A New Numerical Method to Solve Nonlinear PDEs

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Abstract—In this paper, we show that a new numerical method, the Constrained Interpolation Profile - Basis Set (CIP-BS) method, is effective in solving nonlinear partial differential equations. This method uses a simple polynomial basis set that is easily extendable to any desired higher-order accuracy. The interpolating profile is chosen so that the subgrid scale solution approaches the local real solution by constraints on the spatial derivatives of the master equations. Then, introducing scalar products, the linear and nonlinear partial differential equations are uniquely reduced to ordinary differential equations for values and spatial derivatives at the grid points. The method gives stable, less diffusive, and accurate results. It is successfully applied to the Korteweg-de Vries equation, and the coupled nonlinear Schrödinger equation describing soliton dynamics.

1. Introduction

During the past three decades there has been significant progress in numerical analysis for nonlinear partial differential equations (PDEs). There are basically two types of methods for numerical solutions of PDEs: spectral and grid methods. The main difference between these two methods comes from the methodology in treating the spatial derivatives. Since spectral methods typically consist of expanding the total solution in terms of differentiable basis functions such as used in the Fourier transformation, they do not suffer from numerical inaccuracies for derivatives. Therefore, in general, these methods give accurate solutions with a minimum number of discretization points, only if appropriate problem specific basis functions which satisfy the boundary conditions are applicable. On the other hand, grid methods, such as finite element methods or finite difference methods, consist of approximating derivatives by finite differences. It is often difficult to approximate the derivatives with sufficient accuracy, because the derivatives are estimated by using only the values of the function on a compact set of grid points. However, since finite difference derivatives often lead to structured matrices, which are easily adapted to a number of standard techniques, they are typically more flexible and easier to implement than spectral methods for systems with complex boundary conditions. Therefore, it is to be said that improvements in grid methods which exemplify the spectral method's accuracy is the primary goal of a numerical method.

In 1991, Yabe and Aoki proposed the Constrained Interpolation Profile (CIP) method[1, 3], in which not only values but also their first derivatives are treated as independent variables associated with the grid point, and the information lost inside the grid cell is retrieved by a Hermite type interpolation function[2]. It is worth noting that the CIP method does not include any algorithm-dependent parameter. If the size of the system and grid intervals for the problem are defined, the governing equations are uniquely transformed into a discretized form, in which no matrix solution is used. However, methods using matrix operations are more advantageous because a number of numerical methods for large, sparse systems developed for the finite difference method or the finite element method can be adopted. Recently, a new numerical method, the CIP-Basis Set (CIP-BS) method[4], has been proposed by generalizing the concept of the CIP method from the viewpoint of the basis set. The governing equations are unambiguously discretized into matrix form equations requiring the residuals to be orthogonal to the basis functions via the same procedure as the Galerkin method. The CIP-BS method, in which the local polynomial basis functions corresponding to the values and spatial derivatives at each grid point belong to the complete set and the C^K class, is called the CIP-BS^K method. Numerical results in the solution of the Schrödinger equation have demonstrated that accurate solutions are obtained by the CIP-BS method and the use of a higher order basis set is essential in increasing accuracy.

Furthermore, we have found that the CIP-BS method can be extended to nonlinear PDEs by introducing differential algebra to discretize nonlinear functional operations. The purpose of this paper is to show that the method can be applied to nonlinear PDEs exemplified by solutions of the Korteweg-de Vries (KdV) equation, and the coupled nonlinear Schrödinger (CNLS) equation which describe the dynamics of solitons.

2. Numerical Method

Since the CIP-BS method is new and not widely known, we first summarize the method adding extensions to adopt the method to nonlinear hyperbolic equations.

