Numerical solutions of nonlinear wave equations

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Accurate, stable numerical solutions of the (nonlinear) sine-Gordon equation are obtained with particular consideration of initial conditions that are exponentially close to the phase space homoclinic manifolds. Earlier local, grid-based numerical studies have encountered difficulties, including numerically induced chaos for such initial conditions. The present results are obtained using the recently reported distributed approximating functional method for calculating spatial derivatives to high accuracy and a simple, explicit method for the time evolution. The numerical solutions are chaos-free for the same conditions employed in previous work that encountered chaos. Moreover, stable results that are free of homoclinic-orbit crossing are obtained even when initial conditions are within 10^{-7} of the phase space separatrix value π. It also is found that the present approach yields extremely accurate solutions for the Korteweg–de Vries and nonlinear Schrödinger equations. Our results support Ablowitz and co-workers' conjecture that ensuring high accuracy of spatial derivatives is more important than the use of symplectic time integration schemes for solving solitary wave equations. [S1063-651X(99)02601-X]

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Ablowitz, Herbst, and Schober [1,2] have recently called attention to the problem of numerically induced spatial and temporal chaos in computational solutions of the sine-Gordon equation (which has applications in physics, chemistry, and biology). Similar numerical difficulties are encountered in solving other important equations, such as the nonlinear Schrödinger equation [3,4] and modified Korteweg–de Vries (KdV) equation [5]. This numerical instability is problematic since it is possible that at least some previous reports of chaos might in fact have been the result of numerical inaccuracy. From the analytical point of view, for an integrable system, such numerical instability is associated with singularities in action-angle variables, which produce the so-called homoclinic orbits in the phase space geometry [1–4,6–8]. The presence of homoclinic orbits leads to exponentially unstable numerical solutions, characterized by oscillations between solutions on ''opposite sides'' of the homoclinic orbit. These ocillations can result from small perturbations in the numerical parameters and/or small numerical errors in the calculated solution. Such ocillations differ from the Gibbs oscillations occurring in the numerical solution of the Burgers equation with high Reynolds number (describing inviscid fluid flow), which are caused by the sharp spatial changes in the solution over a small distance [9]. From a computational point of view, a universal feature of these instabilities is that they typically occur when the numerical method is not adequate for describing sufficiently accurately the actual changes in a solution for the given space and time meshes. Ablowitz, Herbst, and Schober found that pseudospectral methods perform significantly better for the sine-Gordon equation than lattice type symplectic schemes [2]. However, for nonlinear equations, spectral and pseudospectral methods are not as simple to implement as various lattice methods. Therefore, it would be extremely useful to have accurate, efficient, simple, and general grid-based methods for solving the various nonlinear solitary equations that play an important role in modern science and technology.

In this paper we apply a reliable and robust approach that has global method accuracy and local or grid method flexibility for treating nonlinear solitary waves. All calculations reported were carried out on an IBM RISC-6000, model 560 workstation in double precision (16 bit arithmetic). The numerical examples studied are the sine-Gordon equation, the KdV equation, and the nonlinear Schrödinger equation. Our approach combines a recently developed Lagrange distributed approximating functional (LDAF) method [10] for spatial discretization and a fourth-order Runge-Kutta scheme [12] for time discretization. The general distributed approximating functional (DAF) method has been introduced [11] as a computational tool for approximating functions and their derivatives to a similar level of accuracy. It has been shown to provide accurate solutions for a number of different types of nonlinear partial differential equations, including the Burgers equation [9,13] and the nonlinear Fokker-Planck equations [14]. The present study focuses on nonlinear solitary wave equations with particular emphasis on the phase space regimes that are ''exponentially close'' [1] to homoclinic orbits, where earlier local methods [15,16] have encountered difficulty in providing correct numerical results. In the present computations we employ the LDAF to evaluate spatial derivatives. The LDAF parameters used are $M=80$ and $\sigma/\Delta=2.88$ for all cases [10]. Here the parameter M determines the degree of a Lagrange interpolating polynomial, which is multiplied by a Gaussian. The width of the Gaussian is determined by the ratio of a width parameter σ to the uniform grid spacing Δ.

