 1. Errors of the potential by standard FFT solver in Example 3.1.

	$h = 1$	$h = 1/2$	$h = 1/4$	$h = 1/8$	$h = 1/16$
$L = 8$	2.08E-01	2.22E-02	2.38E-03	2.38E-03	2.38E-03
$L = 16$	2.05E-01	2.12E-02	5.95E-04	5.95E-04	5.95E-04
	$L = 8$	$L = 16$	$L = 32$	$L = 64$	$L = 128$
$h= 1/16$	2.38E-03	5.95E-04	1.49E-04	3.72E-05	9.30E-06

TABLE 2. Errors of the potential by the NUFFT solver in Example 3.1.

	$h = 1$	$h = 1/2$	$h = 1/4$	$h = 1/8$	$h = 1/16$
$L = 8$	2.04E-01	2.08E-02	2.53E-04	1.56E-10	2.69E-15
$L = 16$	2.04E-01	2.08E-02	2.53E-04	1.56E-10	2.83E-15

TABLE 3. Errors and computational time of Example 3.1 on $[-32, 32]^2$. T_{HF}: time for high frequency part I_1 in (2.8), T_{NUFFT}: time for NUFFT part I_2 in (2.8).

	T_{HF}	T_{NUFFT}	T_{Total}	E
$h = 1/2$	2.00E-02	1.00E-02	3.00E-02	2.08E-02
$h = 1/4$	9.00E-02	4.00E-02	1.30E-01	2.53E-04
$h = 1/8$	3.70E-01	1.50E-01	5.20E-01	1.56E-10
$h= 1/16$	1.66	5.80E-01	2.24	2.69E-15

Second, the efficiency of NUFFT is shown in terms of CPU time. Table 3 displays the errors and computational cost of the NUFFT solver on $[-32, 32]^2$. The algorithm is implemented in Fortran, the code is compiled by ifort 13.1.2 using the option -O3, and executed on 32 bit Ubuntu Linux on a 2.90GHz Intel(R) Core(TM) i7-3520M CPU with 6MB cache.

Thirdly, we compare NUFFT and FFT in terms of computation time needed to achieve a given accuracy. We just report one comparison result for the sake of brevity. It takes 0.12 seconds for the FFT solver on $[-32, 32]^2$ with $h = 1/16$ and the achieved accuracy is 1.49E$-$04. For the NUFFT solver on $[-8, 8]^2$ with $h = 1/4$, a time of 0.02 seconds is needed, and the obtained accuracy is 2.53E$-$04, which is comparable in size to the accuracy of the previous case. So the new method clearly achieves a time benefit.

From Tables 1$-$3, we can conclude that: (i) The accuracy by the standard FFT solver reaches a saturation as the mesh size decreases, where the errors coming from the periodic boundary condition approximation dominate; (ii) For the standard FFT solver, the boundary condition error decreases as the domain increases, and the convergence rate with respect to volume of the domain is one; (iii) The NUFFT solver approximates the potential with spectral accuracy and the computational cost is $O(N \log(N))$ (with N being the total number of grid points in physical domain). The accuracy of this solver is better than the best accuracy achieved by the standard FFT solver on a much larger domain. Thus the new solver is quite efficient, which shall make it an ideal choice in long time dynamics of DS.

Example 3.2. Arkadiev's exact solution with geometric decay.

In the exact solution given by Arkadiev [6], the density and the corresponding potential are given explicitly as follows

$$\rho(\mathbf{x}) = \frac{4}{((x + 1)^2 + y^2 + 1)^2}, \quad \Phi(\mathbf{x}) = -2 \, \frac{y^2 - (x + 1)^2 + 1}{((x + 1)^2 + y^2 + 1)^2}. \tag{3.23}$$

TABLE 4. Errors of the potential by standard FFT solver in Example 3.2.

	$h = 1$	$h = 1/2$	$h = 1/4$	$h = 1/8$	$h = 1/16$
$L = 8$	3.40E-02	2.51E-02	2.63E-02	2.69E-02	2.73E-02
$L = 16$	2.44E-02	6.11E-03	6.24E-03	6.31E-03	6.34E-03
$L = 32$	2.20E-02	1.50E-03	1.51E-03	1.52E-03	1.53E-03
$L = 64$	2.13E-02	4.41E-04	3.73E-04	3.74E-04	3.74E-04

TABLE 5. Errors of the potential by NUFFT solver in Example 3.2.

