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Short Note

A note on the basis set approach in the constrained interpolation profile method

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Abstract

We propose a simple polynomial basis set that is easily extendable to any desired higher-order accuracy. This method is based on the Constrained Interpolation Profile (CIP) method and the profile is chosen so that the subgrid scale solution approaches the real solution by the constraints from the spatial derivative of the original equation. By adopting the higher-order derivatives of the master equations as constraints to generate a self-consistent subgrid profile, this solution quickly converges. 3rd and 5th order polynomials are tested on the one-dimensional Schrödinger equation and are proved to give solutions a few orders of magnitude higher in accuracy than conventional methods for lower-lying eigenstates.

Keywords: Basis set; CIP-BS method; CIP method; Time-dependent Schrödinger equation; Generalized eigenvalue equation; Dirichlet boundary conditions; Neumann boundary conditions

There is a growing interest in the accurate solutions of the excited states of atoms and their time-dependent solutions for computational design of material properties, catalysis, medical drugs, and so on, or to elucidate non-linear phenomena in strong interactions. Much pioneering work has been performed with this goal in mind [1–4].

The purpose of this paper is to establish a systematic and simple method to get solutions of the Schrödinger equation with any desired accuracy by generalizing the concept of the Constrained Interpolation Profile (CIP) method. The CIP method was first proposed by one of the authors for the solution of hyperbolic-type equations [5–9]. In its original form, it used a cubic polynomial to describe the subgrid-

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scale profile. All the coefficients of the polynomial are determined so that the piece-wise polynomial can reproduce a local analytical solution within a grid cell by the constraints from the spatial derivatives of the original equation. Resultingly, the CIP method can accurately describe the solution of a propagating wave having a wavelength of only two grid cells, which is beyond the capability of existing schemes. In this paper, we apply the proposed method to the one-dimensional Schrödinger equation and obtain very accurate solutions which are a few orders of magnitude better than conventional methods for lower-lying eigenstates.

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

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

where $f_i^{(k)}$ is the kth 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

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

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:

$$\begin{aligned} &D_x^l \phi_{k,i\pm}(x_i) = \begin{cases} 1 & \text{for } l = k, \\ 0 & \text{for } l = 0, 1, \ldots, k-1, k+1, \ldots, K, \end{cases} \\ &D_x^l \phi_{k,i\pm}(x_{i\pm1}) = 0 \quad \text{for } k = 0, 1, \ldots, K, \end{aligned} \tag{3}$$

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 $\phi_{k,i}(x) = \phi_{k,i-n}(x - x_n)$.

Especially, the interpolating function in $[x_i, x_{i+1}]$ for the CIP-BS^1 method is written by the Hermite type interpolation as $f(x) = c_0 + c_1\bar{x} + c_2\bar{x}^2 + c_3\bar{x}^3$, where

$$\begin{aligned} &c_0 = f_i, c_1 = f_i', \\ &c_2 = 3(f_{i+1} - f_i)/\Delta x^2 - (2f_i' + f_{i+1}')/\Delta x, \\ &c_3 = 2(f_i - f_{i+1})/\Delta x^3 + (f_i' + f_{i+1}')/\Delta x^2 \end{aligned} \tag{4}$$

and $\bar{x} = x - x_i$, $\Delta x = x_{i+1} - x_i$. The coefficients c_0, c_1, c_2, c_3 are the same as those of the CIP method determined with the constraints: $f(x_i) = f_i$, $f'(x_i) = f_i'$, $f(x_{i+1}) = f_{i+1}$, $f'(x_{i+1}) = f_{i+1}'$.

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 $\phi_{k,i\pm}(x)\delta(x - x_{i\pm1}) = 0$ 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 lth order derivatives of $\phi_{k,i}(x)$ for $l \leqslant K+1$ 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 kth 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 $N \to \infty$ or $K \to \infty$. 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 $\mathbf{f} = (\mathbf{f_1}, \mathbf{f_2}, \ldots, \mathbf{f_N})$, where $\mathbf{f_i} = (f_i^{(0)}, f_i^{(1)}, \ldots, f_i^{(K)})$.