We need a basis set where it is easy to define values and derivatives of an arbitrary function, $f(x)$, at the grid

points. Therefore, we assume that the functions in the domain of R^1 can be approximated by the CIP-basis set of degree K method (CIP-BS^K), where K refers to the order of the derivatives we retain in the calculation, through the expression

$$f(x) = \sum_{i=1}^{N} \sum_{k=0}^{K} f_i^{(k)} \phi_{k,i}(x), \qquad (1)$$

where $f_i^{(k)}$ is the k-th coefficient at the grid point x_i, the summation on the index i is taken over all grid points, and the basis functions, $\phi_{k,i}(x)$, on the local support $[x_{i-1}, x_{i+1}]$ are expressed in the form

$$\phi_{k,i}(x) = \theta_{i-1,i}(x)\phi_{k,i-}(x) + \theta_{i,i+1}(x)\phi_{k,i+}(x), \qquad (2)$$

where $\theta_{i,i+1}(x) = \theta(x - x_i) - \theta(x - x_{i+1})$, $\theta(x)$ is the Heaviside step function, and $\phi_{k,i-}(x), \phi_{k,i+}(x)$ are polynomials of degree $(2K + 1)$ determined from the constraints:

$$
\begin{aligned}
D_x^l \phi_{k,i\pm}(x_i) &= \begin{cases} 1 & for & l = k \\ 0 & for & l = 0, 1, \cdots, k-1, k+1, \cdots, K \end{cases} \\
D_x^l \phi_{k,i\pm}(x_{i\pm 1}) &= 0 \quad for \quad k = 0, 1, \cdots, K,
\end{aligned} \qquad (3)
$$

where D_x is the derivative operator in x, and $D_x^0 = 1$. For a uniform grid system the basis function satisfies the translational relation $\phi_{k,i}(x) = \phi_{k,i-n}(x - x_n)$.

The first derivative of the basis function is expressed as $D_x \phi_{k,i}(x) = \theta_{i-1,i}\phi'_{k,i-}(x) + \theta_{i,i+1}\phi'_{k,i+}(x)$. Here, we have used the fact that $\phi_{k,i\pm}(x)\delta(x - x_{i\pm 1}) = 0$ due to the relation $x\delta(x) = 0$, and $\phi_{k,i-}(x_i) = \phi_{k,i+}(x_i)$, where $\delta(x)$ is the Dirac delta function. Similarly, we can obtain the l-th order derivatives of $\phi_{k,i}(x)$ for $l \leq K + 1$ as $D_x^l \phi_{k,i}(x) = \theta_{i-1,i}\phi_{k,i-}^{(l)}(x) + \theta_{i,i+1}\phi_{k,i+}^{(l)}(x)$. Although the basis functions are constructed by using distribution functions, the functions represented in the CIP-BS^K method belong to the C^K class. Therefore, it is easily found that the k-th spatial derivative of $f(x)$ at the grid point x_i equals the coefficient $f_i^{(k)}$, i.e. $D_x^k f(x)|_{x=x_i} = f_i^{(k)}$. We can say that the basis set belongs to a complete set in the sense that the expansion (1) could represent the exact solution with any degree of accuracy in the limit $N \rightarrow \infty$ or $K \rightarrow \infty$. If $f(x) = 0$ in Eq.(1), we can deduce that all the coefficients $f_i^{(k)}$ are zero, and that the basis functions are linearly independent. Then the function $f(x)$ can also be represented by this basis set as $\boldsymbol{f} = (\boldsymbol{f}_1, \boldsymbol{f}_2, \cdots, \boldsymbol{f}_N)$ where $\boldsymbol{f}_i = (f_i^{(0)}, f_i^{(1)}, \cdots, f_i^{(K)})$.

Let us define addition and multiplication of the functions as follows:

$$f(x) + g(x) \Leftrightarrow \boldsymbol{f} + \boldsymbol{g} = (\boldsymbol{f}_1 + \boldsymbol{g}_1, \boldsymbol{f}_2 + \boldsymbol{g}_2, \cdots, \boldsymbol{f}_N + \boldsymbol{g}_N) \quad (4)$$

$$cf(x) \Leftrightarrow c\boldsymbol{f} = (c\boldsymbol{f}_1, c\boldsymbol{f}_2, \cdots, c\boldsymbol{f}_N) \qquad (5)$$

$$f(x) \cdot g(x) \Leftrightarrow \boldsymbol{f} \cdot \boldsymbol{g} = (\boldsymbol{f}_1 \cdot \boldsymbol{g}_1, \boldsymbol{f}_2 \cdot \boldsymbol{g}_2, \cdots, \boldsymbol{f}_N \cdot \boldsymbol{g}_N), \quad (6)$$