	$h = 1$	$h = 1/2$	$h = 1/4$	$h = 1/8$	$h = 1/16$
$L = 8$	2.12E-02	2.51E-04	8.27E-05	8.76E-05	9.02E-05
$L = 16$	2.12E-02	2.49E-04	4.28E-06	4.40E-06	4.46E-06
$L = 32$	2.11E-02	2.49E-04	1.11E-06	2.47E-07	2.48E-07
$L = 64$	2.11E-02	2.49E-04	1.11E-06	1.46E-08	1.47E-08

TABLE 6. Errors and computational time of Example 3.2 on $[-64, 64]^2$.

	T_{HF}	T_{NUFFT}	T_{Total}	E
$h = 1$	0.04	0.01	0.05	2.11E-02
$h = 1/2$	0.18	0.03	0.21	2.49E-04
$h = 1/4$	0.96	0.12	1.08	1.11E-06
$h = 1/8$	4.90	0.55	5.45	1.46E-08

Note that density and the potential both decay geometrically. It is known that these rational decay solutions are notoriously hard to simulate numerically due to their slow decay at far field, which in turn requires large computational domains so as to achieve satisfactory results.

We present the accuracy results by the standard FFT and NUFFT solver and the efficiency performance of NUFFT. Table 4 presents errors of the potential obtained by the standard FFT solver on $[-L, L]^2$ with different h. Table 5 shows errors of the potential by the NUFFT solver on $[-L, L]^2$. Table 6 displays errors and computational cost of the NUFFT solver on $[-64, 64]^2$ on the same computer as in Example 3.1.

Also in this example, from Tables 4−6 we can observe a saturation due to the truncation and the periodic boundary condition approximation for FFT solver. The NUFFT solver does not perform as well as in Example 3.1, and the main reason should be the geometric decay of the potential and density. However, we could still achieve much better accuracy than standard FFT for equal discretization step and domain size, *i.e.* several orders of magnitude for the finest resolution tested. Thus the NUFFT solver is still an ideal choice for the simulation of long time dynamics.

3.2. Comparison for Hyperbolic-Elliptic DS simulation

As shown in the last subsection, the NUFFT solver proves to be accurate and efficient for evaluation of the nonlocal potential. In this subsection, we compare these two solvers in terms of accuracy when applied to simulate the complete dynamics of the DS equations (1.1)−(1.3). In this subsection, we use the relative discrete l^2 norm as error measure for all reported examples.

Example 3.3. Hyperbolic-Elliptic DS equation.

We first study the defocusing H-E Case with $\alpha = 1$, $\beta = -1$. In this case, we consider the following two initial values:

(1) **Case I** *(Arkadiev's solution)*. We consider again the exact solution given in [6]. The initial value is

$$u_0(\mathbf{x}) = \frac{2\mathrm{e}^{i2y}}{(x+1)^2 + y^2 + 1}, \tag{3.24}$$

and for the evolution,

$$u(x, y, t) = \frac{2\mathrm{e}^{i(2y+4t)}}{(x+1)^2 + (y+4t)^2 + 1}, \tag{3.25}$$

$$\Phi(x, y, t) = -2 \frac{(y+4t)^2 - x(x+2)}{\left((x+1)^2 + (y+4t)^2 + 1\right)^2}. \tag{3.26}$$

(2) **Case II** *(Gaussian initial value)*. Consider a Gaussian initial value as

$$u_0(x, y) = \mathrm{e}^{-\frac{(x^2+y^2)}{4}}. \tag{3.27}$$

We use a highly resolved reference solution, obtained by applying a *fourth-order time splitting Fourier pseudo spectral method* (TSFP4) [23] coupled with NUFFT potential solver on $[-64, 64]^2$ with a fine mesh size $h = 1/8$ and time step $\Delta t = 0.001$.

We truncate the problem onto a bounded domain, *i.e.* a rectangle $[-L, L]^2$, and impose periodic boundary conditions for u, which could be well resolved by the Fourier pseudo-spectral method. The integrator was chosen as fourth-order time splitting method [23] with a small time step, *i.e.* $\Delta t = 0.001$, such that errors coming from the temporal discretization are negligible. The potential Φ is evaluated by FFT or NUFFT solver on the same uniform mesh grid as the wave function. For brevity, we shall denote the TSFP4 coupled with FFT potential solver by FFT, and TSFP4 coupled with NUFFT potential solver by NUFFT.