To better understand the procedure we use to solve the differential equation that will be given below, we review the process of the CIP method in comparison with the CIP-BS method. If the equation to be solved has a form like $\partial f/\partial t = L[f]$, where L is the spatial operator, then the time evolution of f at the grid point is given by this equation. The CIP method uses the derivative of this equation, $\partial f'/\partial t = \partial L[f]/\partial x$, to determine the time evolution of f' at the grid point. Thus the profile inside the grid cell is described by Eq. (1). Instead of using such an equation at each local grid point, we here use the integrated equation over the grid cell. Since $\phi_{0,i}$ peaked at the point i and $\phi_{1,i}$ is zero at i, these are almost orthogonal. Therefore, integration of the equation multiplied by $\phi_{0,i}$ picks up the contribution from f and corresponds to $\partial f/\partial t = L[f]$ while the integration with $\phi_{1,i}$ corresponds to $\partial f'/\partial t = \partial L[f]/\partial x$ as in the CIP method. The prediction of the value and derivative based on the original equation is thus realized by the scalar product $\langle g|h\rangle \equiv \int_R \overline{g}(x)h(x)\mathrm{d}x$, where $\overline{g}(x)$ is the f conjugate of $g(x)$. When L is a linear operator, multiplying $\langle\phi_{k,i}|$ from the left to the equation, we obtain the matrix equation $S\mathrm{d}\mathbf{f}/\mathrm{d}t = L\mathbf{f}$, where S is a positive-definite matrix with the element $S_{ki,k'i'} = \langle\phi_{k,i}|\phi_{k',i'}\rangle$. 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 matrix representation of the operator L also has the same structure as the matrix S, and the matrix elements $\langle\phi_{k,i}|L|\phi_{k',i'}\rangle$ can be analytically calculated. The subset of the matrix equation resulting from the multiplication of $\langle\phi_{k,i}|$ corresponds to the equation $\partial f^k/\partial t = \partial^k L[f]/\partial x^k$, for example, the subset using $\langle\phi_{2,i}|$ corresponds to the equation $\partial f''/\partial t = \partial^2 L[f]/\partial x^2$, and so on for higher order ($\leqslant K$) derivatives. This procedure is equivalent to the one in the Galerkin method in which the residual $\mathrm{i}\frac{\partial f}{\partial t} - L[f]$ is required to be orthogonal to the basis functions $\phi_{k,i}$. The matrix elements of the differential operator $\langle\phi_{k,i}|D_x^l|\phi_{k',i'}\rangle$, which appear in L, can be defined properly for $l \leqslant K+2$ and using integration by parts the relation $\langle\phi_{k,i}|D_x^l|\phi_{k',i'}\rangle = (-1)^m\langle D_x^m\phi_{k,i}|D_x^{l-m}|\phi_{k',i'}\rangle$ holds for $m = 0, 1, \ldots, l$. It is worth noting that the matrix elements for $l \geqslant K+3$ are not defined, because the terms like $\theta(x)\delta'(x)$ cannot be regularized.

Writing the wavefunction as $\varphi(x,t) = \sum_{i=1}^{N}\sum_{k=0}^{K} a_i^{(k)}(t)\phi_{k,i}(x)$, where $a_i^{(k)}(t)$ is a complex number, the one-dimensional time-dependent Schrödinger equation in an external potential $V(x,t)$

$$\mathrm{i}\frac{\partial\varphi(x,t)}{\partial t} = -\frac{1}{2m}D_x^2\varphi(x,t) + V(r,t)\varphi(x,t) \tag{5}$$

is reduced to the ordinary differential equation

$$\mathrm{i}S\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{a}(t) = (H_0 + H_I(t))\mathbf{a}(t), \tag{6}$$