where c is a scalar value. Addition and scalar multiplication for $\boldsymbol{f}_i$ are

$$\boldsymbol{f}_i + \boldsymbol{g}_i = (f_i^{(0)} + g_i^{(0)}, f_i^{(1)} + g_i^{(1)}, \cdots, f_i^{(K)} + g_i^{(K)}) \quad (7)$$

$$c\boldsymbol{f}_i = (cf_i^{(0)}, cf_i^{(1)}, \cdots, cf_i^{(K)}) \qquad (8)$$

and multiplication is given by

$$\boldsymbol{f}_i \cdot \boldsymbol{g}_i = (h_i^{(0)}, h_i^{(1)}, \cdots, h_i^{(K)}), \qquad (9)$$

where $h_i^{(j)} = \sum_{l=0}^{j} \frac{j!}{l!(j-l)!} f_i^{(l)} g_i^{(j-l)}$. The identity of addition and multiplication are $(0, 0, \cdots)$ and $(1, 0, \cdots)$, respectively. Eqs.(7) - (9) are the same as the definition for differential algebra $_K D_1$, (see ref.[5]). Therefore, the functions $f^{-1}(x)$, $\sqrt{f(x)}$, $sin(f(x))$, or $exp(f(x))$ can be uniquely represented by the basis set using the representation of $f(x)$. For Example, $f^{-1}(x)$ is can be expressed $(\frac{1}{f_i^{(0)}}, -\frac{f_i^{(1)}}{f_i^{(0)2}}, \frac{2f_i^{(1)2} - f_i^{(0)} f_i^{(2)}}{f_i^{(0)3}})$ when $K = 2$ and $f_i^{(0)} \neq 0$. However, it is worth noting that, although the operation D_x^n maps $_K D_1$ into $_{K-n} D_1$ in the differential algebra, we represent D_x^n as a matrix by introducing the scalar product of the basis function $\phi_{k,i}(x)$ and $\phi_{k',i'}(x)$ in the domain R as [4]

$$< \phi_{k,i}|\phi_{k',i'} > \equiv \int_R \phi_{k,i}(x)\phi_{k',i'}(x)dx. \qquad (10)$$

Partial differential equations $\partial f(x,t)/\partial t = L[f(x,t)]$, where L is a linear or nonlinear operator, are reduced to ordinary differential equations by the scalar product. Applying $< \phi_{k,i}|$, $(k = 0, 1, 2, \cdots, K, i = 0, 1, 2, \cdots, N)$, to the left of the equation, we obtain

$$S \frac{d\boldsymbol{f}}{dt} = L[\boldsymbol{f}], \qquad (11)$$

where S is a positive-definite matrix with the element $S_{ki,k'i'} = < \phi_{k,i}|\phi_{k',i'} >$, and L is a $m + 1$ dimensional matrix with the element

$$L_{ki,k_1 i_1, \cdots, k_m i_m} = < \phi_{k,i}|D_x^{n_1} \phi_{k_1 i_1} \cdots D_x^{n_m} \phi_{k_m i_m} >, \qquad (12)$$

where m is a power of f and $D_x^{n_l}$ is a differential operator on the lth f. For example, if L contains a term $f\partial f/\partial x$, the element of the corresponding matrix is $L_{ki,k_1 i_1, k_2 i_2} = < \phi_{k,i}|\phi_{k_1 i_1} D_x \phi_{k_m i_m} >$. Since $S_{ki,k'i'}$ is non-zero only for $i' = i - 1, i, i + 1$, S is a band diagonal matrix with bandwidth $3(K + 1)$. The non-zero elements of the matrix representation of the operator L are only $i_l = i - 1, i, i + 1$, and can be analytically calculated. The rank of the differential operator must satisfy one of the following conditions: (1) $n_l \leq K$ for $l = 1, 2, \cdots, m$, (2) the maximum of n_l is $K + 1$, and the other n_l are less than K, (3) the maximum of n_l is $K + 2$, and the other n_l are less than $K - 1$. Otherwise, terms like $\theta(x)\delta(x)'$, which cannot be regularized, would appear. This procedure is equivalent to the one in the Galerkin method in which the residual $\frac{\partial}{\partial t} f(x,t) - L[f(x,t)]$ is required to be orthogonal to the basis functions $\phi_{k,i}(x)$. Roughly speaking, the subset of the equations resulting from the multiplication of $< \phi_{k,i}|$ corresponds to the equation $\partial f^k/\partial t = \partial^k L[f]/\partial x^k$.