Table 7 and 8 present errors of the wave function and potential at time $T = 0.4$ obtained by FFT and NUFFT for Case I. Table 9 and 10 show errors of the wave function and potential at time $T = 0.4$ obtained by FFT and NUFFT for case II.

From Tables 7−10, we can draw the following conclusions: (i) To achieve a fair accuracy in the potential by FFT solver, one needs to choose a very large domain; while the NUFFT solver essentially does not depend on the size of the computational domain. Moreover it is spectrally accurate provided the wave function decays fast enough. (ii) The accuracy for the wave function in Case I does not improve too much by NUFFT. Here the error coming from the the bounded domain truncation of u is dominant. However, all the simulations done with NUFFT show better results than the FFT method. To significantly increase accuracy in this case, a treatment of boundary cutoff errors for the wave function u is necessary; this direction of work will be the subject of a future paper. For Case II, where the wave function decays exponentially fast, the improvement of the NUFFT solver is obviously observed.

3.3. Comparison for Elliptic−Elliptic DS simulation

Here we take the same example as treated in [12, 15]. All the errors presented in this subsection are relative discrete l^2 errors.

Example 3.4. Elliptic−Elliptic DS equation.

TABLE 7. Errors of the wave function (*upper*) and potential (*below*) by FFT solver for Example 3.3: Case I.

	$h = 1$	$h = 1/2$	$h = 1/4$	$h = 1/8$
$L = 8$	3.30E-01	5.36E-02	4.82E-02	4.85E-02
$L = 16$	3.30E-01	3.14E-02	1.73E-02	1.73E-02
$L = 32$	3.30E-01	2.78E-02	8.25E-03	8.26E-03
$L = 64$	3.30E-01	2.68E-02	2.23E-03	2.23E-03
$L = 8$	2.54E-01	1.63E-01	1.63E-01	1.64E-01
$L = 16$	2.22E-01	8.24E-02	8.17E-02	8.17E-02
$L = 32$	2.14E-01	4.23E-02	4.08E-02	4.08E-02
$L = 64$	2.12E-01	2.33E-02	2.04E-02	2.04E-02

TABLE 8. Errors of the wave function (*upper*) and potential (*below*) by NUFFT for Example 3.3: Case I.

	$h = 1$	$h = 1/2$	$h = 1/4$	$h = 1/8$
$L = 8$	3.35E-01	3.81E-02	2.82E-02	2.88E-02
$L = 16$	3.31E-01	3.02E-02	1.42E-02	1.42E-02
$L = 32$	3.30E-01	2.78E-02	7.88E-03	7.89E-03
$L = 64$	3.30E-01	2.68E-02	2.15E-03	2.15E-03
$L = 8$	2.00E-01	1.12E-02	1.91E-03	1.88E-03
$L = 16$	2.08E-01	1.13E-02	4.52E-05	1.72E-04
$L = 32$	2.10E-01	1.13E-02	5.84E-06	4.32E-06
$L = 64$	2.11E-01	1.13E-02	4.15E-06	5.06E-07

TABLE 9. Errors of the wave function (*upper*) and potential (*below*) by FFT for Example 3.3: Case II.

	$h = 1$	$h = 1/2$	$h = 1/4$	$h = 1/8$
$L = 8$	2.03E-02	1.96E-02	1.96E-02	1.96E-02
$L = 16$	7.16E-03	4.91E-03	4.91E-03	4.91E-03
$L = 32$	5.36E-03	1.23E-03	1.23E-03	1.23E-03
$L = 64$	5.22E-03	3.07E-04	3.07E-04	3.07E-04
$L = 8$	1.91E-01	1.91E-01	1.91E-01	1.91E-01
$L = 16$	9.55E-02	9.53E-02	9.53E-02	9.53E-02
$L = 32$	4.79E-02	4.77E-02	4.77E-02	4.77E-02
$L = 64$	2.42E-02	2.38E-02	2.38E-02	2.38E-02

TABLE 10. Errors of the wave function (*upper*) and potential (*below*) by NUFFT for Example 3.3: Case II.

	$h = 1$	$h = 1/2$	$h = 1/4$	$h = 1/8$
$L = 8$	5.14E-03	8.03E-06	5.09E-07	4.69E-07
$L = 16$	5.21E-03	8.07E-06	3.26E-11	3.09E-13
$L = 32$	5.21E-03	8.01E-06	3.26E-11	5.02E-13
$L = 8$	3.34E-03	2.01E-05	1.90E-08	1.28E-08
$L = 16$	3.85E-03	2.05E-05	8.84E-11	4.22E-13
$L = 32$	3.98E-03	2.07E-05	8.91E-11	8.11E-14

TABLE 11. Errors of the wave function (*upper*) and potential (*below*) by standard FFT for Example 3.4.

