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 oscillations can result from small perturbations in the numerical parameters and/or small numerical errors in the calculated solution. Such oscillations 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 the 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 $\sigma$ to the uniform grid spacing $\Delta$.

As the first example we consider the sine-Gordon equation...
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

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

(1)

with periodic boundary conditions

\[ u(x,t) = u(x + L,t). \]  

(2)

By doing this, one starts with a breather solution

\[ u(x,t) = \pi + 4 \tan^{-1}[\epsilon^2], \]  

(3)

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

\[(x, t, u) \rightarrow (t, x, u + \pi).\]  

(5)

By choosing \(\epsilon = 0.05\) 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 \(2\pi\)’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 \(\epsilon = 0.05\) 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 \(2\pi\) and no high-frequency oscillations occur even if the solution is integrated for a long time. The case of \(\epsilon = 0.1\) was found by Ablowitz, Herbst, and Schober [1] to involve spatial and temporal chaos after a long-time integration (\(t \approx 300\) time units). We consider the numerical solution of Eq. (1) subject to the same initial conditions used in Ref. [1]:

\[ u(x,0) = \pi + \epsilon_1 \cos(\mu x), \quad u_x(x,0) = 0, \]  

(9)

with \(\mu = 2\pi/L\), \(L = 2\sqrt{2}\pi\), and \(\pi\) calculated as \(\cos^{-1}(-1)\). Using a doubly discrete, integrable discretization scheme [15], Ablowitz, Herbst, and Schober [1] have shown that for small \(\epsilon_1\)’s, these initial values are exponentially close to the homoclinic orbit than was previously feasible.

It is possible to obtain solutions much closer to the homoclinic orbit than was previously feasible.
present integrator, we introduce a small perturbation \( \epsilon_0 \) to the zeroth-order homoclinic orbit and modify the initial condition (9) to read

\[
u(x,0) = (\pi + \epsilon_0) + \epsilon_1 \cos(\mu x), \quad \nu_t(x,0) = 0,\]

(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 \( \epsilon_0 \) is sufficiently large. For small \( \epsilon_0 \) values, the solutions are still extremely close to the homoclinic orbits. Our method has achieved numerical convergence and yielded homoclinc-orbit-crossing-free results for \( (\pi + \epsilon_0) = 3.1415926 \) when the number of grid points \( N \) is larger than 700.

As the second example we consider the nonlinear Schrödinger equation

\[
i \frac{\partial u(x,t)}{\partial t} + \frac{\partial^2 u(x,t)}{\partial x^2} + 4|u(x,t)|^2 u(x,t) = 0,\]

(11)

with periodic boundary conditions (period \( L = 2\sqrt{2} \pi \)) and initial values \( u(x,0) = 0.5 + 0.05 \cos(4 \pi / L) \). Numerically induced chaos in this equation has been studied by Ablowitz and Herbst [3] and by McLaughlin and Schober [4]. The present LDAPF 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 LDAPF 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 LDAPF method by numerically solving the KdV equation

\[
\frac{\partial u(x,t)}{\partial t} + u(x,t) \frac{\partial u(x,t)}{\partial x} + \beta \frac{\partial^3 u(x,t)}{\partial x^3} = 0
\]

(12)

with Dirichlet boundary conditions, assuming the initial solitary wave packet [18] \( u(x,0) = 3 \eta \text{sech}^2(\Delta x - 6) \) \( \eta = 0.3, \beta = 4.84 \times 10^{-4} \) and \( A = \frac{1}{4} (\eta / \beta)^{1/2} \). 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.

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 \( \sigma / \Delta \) 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 LDAPF 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 LDAPF method provides smooth, chaos-free, and even homoclinic-orbit-crossing-free [if one uses an appropriate value of \( \epsilon_0 \) approximation to \( \pi \) in the initial condition (10)] results using a reasonable number of grid points and time increment. In addition, such results

<table>
<thead>
<tr>
<th>( \Delta t )</th>
<th>( t )</th>
<th>( L_2^a )</th>
<th>( L_{\infty}^a )</th>
<th>( L_2^b )</th>
<th>( L_{\infty}^b )</th>
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<tr>
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<td>5.7[-4]</td>
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<td>3.0[-5]</td>
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</tr>
<tr>
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<td>7.4[-4]</td>
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<td>3.0[-10]</td>
<td>5.8[-10]</td>
<td></td>
<td></td>
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</tr>
</tbody>
</table>

\begin{itemize}
\item \( ^a \)Reference [18].
\item \( ^b \)Present work.
\end{itemize}

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

<table>
<thead>
<tr>
<th>( \Delta t )</th>
<th>( t )</th>
<th>( L_2 )</th>
<th>( L_{\infty} )</th>
</tr>
</thead>
<tbody>
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<tr>
<td>0.4</td>
<td>1.9[-14]</td>
<td>2.6[-14]</td>
<td></td>
</tr>
<tr>
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<td>2.0[-14]</td>
<td>2.6[-14]</td>
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</tr>
<tr>
<td>1.0</td>
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<td>6.0[-14]</td>
<td>7.3[-14]</td>
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</tbody>
</table>

**TABLE II.** Errors of the numerical solutions for the Klein-Gordon equation (\( \Delta t = 0.001 \) and \( \Delta x = 0.333 \)).
are obtained using an explicit (as opposed to implicit) algorithm for the time evolution. We note that when \( \pi \) 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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