3. Numerical Results

Here, we solve the KdV, and CNLS equations to demonstrate the effectiveness of the CIP-BS method. For simplicity, we consider one-dimensional problems with a uniform

grid. The implicit solver with general sparse Jacobian matrices developed by Hindmarsh and Balsdon [6] is used to time propagate the discretized equations (Eq.(11)).

3.1. KdV Equation

We solve the KdV equation:

$$\frac{\partial f}{\partial t} + f\frac{\partial f}{\partial x} = -\mu\frac{\partial^3 f}{\partial x^3}, \qquad (13)$$

on the two length periodic interval with the initial condition $f(x,0) = \cos \pi x$ and the dispersion coefficient $\mu = 0.022^2$. This problem was ﬁrst calculated by Zabusky and Kruskal [7], using the ﬁnite differencing method where the momentum is identically conserved. Here, we discretize the equation as follows:

$$S_{ki,k'i'}\frac{df_{i'}^{(k')}}{dt} = -L_{ki,i_1k_1,i_2k_2}^{(001)}f_{i_1}^{(k_1)}f_{i_2}^{(k_2)} - \mu L_{ki,i_1k_1}^{(03)}f_{i_1}^{(k_1)}, \quad (14)$$

for $i = 1, 2, \cdots, N, k = 0, 1, \cdots, K$, where $L_{ki,i_1k_1}^{(03)} = < \phi_{k,i}|D_x^3\phi_{k_1i_1} >$. The summations for k', k_1, k_2 are taken on $0, 1, \cdots, K$, and those for i', i_1, i_2 on $i-1, i, i+1$. Hereafter, if a subscript appears twice in a term, this summation is assumed.

Figure 1 depicts the temporal development of the wave form, and Fig. 2 gives the space-time trajectories of the solitons calculated by the CIP-BS[1] method. The results in Ref.[7] are well reproduced. We can observe that the soliton retains its identity after strong nonlinear interactions with other solitons. In addition, all the solitons almost reconstruct the initial state after each recurrence time T_R. These calculations are carried out by the CIP-BS[1] or CIP-BS[2] method, since the KdV equation contains 3rd order spatial derivatives and cannot be solved by the CIP-BS[0] method as explained in the previous section. The quantity $\int f(x,t)dx$ is conserved for $0 \le t \le 3T_R$ within 10^{-11} and 10^{-14} when solved by the CIP-BS[1] and CIP-BS[2] method, respectively.

3.2. CNLS Equation

Next, we solve CNSL equation,

$$i\frac{\partial u}{\partial t} + \frac{\partial^2 u}{\partial x^2} + (|u|^2 + \beta|v|^2)u = 0,$$
$$i\frac{\partial v}{\partial t} + \frac{\partial^2 v}{\partial x^2} + (|v|^2 + \beta|u|^2)u = 0, \qquad (15)$$

where u and v are complex functions, and β is a coupling constant. Letting $u = p + iq, v = r + is$, the CNLS equation(Eq.(15)) can be written as

$$\frac{\partial p}{\partial t} = -\frac{\partial^2 q}{\partial x^2} - ((p^2 + q^2) + \beta(r^2 + s^2))q,$$
$$\frac{\partial q}{\partial t} = \frac{\partial^2 p}{\partial x^2} + ((p^2 + q^2) + \beta(r^2 + s^2))p,$$
$$\frac{\partial r}{\partial t} = -\frac{\partial^2 s}{\partial x^2} - ((r^2 + s^2) + \beta(p^2 + q^2))s,$$
$$\frac{\partial s}{\partial t} = \frac{\partial^2 r}{\partial x^2} + ((r^2 + s^2) + \beta(p^2 + q^2))r. \qquad (16)$$
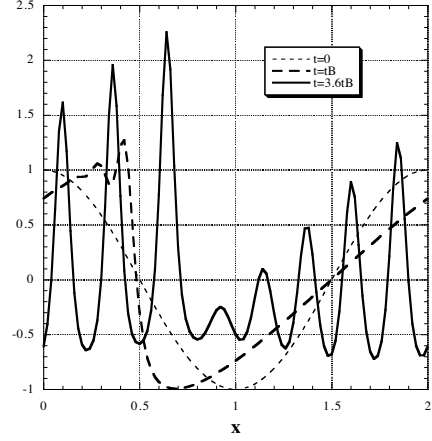