where atomic units ($\hbar = e = m_e = 1$) are used. In general, this procedure is used to form equations for the coefficients $f_i^{(k)}$ from the the partial differential equations for $f(x)$. Even if nonlinear terms are involved, for example $H_I = c\varphi(x,t)^2$, the structure of the matrices is same as the one for the linear equation except that the coefficients $f_i^{(k)}$ would be included. In the case of the stationary potential, the energy spectrum is obtained by setting $a_i^{(k)}(t) = \exp(-\mathrm{i}\lambda t)a_i^{(k)}$ and solving the generalized eigenvalue equation

$$(H_0 + H_I)\mathbf{a} = \lambda S\mathbf{a}. \tag{7}$$

We have applied the proposed idea to the Schrödinger equation to demonstrate its efficiency and accuracy. For simplicity we consider the one-dimensional eigenvalue problem Eq. (7) with a uniform grid. The extension to multidimensional problems or non-uniform grid systems is straightforward in a manner similar to the CIP method [7]. Furthermore, it is easy to solve the time-dependent Schrödinger equation (6) by means of either an explicit or implicit time propagation scheme [10].

For the first case, we consider the eigenvalue spectrum for the Schrödinger equation for the free electron in a box. The results are shown in Tables 1 and 2, where the box size is taken to be 1.0 a.u. As seen from the error for the number of grid points $N = 50$, the results by the CIP-BS^2 method, which includes second derivatives, are 10^5–10^6 times more accurate than those by the CIP-BS^1 method. It takes 0.069 s with a

Table 1
Relative errors of eigenvalues of the free electron and the CPU time on the Alpha EV60 processor with 833 MHz

n	Analytical	CIP-BS^1, $N = 50$	CIP-BS^1, $N = 100$	CIP-BS^2, $N = 24$	CIP-BS^2, $N = 50$
1	1.2337005501	8.54×10^{-13}	7.90×10^{-13}	1.19×10^{-13}	6.75×10^{-13}
2	11.103304951	2.31×10^{-11}	4.99×10^{-13}	1.51×10^{-14}	1.23×10^{-13}
3	30.842513753	4.92×10^{-10}	8.79×10^{-12}	2.04×10^{-14}	4.07×10^{-14}
4	60.451326957	3.68×10^{-9}	5.92×10^{-11}	3.11×10^{-14}	1.12×10^{-14}
5	99.929744561	1.64×10^{-8}	2.62×10^{-10}	7.48×10^{-13}	2.70×10^{-14}
10	445.36589860	1.33×10^{-6}	2.26×10^{-8}	1.78×10^{-10}	1.33×10^{-12}
15	103.75421627	1.45×10^{-5}	2.75×10^{-7}	1.77×10^{-7}	1.04×10^{-10}
CPU (s)		0.024	0.149	0.015	0.069

The box size = 1.0 a.u. and N is the number of grid points. The boundary condition for the wavefunction is zero at $r = 0$ a.u., and zero derivative at $r = 1.0$ a.u.

Table 2
Same as Table 1. The boundary condition for the wavefunction is zero at $r = 1.0$ a.u

No.	Analytical	CIP-BS^1, $N = 50$	CIP-BS^1, $N = 100$	CIP-BS^2, $N = 25$	CIP-BS^2, $N = 50$
1	4.9348022005	2.83×10^{-12}	1.63×10^{-12}	1.79×10^{-13}	1.47×10^{-13}
2	19.739208802	1.30×10^{-10}	2.71×10^{-12}	3.73×10^{-14}	1.04×10^{-13}
3	44.413219805	1.46×10^{-9}	2.39×10^{-11}	1.10×10^{-14}	2.35×10^{-13}
4	78.956835209	8.15×10^{-9}	1.30×10^{-10}	2.19×10^{-13}	3.26×10^{-14}
5	123.37005501	3.07×10^{-8}	4.93×10^{-10}	2.22×10^{-12}	2.53×10^{-14}
10	493.48022005	1.78×10^{-6}	3.07×10^{-8}	3.03×10^{-9}	2.31×10^{-12}
15	111.03304951	1.75×10^{-5}	3.35×10^{-7}	2.50×10^{-7}	1.47×10^{-10}
CPU (s)		0.024	0.149	0.015	0.069