As the first example we consider the sine-Gordon equation

$$\frac{\partial^2 u(x,t)}{\partial t^2} = \frac{\partial^2 u(x,t)}{\partial x^2} - \sin[u(x,t)], \tag{1}$$

with periodic boundary conditions

$$u(x,t) = u(x+L,t). \tag{2}$$

The sine-Gordon equation (1) is associated with a completely integrable Hamiltonian system [6,1]; its phase space geometry has been analyzed recently by Ercolani, Forest, and McLaughlin [6]. Its homoclinic orbits have been shown to be associated with chaos and numerical instabilities [6,1]. The simplest such orbit can be obtained by examining the spatially homogeneous sine-Gordon equation, i.e., the integrable periodic pendulum equation

$$\frac{\partial^2 u}{\partial t^2} + \sin(u) = 0, \tag{3}$$

which has a well-known ''pendulum homoclinic'' orbit

$$u(x,t) = \pi + 4\tan^{-1}[e^t] \tag{4}$$

corresponding to the phase space separatrix at $(u,u_t) = (\pi,0)$. A family of homoclinic orbits can be constructed [6,1] from the sine-Gordon equation's symmetry

$$(x,t,u) \rightarrow (t,x,u+\pi). \tag{5}$$

By doing this, one starts with a breather solution

$$u(x,t) = 4\tan^{-1}\left[\frac{\tan(\nu)\cos[\cos(\nu)t]}{\cosh[\sin(\nu)x]}\right], \tag{6}$$

where the parameter ν satisfies

$$|\nu| \ll 1. \tag{7}$$

This breather can be regarded as a kink-antikink bounded pair in space with a $2\pi/\cos(\nu)$ periodic oscillation in time. The sine-Gordon symmetry (5) leads to a family of real-valued homoclinic orbits

$$u(x,t) = \pi + 4\tan^{-1}\left[\frac{\tan(\nu)\cos[\cos(\nu)x]}{\cosh[\sin(\nu)t]}\right]. \tag{8}$$

In contrast to the spatially homogeneous homoclinic orbit (4), this family of homoclinic orbits also has a $2\pi/\cos(\nu)$ periodic spatial structure, i.e., a tangent cone associated with a phase space limit point $(\pi,0)$. We refer the reader to Ref. [6] for the construction of more general homoclinic states and a detailed spectral analysis. We emphasize that a thorough numerical analysis of chaotic behavior in various discretizations of the sine-Gordon equation for a wide range of parameter values, initial conditions, and time durations is beyond the scope of the present work. Such an analysis, as has been initiated by Ablowitz, Herbst, and Schober [1], is certainly important, particularly in the case of numerical chaotic behavior in high-dimensional conservative systems. Our purpose here is to demonstrate that the present LDAF approach is not only stable for numerical parameter values and initial conditions that led to numerical chaos when other spatial discretizations have been employed [1,2], but also makes it possible to obtain solutions much closer to the homoclinic orbit than was previously feasible.

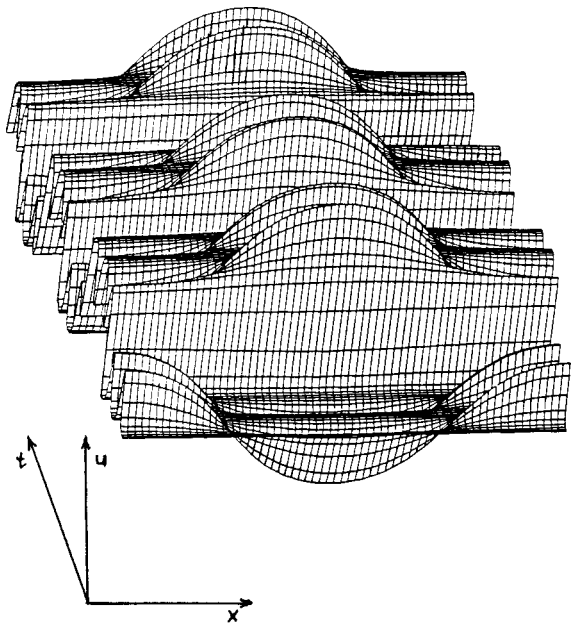

FIG. 1. Numerical solutions of the sine-Gordon equation.

We consider the numerical solution of Eq. (1) subject to the same initial conditions used in Ref. [1]:

$$u(x,0) = \pi + \epsilon_1 \cos(\mu x), \quad u_t(x,0) = 0, \tag{9}$$

with $\mu = 2\pi/L$, $L = 2\sqrt{2}\pi$, and π calculated as $\cos^{-1}(-1)$. Using a doubly discrete, integrable discretization scheme [15], Ablowitz, Herbst, and Schober [1] have shown that for small ϵ_1's, these initial values are exponentially close to the homoclinic manifold and produce numerical instability when one uses the Hirota solution algorithm [15]. Both spatial and temporal chaos are easily excited by very small perturbations (including roundoff error). A more troubling aspect is that these numerical instabilities persist as the mesh is refined and the temporal evolution of the numerical solution remains unstable even if all the conserved quantities are well preserved (by employing a very fine grid). In the present study we choose $\epsilon_1 = 0.05$ and 0.1 and the number N of grid points in x is taken to be 64. These values are identical to those leading to chaos in the calculations of Ablowitz, Herbst, and Schober [1]. No irregular oscillations occur when the solution is translated though a multiple of 2π and no high-frequency oscillations occur even if the solution is integrated for a long time. The case of $\epsilon_1 = 0.1$ was found by Ablowitz, Herbst, and Schober [1] to involve spatial and temporal chaos after a long-time integration ($t \geqslant 300$ time units). We have propagated our numerical solution for 650 time units without detecting any trace of chaotic instability. The results of integrating Eq. (1) with initial conditions (9) over a period of 450–550 time units for $\epsilon_1 = 0.1$ are presented in Fig. 1.

While the present calculations for the above examples are free of numerical chaos, we note that homoclinic orbit crossing occurs when the solution is translated through a multiple of 2π (see Fig. 1). In order to test the reliability of the

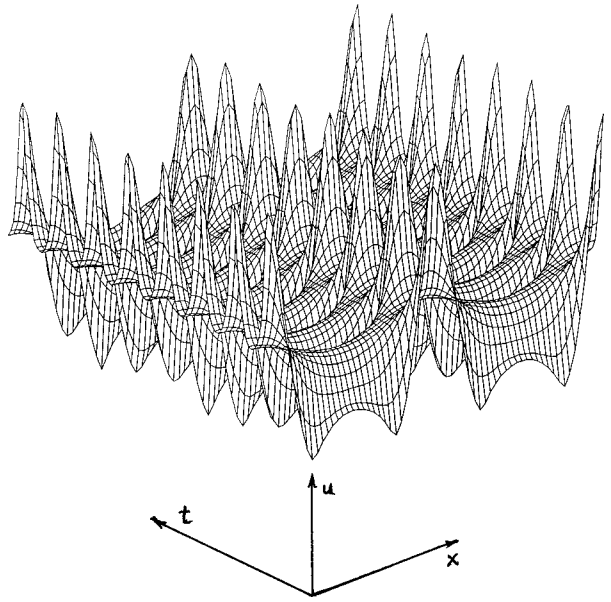

FIG. 2. Numerical solutions of the nonlinear Schrödinger equation up to $t=100$.

present integrator, we introduce a small perturbation ϵ_0 to the zeroth-order homoclinic orbit and modify the initial condition (9) to read

$$u(x,0)=(\pi+\epsilon_0)+\epsilon_1\cos(\mu x), \quad u_t(x,0)=0, \qquad (10)$$

with $\mu=2\pi/L$, $L=2\sqrt{2}\pi$, and $\epsilon_1=0.05$. This represents a stable phase space structure when the perturbation ϵ_0 is sufficiently large. For small ϵ_0 values, the solutions are still extremely close to the homoclinic orbits. Our method has achieved numerical convergence and yielded homoclinic-orbit-crossing-free results for $(\pi+\epsilon_0)=3.141\,592\,6$ when the number of grid points N is larger than 700.

As the second example we consider the nonlinear Schrödinger equation

$$i\,\frac{\partial u(x,t)}{\partial t}+\frac{\partial^2 u(x,t)}{\partial x^2}+4|u(x,t)|^2u(x,t)=0, \qquad (11)$$

with periodic boundary conditions (period $L=2\sqrt{2\pi}$) and initial values [3] $u(x,0)=0.5+0.05\cos(4\pi/L)$. Numerically induced chaos in this equation has been studied by Ablowitz and Herbst [3] and by McLaughlin and Schober [4]. The present LDAF approach provides stable numerical solutions (see Fig. 2) under the same integration conditions. Ablowitz, Herbst, and [2] have recently advanced the conjecture that the crucial factor in the occurrence of this numerical chaos is the accuracy of the discretization of spatial derivatives. This suggests that the success of the LDAF approach is due to its accuracy in representing $u(x,t)$ and its spatial derivatives. To further test this conjecture we examine the accuracy of the LDAF method by numerically solving the KdV equation

$$\frac{\partial u(x,t)}{\partial t}+u(x,t)\,\frac{\partial u(x,t)}{\partial x}+\beta\,\frac{\partial^3 u(x,t)}{\partial x^3}=0 \qquad (12)$$

with Dirichlet boundary conditions, assuming the initial solitary wave packet [18] $u(x,0)=3\eta\,\mathrm{sech}^2(Ax-6)$ [$\eta=0.3$, $\beta=4.84\times10^{-4}$, and $A=\frac{1}{2}(\eta/\beta)^{1/2}$]. Sanz-Serna and Christie obtained accurate results for this exactly soluble problem by using their modified Petrov-Galerkin method. Our results, as shown in Tables I and II, are more accurate than theirs, while using a much larger grid spacing.