Figure 1: The solution of the KdV equation by the CIP-BS[1] method with an initial condition of $f(x,0) = \cos \pi x$. CFL number =0.1, and $\Delta x = 0.01$. The curves are drawn depending on the breakdown time of $tB = 1/\pi$.
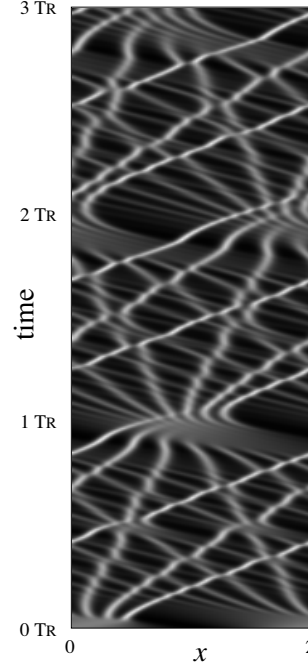

Figure 2: Soliton trajectories in a space-time diagram. $T_R(= 30.4tB = 30.4/\pi)$ is the recurrence time. The white and black color correspond to the value 3 and -1, respectively.

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In the CNLS system the global norm N_u, N_v, momentum $J = J_u + J_v$, and energy $E = E_u + E_v + E_I$, where $E_u = \int_R \mathcal{E}_u dx$, $E_v = \int_R \mathcal{E}_v dx$, $E_I = \int_R \mathcal{E}_I dx$, $\mathcal{E}_u = \frac{1}{2}(p^2 + q^2)^2 - ((\frac{\partial p}{\partial x})^2 + (\frac{\partial q}{\partial x})^2)$, $\mathcal{E}_v = \frac{1}{2}(r^2 + s^2)^2 - ((\frac{\partial r}{\partial x})^2 + (\frac{\partial s}{\partial x})^2)$, and $\mathcal{E}_I = \beta(p^2 + q^2)(r^2 + s^2)$, are conserved.

The discretized CNLS equations are straightforwardly obtained as:

$$S_{ki,k'i'}\frac{dp_i^{(k')}}{dt} = -L_{ki,i_1k_1}^{(02)}q_{i_1}^{(k_1)} - L_{ki,i_1k_1,i_2k_2}^{(000)}((p^2{}_{i_1}^{(k_1)} + q^2{}_{i_1}^{(k_1)}) + \beta(r^2{}_{i_1}^{(k_1)} + s^2{}_{i_1}^{(k_1)}))q_{i_2}^{(k_2)},$$

$$S_{ki,k'i'}\frac{dq_i^{(k')}}{dt} = L_{ki,i_1k_1}^{(02)}p_{i_1}^{(k_1)} + L_{ki,i_1k_1,i_2k_2}^{(000)}((p^2{}_{i_1}^{(k_1)} + q^2{}_{i_1}^{(k_1)}) + \beta(r^2{}_{i_1}^{(k_1)} + s^2{}_{i_1}^{(k_1)}))p_{i_2}^{(k_2)},$$

$$S_{ki,k'i'}\frac{dr_i^{(k')}}{dt} = -L_{ki,i_1k_1}^{(02)}s_{i_1}^{(k_1)} - L_{ki,i_1k_1,i_2k_2}^{(000)}((r^2{}_{i_1}^{(k_1)} + s^2{}_{i_1}^{(k_1)}) + \beta(p^2{}_{i_1}^{(k_1)} + q^2{}_{i_1}^{(k_1)}))s_{i_2}^{(k_2)},$$

$$S_{ki,k'i'}\frac{ds_i^{(k')}}{dt} = L_{ki,i_1k_1}^{(02)}r_{i_1}^{(k_1)} + L_{ki,i_1k_1,i_2k_2}^{(000)}((r^2{}_{i_1}^{(k_1)} + s^2{}_{i_1}^{(k_1)}) + \beta(p^2{}_{i_1}^{(k_1)} + q^2{}_{i_1}^{(k_1)}))r_{i_2}^{(k_2)},$$