	$h = 1$	$h = 1/2$	$h = 1/4$	$h = 1/8$
$L = 8$	1.26E-02	9.82E-03	9.82E-03	9.82E-03
$L = 16$	6.95E-03	2.46E-03	2.45E-03	2.45E-03
$L = 32$	6.16E-03	6.17E-04	6.14E-04	6.14E-04
$L = 8$	1.84E-01	1.83E-01	1.83E-01	1.83E-01
$L = 16$	9.25E-02	9.14E-02	9.14E-02	9.14E-02
$L = 32$	4.74E-02	4.57E-02	4.57E-02	4.57E-02

TABLE 12. Errors of the wave function (*upper*) and potential (*below*) by NUFFT for Example 3.4.

	$h = 1$	$h = 1/2$	$h = 1/4$	$h = 1/8$
$L = 8$	5.88E-03	6.15E-05	7.52E-08	6.05E-08
$L = 16$	5.97E-03	6.21E-05	3.17E-08	5.59E-13
$L = 32$	5.99E-03	6.22E-05	3.18E-08	7.37E-13
$L = 8$	1.18E-02	9.52E-05	1.06E-07	9.60E-11
$L = 16$	1.22E-02	9.82E-05	1.08E-07	7.08E-13
$L = 32$	1.23E-02	9.90E-05	1.08E-07	2.52E-13

$$i \, \partial_t u = -(\partial_{xx} + \partial_{yy}) \, u + \chi \, |u|^2 u + u \, \phi, \quad \mathbf{x} \in \mathbb{R}^2, \quad -(\partial_{xx} + \partial_{yy})\phi = \gamma \, |u|^2_{xx},$$

with initial value chosen as a Gaussian, *i.e.* $u(\mathbf{x}, 0) = u_0(\mathbf{x}) = 4 \, e^{-\frac{x^2+y^2}{4}}$. In this example, it is known that finite time blowup can occur. We choose a maximal computation time smaller than the time of blow-up to test the accuracy performance of the NUFFT solver. We take $\chi = -1$ (focusing interaction), $\gamma = 1$ and final time $T = 0.05$, which is smaller than the blow up critical time $T_* \approx 0.1311$. The reference solution used to measure the errors is obtained numerically by applying TSFP4 coupled with the NUFFT solver on the domain $[-64, 64]^2$ with a fine mesh size $h = 1/8$ and very fine time step $\Delta t = 0.0001$ such that errors coming from the temporal discretization are negligible.

Table 11 and 12 present errors of the wave function and potential at time $T = 0.05$ obtained by FFT and NUFFT respectively, from which we can draw similar conclusions as in Example 3.3.

4. CONCLUSION

We propose an efficient and accurate solver for the nonlocal potential in Davey−Stewartson system utilizing a nonuniform FFT (NUFFT) fast algorithm. We show in this paper that the NUFFT solver helps to achieve much better accuracy in the calculation of the nonlocal coupling term while still maintaining $O(N \log N)$ complexity, the same as uniform FFT. Extensive numerical results are presented to show its efficiency and accuracy.

For a wave function with exponential decay, the new solver reaches machine precision, while for the lump solution according to Arkadiev with algebraic decay, there still is a significant gain in accuracy. For the latter case, the dominant error comes from the truncation of the wave function and the advantage of NUFFT is masked. In this case, the NUFFT solver should be coupled to a method for removing cutoff errors of the wave function u, and future work in this direction is planned. The dramatic improvement in the nonlocal potential evaluation also benefits greatly the simulation of the DS equations. The gain in accuracy and efficiency makes the new solver a good alternative in simulations. Further extensions of the NUFFT solver to other nonlocal potentials are possible.

References

[1] M. Ablowitz and R. Haberman, Nonlinear evolution equations in two and three dimensions. *Phys. Rev. Lett.* **35** (1975) 1185–1188.

[2] M.J. Ablowitz and H. Segur, Solitons and the inverse scattering transform. *Studies in Applied and Numerical Mathematics.* SIAM, Philadelphia (1981).

[3] X. Antoine, A. Arnold, C. Besse, M. Ehrhardt and A. Schädle, A review of transparent and artificial boundary conditions techniques for linear and nonlinear Schrödinger equations. *Commun. Comput. Phys.* **4** (2008) 729–796.