TABLE I. Errors of the numerical solutions for the KdV equation. The numbers in square brackets denote powers of 10.

Δt	t	L_2[a]	L_∞[a]	L_2[b]	L_∞[b]
0.005		$\Delta x=0.01$		$\Delta x=0.025$	
	0.25	2.1[−4]	7.0[−5]	2.1[−5]	5.3[−5]
	0.50	3.8[−4]	1.1[−4]	2.7[−5]	6.0[−5]
	0.75	5.7[−4]	1.7[−4]	3.0[−5]	6.2[−5]
	1.00	7.4[−4]	2.1[−4]	3.3[−5]	6.6[−5]
0.0005				$\Delta x=0.013$	
	0.25			2.1[−10]	4.7[−10]
	0.50			2.3[−10]	4.1[−10]
	0.75			2.6[−10]	6.0[−10]
	1.00			3.0[−10]	5.8[−10]

[a]Reference [18].
[b]Present work.

These results provide very strong support for the earlier statement of Ablowitz, Herbst, and Schober that the occurrence of numerical chaos is primarily the result of inaccurate approximation of the spatial derivatives in discretizing the partial differential equation [2], as opposed to the treatment of the temporal evolution. By an appropriate choice of the DAF parameters M and σ/Δ one can control the accuracy of the DAF derivatives to the limit of machine accuracy (even higher accuracy should be attainable by use of extended precision). This should enable one to obtain stable, converged solutions for initially even closer to the separatrix.

In conclusion, in this paper, we have employed the LDAF integrator [10,17] to solve the nonlinear sine-Gordon, Schrödinger, and KdV equations numerically. Particular consideration was given to cases where the initial values are exponentially close to the homoclinic manifolds. Previous local or grid-based algorithms have encountered difficulties, including numerically induced spatiotemporal chaos [1]. So far, no numerical method totally free from homoclinic orbit crossing has been reported. However, the LDAF method provides smooth, chaos-free, and even homoclinic-orbit-crossing-free [if one uses an appropriate value of ϵ_0 approximation to π in the initial condition (10)] results using a reasonable number of grid points and time increment. In addition, such results

TABLE II. Errors of the numerical solutions for the Klein-Gordon equation ($\Delta t=0.001$ and $\Delta x=0.333$).

t	L_2	L_∞
0.1	5.7[−15]	8.0[−15]
0.2	1.1[−14]	1.6[−14]
0.3	1.6[−14]	2.2[−14]
0.4	1.9[−14]	2.6[−14]
0.5	2.0[−14]	2.6[−14]
1.0	2.3[−14]	3.8[−14]
2.0	6.0[−14]	7.3[−14]

are obtained using an explicit (as opposed to implicit) algorithm for the time evolution. We note that when π is generated as $\cos^{-1}(-1)$ in the computer (and $\epsilon_0=0$), corresponding to initial conditions that are extremely close to the separatrix, zeroth-order homoclinic orbit crossings can occur for certain numerical parameters, which were not eliminated by increasing the number of grid points up to 3000. Such initial conditions place extremely high demands on the accuracy with which spatial derivatives must be computed. In order to demonstrate the reliability of the LDAF approach, we have introduced initial conditions that are within 10^{-7} of the zeroth-order homoclinic orbit in the initial values. In this circumstance, the LDAF approach is able to provide results free from homoclinic orbit crossing and numerical chaos for $\pi+\epsilon_0$ equal to 3.141 592 6. A spectral analysis indicates that the LDAF method preserves the action of the sine-Gordon linear operator (the spatial part of the Lax pair) at least as well as or better than a previous pseudospectral approach [19–22].

In the past, symplectic numerical methods have been emphasized and regarded as superior to explicit methods for preserving the phase space structures of low-dimensional Hamiltonian systems. Only very recently have Ablowitz, Herbst, and Schober [2] suggested that this is not the relevant issue, but rather that the accuracy of the spatial discretization is more important. This was based on results obtained by a pseudospectral approach [2]. The present results, obtained with the LDAF approach, provide convincing support for their conjecture.

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