single CPU of the Alphaserver ES40 for the $N = 50$ grid point case of the CIP-BS^2 method. We can see from Tables 1 and 2 that the CPU times approximately proportional to the number of matrix elements, i.e. $((K+1)N)^2$, when the routine DSYGV of the LAPACK library is used to solve the generalized eigenvalue problem. The zero derivative boundary condition at grid point N is built in by setting $a_N^1 = 0$ (i.e., $\varphi'(r_N) = 0$). In the same way setting the boundary to zero is done by setting $a_N^0 = 0$ (i.e., $\varphi(0) = 0$). Since the derivatives are included in the state vector **a**, incorporation of the boundary conditions can be achieved keeping a one-to-one correspondence to the analytical ones. Periodic or other types of boundary conditions can also be treated in the same manner. Although we use basis functions that do not satisfy boundary conditions, it is not necessary to add a Bloch operator to the Hamiltonian as in the discrete variable representation (DVR) method [3]. The numerical results in Tables 1 and 2 indicate good agreement with the exact values.

For the second case, we consider the eigenvalue spectrum for the radial Schrödinger equation of the hydrogen atom. The system size is set to 1000 a.u. in order to obtain sufficient precision for states with a high principal quantum number n. In Table 3, we present the results of energy levels for s-, p-, and d-orbitals. Here the grid interval is 1 a.u. and the boundary condition $\varphi(0) = \varphi(r_N) = 0$ is imposed for this eigenvalue problem. We can see that the eigenvectors simultaneously contain derivatives consistent with the eigenfunctions from samples of the calculated orbitals shown in Fig. 1. The results show excellent agreement with the analytical spectrum. It should be emphasized that the singularities due to the kinetic operator $(1/r^2)$ and the Coulomb potential $(1/r)$ at $r = 0$ are eliminated in the Hamiltonian by taking the scalar product.

Table 3
Relative errors of energy levels of bound states of the hydrogen atom with the CIP-BS^2 method

n	Analytical	$l = 0$	$l = 1$	$l = 2$
1	$-5.0000000000 \times 10^{-1}$	8.21×10^{-9}		
2	$-1.2500000000 \times 10^{-1}$	2.77×10^{-10}	8.16×10^{-11}	
3	$-5.5555555556 \times 10^{-2}$	7.34×10^{-11}	3.10×10^{-11}	1.40×10^{-12}
4	$-3.1250000000 \times 10^{-2}$	3.88×10^{-11}	1.48×10^{-11}	3.63×10^{-13}
5	$-2.0000000000 \times 10^{-2}$	2.37×10^{-11}	3.12×10^{-11}	6.25×10^{-12}
8	$-7.8125000000 \times 10^{-3}$	4.09×10^{-12}	2.84×10^{-12}	1.32×10^{-12}
10	$-5.0000000000 \times 10^{-3}$	2.17×10^{-12}	3.14×10^{-12}	7.90×10^{-12}
15	$-2.2222222222 \times 10^{-3}$	1.11×10^{-11}	1.49×10^{-11}	5.34×10^{-12}
17	$-1.7301038062 \times 10^{-3}$	7.61×10^{-12}	2.53×10^{-12}	3.48×10^{-12}

The system size is 1000.0 a.u. and the grid interval is 1.0 a.u. The boundary condition for the wavefunction is zero at $r = 0$ and $r = 1000.0$ a.u.