[4] X. Antoine, W. Bao and C. Besse, Computational methods for the dynamics of the nonlinear Schrödinger/Gross-Pitaevskii equations. *Comput. Phys. Commun.* **184** (2013) 2621–2633.

[5] X. Antoine, C. Besse and P. Klein, Numerical solution of time-dependent nonlinear Schrödinger equation using domain truncation techniques coupled with relaxation scheme. *Laser Phys.* **21** (2011) 1491–1502.

[6] V.A. Arkadiev, A.K. Pogrebkov and M.C. Polivanov, Inverse scattering transform method and soliton solutions for the Davey−Stewartson II equation. *Physica D* **36** (1989) 189–196.

[7] W. Bao, S. Jiang, Q. Tang and Y. Zhang, Computing the ground state and dynamics of the nonlinear Schrödinger equation with nonlocal interactions via the nonuniform FFT. *J. Comput. Phys.* **296** (2015) 72–89.

[8] W. Bao, S. Jin and P.A. Markowich, Time-splitting spectral approximations for the Schrödinger equation in the semiclassical regime. *J. Comput. Phys.* **175** (2002) 487–524.

[9] W. Bao, S. Jin and P.A. Markowich, Numerical studies of time-splitting spectral discretizations of nonlinear Schrödinger equations in the semiclassical regime. *SIAM J. Sci. Comput.* **25** (2003) 27–64.

[10] W. Bao, N.J. Mauser and H.P. Stimming, Effective one particle quantum dynamics of electrons: A numerical study of the Schrödinger-Poisson-Xα model. *Commun. Math. Sci.* **1** (2003) 809–831.

[11] W. Bao, Q. Tang and Y. Zhang, Accurate and efficient numerical methods for computing ground states and dynamics of dipolar Bose-Einstein condensates via the nonuniform FFT. *Commun. Comput. Phys.* **19** (2016) 1141–1166.

[12] C. Besse, N.J. Mauser and H.P. Stimming, Numerical Study of the Davey−Stewartson System. *ESAIM: M2AN* **38** (2004) 1035–1054.

[13] V.D. Djordjević and L.G. Redekopp, On two-dimensional packets of capillary-gravity waves. *J. Fluid Mech.* **79** (1977) 703–714.

[14] A. Dutt and V. Rokhlin, Fast Fourier transforms for nonequispaced data. *SIAM J. Sci. Comput.* **14** (1993) 1368–1393.

[15] J.M. Ghidaglia and J.C. Saut, On the initial value problem for the Davey−Stewartson systems. *Nonlinearity* **3** (1990) 475–506.

[16] L. Greengard and J.Y. Lee, Accelerating the nonuniform fast Fourier transform. *SIAM Rev.* **46** (2004) 443–454.

[17] S. Jiang, L. Greengard and W. Bao, Fast and accurate evaluation of nonlocal Coulomb and dipole-dipole interactions via the nonuniform FFT. *SIAM J. Sci. Comput.* **36** (2014) B777–B794.

[18] C. Klein, B. Muite and K. Roidot, Numerical study of blowup in the Davey−Stewartson system. *Discrete Contin. Dyn. Syst.* *− Ser. B* **5** (2013) 1361–1387.

[19] C. Klein and K. Roidot, Fourth order time-stepping for Kadomtsev-Petviashvili and Davey−Stewartson equations. *SIAM J. Sci. Comput.* **33** (2011) 3333–3356.

[20] Y. Ohta and J.K. Yang, Dynamics of rogue waves in the Davey−Stewartson II equation. *J. Phys. A* **46** (2013) 105–202.

[21] A. Scrinzi, H.P. Stimming and N.J. Mauser, On the non-equivalence of perfectly matched layers and exterior complex scaling. *J. Comput. Phys.* **269** (2014) 98–107.

[22] Z. Xu, H. Han and X. Wu, Adaptive absorbing boundary conditions for Schrödinger-type equations: Application to nonlinear and multi-dimensional problems. *J. Comput. Phys.* **225** (2007) 1577–1589.

[23] H. Yoshida, Construction of higher order symplectic integrators. *Phys. Lett. A.* **150** (1990) 262–268.

[24] Y. Zhang and X. Dong, On the computation of ground state and dynamics of Schrödinger-Poisson-Slater system. *J. Comput. Phys.* **230** (2011) 2660–2676.