Also, the discretized expressions for the global norm, momentum, and energy are obtained in the same procedure. For example, the global norm is calculated as $N_u = L_{i_1k_1,i_2k_2}^{(00)}(p_{i_1}^{(k_1)}p_{i_2}^{(k_2)} + q_{i_1}^{(k_1)}q_{i_2}^{(k_2)})$, where $L_{ki,i_1k_1}^{(00)} = <\phi_{k,i}|\phi_{k_1i_1}>$.

We consider the CNLS equation with the initial condition [8, 9]: $u(x, 0) = \sqrt{2}r_1 sech(r_1x - \xi_1)e^{iv_1x}$, $v(x, 0) = \sqrt{2}r_2 sech(r_2x - \xi_2)e^{iv_2x}$. We take $r_1 = 1.2$, $r_2 = 1.0$, $\xi_1 = -\xi_2 = d_0/2 = 12.5$, and $v_1 = -v_2 = -v_0/4 > 0$ such that the two solitons with different amplitudes approach with the velocity v_0 and collide at $x \approx 0$ after $t \approx d_0/v_0$.

Figure 3 shows the results for $\beta = 1$. The computations are carried out over the range $-30 \leq x \leq 30$, $0 \leq t \leq 50$ with a time step $\Delta t = 0.01$ and a space interval $\Delta x = 0.3$ by the CIP-BS[1] method. From Fig.3, we can observe that the soliton retains its identity after nonlinear interactions with the other soliton. The errors of the global norm N_u, N_v, momentum J, and energy E are also shown in the gure. Although it seems that the errors of the momentum and energy increase during strong interaction, it is only due to the lack of approximation accuracy for monitoring variables, *i.e.* the error is reduced soon after the interaction ended. The conservation property of the energy by the CIP-BS method compared well with those in Ref.[9], in which the multi-symplectic method is used. The errors of the energy versus Δx and K at the end of computation (not shown here), we have con rmed the CIP-BS[1] and CIP-BS[2] methods have 4th and 6th order accuracy despite nonlinear interactions.

4. Conclusion

We have generalized the CIP-BS method by introducing matrix representations and clarifying the relation with differential algebra to accommodate it to nonlinear partial differential equations. The nonlinear PDEs are uniquely reduced to ODEs for values and spatial derivatives at the grid points. Furthermore, since the matrix, S and L, are sparse and sufficient to be calculated only at the beginning of the simulation, the method is computationally efficient. It is successfully applied to typical nonlinear PDEs describing soliton dynamics: the KdV and CNLS equations. It is
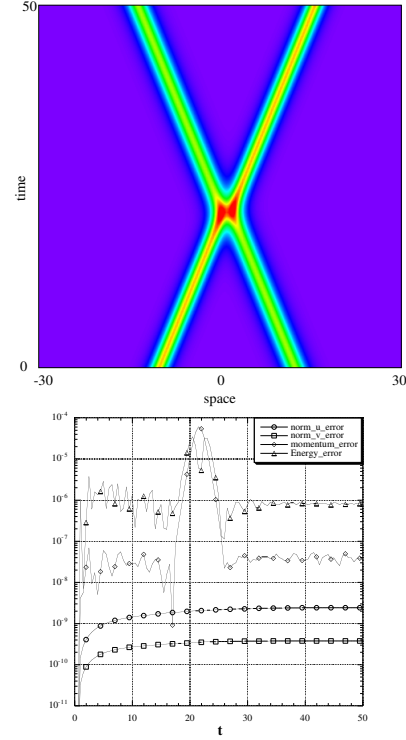

Figure 3: The solutions of the CNLS equation for the interaction of two solitons with $\beta = 1$. The surface plots show the amplitude of solitons. The bottom plot shows numerical results of norm, momentum, and energy error.

proved that the method gives stable, less diffusive, and accurate results.

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