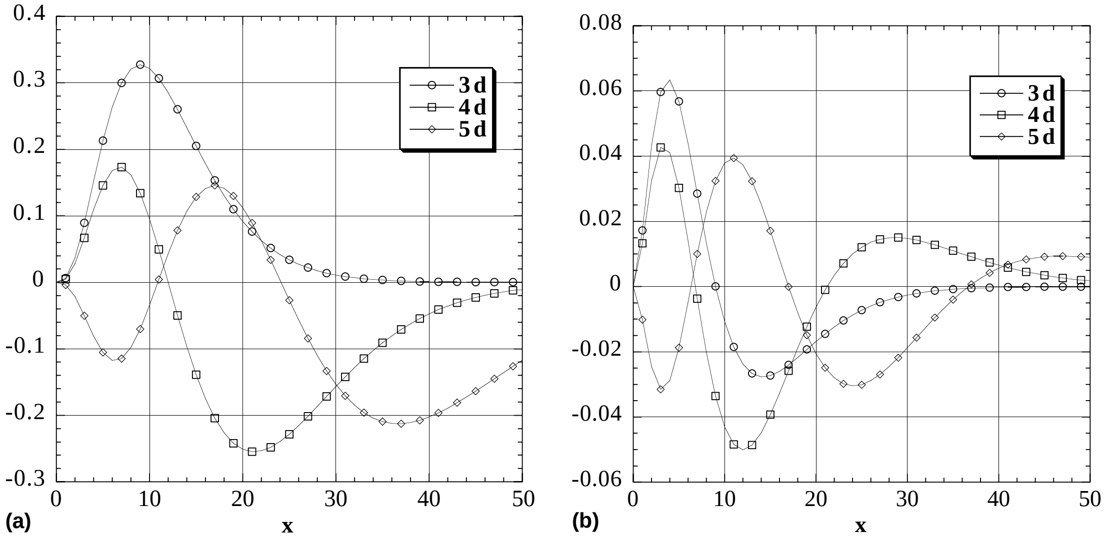

Fig. 1. The calculated (a) eigenfunctions and (b) their first derivatives for the 3d, 4d, 5d orbitals of the hydrogen atom. They are not normalized or interpolated.

For the third case, we consider the eigenvalue spectrum for the Schrödinger equation in the Morse potential, $V(x) = D[(e^{-2\alpha x} - 2e^{-\alpha x}) + 1]$, which accurately describes the vibrations of a two-atom molecule. Using the variable $z = \frac{2\gamma}{\alpha} e^{-\alpha x}$, where $\gamma = (2mD)^{1/2}$, the equation turns out to be a confluent hypergeometric equation so that the complete solution becomes [11]

$$\varphi(z) = z^{\beta/\alpha} e^{-z/2} \{C_1 M(a, b, z) + C_2 U(a, b, z)\}, \tag{8}$$

where $\beta = (2m(D - E))^{1/2}$, $c = \frac{2\beta}{\alpha} + 1$, $a = \frac{c}{2} - \frac{\gamma}{\alpha}$, $M(a, b, z)$ and $U(a, b, z)$ are Kummer's functions, m is the reduced mass, and E is the energy of the system. For the bound state, the constant C_2 must vanish, the constant C_1 is fixed by the normalization, and the eigenenergy must be determined from the relation $a = -n$, where n is a non-negative integer which satisfies $0 < E < D$. The results are shown in Table 4,

Table 4
Relative errors of energy levels of bound states in the Morse potential with the CIP-BS^2 method for different grid numbers N

n	Analytical	$N = 80$	$N = 100$	$N = 140$	Braun et al.[a]	Wei et al.[b]
0	$2.8617197881\times10^{-4}$	9.53×10^{-14}	6.95×10^{-14}	1.73×10^{-13}		
1	$8.5299662358\times10^{-4}$	7.07×10^{-13}	1.10×10^{-13}	4.56×10^{-14}	1.18×10^{-8}	1.64×10^{-11}
2	$1.4124621846\times10^{-3}$	2.77×10^{-12}	3.41×10^{-13}	2.09×10^{-14}	2.13×10^{-8}	3.05×10^{-11}
3	$1.9645686617\times10^{-3}$	8.58×10^{-12}	8.39×10^{-13}	6.20×10^{-14}	2.55×10^{-8}	3.57×10^{-11}
4	$2.5093160551\times10^{-3}$	2.24×10^{-11}	2.18×10^{-12}	5.93×10^{-14}	2.80×10^{-8}	3.92×10^{-11}
5	$3.0467043647\times10^{-3}$	5.08×10^{-11}	4.94×10^{-12}	1.71×10^{-13}	2.90×10^{-8}	4.28×10^{-11}
6	$3.5767335905\times10^{-3}$	1.95×10^{-10}	1.00×10^{-11}	3.08×10^{-13}	3.08×10^{-8}	4.20×10^{-11}
11	$6.1164934624\times10^{-3}$	1.35×10^{-9}	1.24×10^{-10}	3.71×10^{-12}	3.27×10^{-8}	4.58×10^{-11}
16	$8.4722762394\times10^{-3}$	6.19×10^{-9}	6.15×10^{-10}	1.81×10^{-11}	3.31×10^{-8}	4.77×10^{-11}
20	$1.0224438953\times10^{-3}$	1.79×10^{-8}	1.58×10^{-9}	4.45×10^{-11}	3.39×10^{-8}	2.83×10^{-11}

The boundary condition for the wavefunction is zero at $r = -0.8$ and $r = 2.0$ a.u. *Note*. Errors of $N = 80$ are same as those of $N = 100$ for $n \leqslant 6$.

[a] Ref. [1] ($N = 128$).

[b] Ref. [2] ($N = 100$).

where the parameters are $\alpha = 0.9374$ a.u., $D = 0.0224$ a.u., $m = 119406$ a.u., and $-0.8 \leqslant x \leqslant 2.0$. These parameters are chosen to compare our results with those by Braun et al. [1] who used the block-Lanczos method with the Chebyshev approximation and Wei et al. [2] who used Lagrange Distributed Approximating Functionals (LDAFs). The boundary condition for the wavefunction is zero at $r = -0.8$ and $r = 2.0$ a.u. As seen from the error, our $N = 80$ and $N = 100$ grid point results are 10^4–10^5 times more accurate than those of Braun et al., and 5–100 times more accurate than those of Wei et al. for the lower-lying eigenstates ($n \leqslant 3$). The high eigenvalues can be improved by enlarging the system size, and/or increasing the density of grid points, as shown in our $N = 140$ grid point results in Table 4. Although these dispositions induce the increase of the number of states ($(K + 1)$ per grid point), the computational time does not increase so rapidly due to the inherent locality of the CIP-BS method (narrower bandwidth than LDAFs).

While the CIP method has provided accurate solutions for various differential equations, especially for hydrodynamics, the CIP-BS method is more attractive for the analysis of quantum mechanical processes. The CIP-BS method, which is the reconstruction of the CIP method from the view point of the basis function of the Hermite type interpolating functions, has incorporated the two important properties in the CIP method: (i) Any variable inside the grid cell is approximated not only by values but also the derivatives consistent with the governing equations. (ii) Interpolating functions are uniquely determined without problem- or algorithm-specific parameters. The system size and grid intervals are essentially inevitable parameters to be adjusted. The CIP-BS method offers additional advantages as follows: (i) It is easily extended to higher order polynomials or to other functions with any desired accuracy by simply adopting the higher-order derivatives of the original equations as constraints to generate a self-consistent subgrid profile. (We have shown the use of higher-order basis set is essential to increase the accuracy.) (ii) It leads to band diagonal matrices, which are easily adapted to a number of numerical methods developed for large, sparse linear systems [10], by transforming the Schrödinger equation. If the system is linear and contains only time-independent interactions, all the relevant matrices are constant and the time propagation of the wavefunction is carried out in a computationally efficient way (low CPU cost and reduced storage). (iii) The boundary conditions are imposed in a simple manner with a one-to-one correspondence to the analytical ones for not only the Dirichlet boundary conditions but also the Neumann boundary conditions. (iv) It provides a proper means to relieve numerical difficulties due to singularities, e.g., Coulomb potential. (v) Although our basis set is non-orthogonal and contains distribution functions, it introduces a close resemblance between quantum mechanics and numerical simulations. (vi) It is straightforwardly extended for solving various linear and nonlinear partial differential equations in the study of the dynamics of a broad spectrum of complex physical processes.

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