Algorithm 986: A Suite of Compact Finite Difference Schemes

MANI MEHRA and KULDIP SINGH PATEL, Indian Institute of Technology Delhi

A collection of Matlab routines that compute derivative approximations of arbitrary functions using high-order compact finite difference schemes is presented. Tenth-order accurate compact finite difference schemes for first and second derivative approximations and sixth-order accurate compact finite difference schemes for third and fourth derivative approximations are discussed for the functions with periodic boundary conditions. Fourier analysis of compact finite difference schemes is explained, and it is observed that compact finite difference schemes have better resolution characteristics when compared to classical finite difference schemes. Compact finite difference schemes for the functions with Dirichlet and Neumann boundary conditions are also discussed. Moreover, compact finite difference schemes for partial derivative approximations of functions in two variables are also given. For each case a Matlab routine is provided to compute the differentiation matrix and results are validated using the test functions.

CCS Concepts: • **Mathematics of computing** → **Numerical differentiation**; **Partial differential equations**;

Additional Key Words and Phrases: Compact finite difference schemes, numerical differentiation, Taylor series expansion, Fourier analysis

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1 INTRODUCTION

High-order compact finite difference schemes in which the value of the function and its first or higher derivatives are considered as unknowns at each discretization point are discussed in this article. High-order compact finite difference schemes have been extensively studied and widely used to compute problems involving incompressible, compressible, and hypersonic flows (Meitz and Fasel 2000; Weinan and Liu 1996), computational aeroacoustic (Cheong and Lee 2001; Sengupta et al. 2003), and several other practical applications (During and Fournie 2012; During et al. 2004; Shang 1999). High-order compact schemes are implicit in nature and provide high-order accuracy for the same number of grid points as compared to classical finite difference schemes. Widening of the computational stencil for high-order approximation in finite difference is one of the major disadvantages. Fortunately, it is possible to derive high-order finite difference approximations

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Authors' addresses: M. Mehra and K. S. Patel, Indian Institute of Technology Delhi, Hauz Khas, New Delhi-110016; emails: {mmehra, kuldip}@maths.iitd.ac.in.

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with compact stencils (commonly known as compact finite difference approximations) at the expense of a small complication in their evaluation. High-order compact finite difference schemes give high-order accuracy and better resolution characteristics as compared to classical finite difference schemes for the same number of grid points. This feature brings them closer to the spectral methods while the freedom in choosing the mesh geometry and the boundary conditions (as in finite difference schemes) is maintained.

There exist various approaches in the literature to derive compact finite difference schemes for derivative approximations. Adam (1975) presented highly accurate difference schemes for the solution of evolution equations of parabolic type. In that same year, Hirsh (1975) discussed higher-order accurate solutions of fluid mechanics problems by a compact finite difference schemes. Two methods based on compact scheme are presented by Adam (1977) to eliminate the second-order derivatives in parabolic equations while keeping the fourth-order accuracy and the tridiagonal nature of the schemes. In Adam (1977), a high-order accurate additional boundary condition is also proposed, which is consistent with the high accuracy of the inner scheme. A fourth-order non-uniform combined compact finite difference scheme using truncated Taylor series is discussed by Geodheer and Potters (1985) and is used by them to solve a model transport problem in one dimension. Lele (1992) discussed various-order compact finite difference approximations for first and second derivatives. Here, an extensive study of high-order compact finite difference schemes using Fourier analysis is discussed, and it is shown that compact finite difference schemes have better resolution characteristics when compared to classical finite difference schemes. Furthermore, compact finite difference schemes are also extended for the third and fourth derivative approximations. Mahesh (1998) discussed combined high-order compact finite difference schemes that evaluate both the first and the second derivatives simultaneously. Chu and Fan (1998) presented sixth-order and eighth-order three-point combined compact finite difference schemes on a uniform grid. Chu and Fan (1998) extended their scheme to a non-uniform grid in Chu and Fan (1999). Compact finite difference approximations for first and second derivatives on a non-uniform grid using method of undetermined coefficient is discussed in Gamet et al. (1999). A fourth-order, nine-point uniform grid compact scheme along with the coordinate transformation from a non-uniform to a uniform grid is used to solve a two-dimensional steady state convection-diffusion equation by Ge and Zhang (2001). Kumar (2009) discussed a high-order compact finite difference scheme for singularly perturbed reaction-diffusion problems on a new mesh of Shishkin type. Polynomial interpolation has also been used to derive an arbitrarily high-order compact finite difference method for the first and second derivatives on non-uniform grids (Shukla et al. 2007; Shukla and Zhong 2005). The same order of accuracy is obtained at interior points as well as at boundary points using polynomial interpolation. However, these compact finite difference schemes are not asymptotically stable on uniform grid. Recently, Sen (2013, 2016) discussed a new family of compact finite difference schemes applicable for unsteady Navier-Stokes equations. In Sen (2016), fourth-order accurate compact finite difference schemes for variable coefficient parabolic problems with mixed derivatives are discussed.

In this article, high-order compact finite difference schemes are discussed that incorporate all types of boundary conditions (periodic, Dirichlet, and Neumann). These are extended to the two-dimensional case for Dirichlet and Neumann boundary conditions. Fourier analysis is discussed, and it is shown that compact schemes have better resolution characteristics when compared to classical finite difference schemes. A uniform grid is assumed throughout the article.

The outline of the article is as follows. In Section 2, high-order compact finite difference schemes for periodic boundary conditions are discussed. High-order compact finite difference schemes for Dirichlet boundary conditions are discussed in Section 3. High-order compact finite difference schemes with Neumann boundary conditions are discussed in Section 4. Our software consists of 23 Matlab functions, which are described in an electronic appendix.

2 HIGH-ORDER COMPACT FINITE DIFFERENCE SCHEMES FOR PERIODIC BOUNDARY CONDITIONS

In this section, high-order compact finite difference schemes are discussed for the functions that are periodic in the independent variable.

2.1 High-Order Compact Finite Difference Schemes in One Dimension with Periodic Boundary Conditions

High-order compact finite difference approximations for first, second, third, and fourth derivatives are discussed in this section. It is shown that up to 10th-order accurate compact approximations for first and second derivatives and up to 6th-order accurate compact approximations for third and fourth derivatives can be obtained by solving systems of linear equations. We use uniform step size $h = \frac{x_{max}-x_{min}}{N}$ and grid point $x_i = x_{min} + h(i-1), \quad 1 \le i \le N+1$. In the case of function of one variable, the differentiation matrix will be of order N.

2.1.1 Approximation of the First Derivative. If $f_i = f(x_i)$ and f'_i represents the first derivative of $f(x)$ at x_i, then an approximation of first derivative may be written as

$$Bf'_{i-2} + Af'_{i-1} + f'_i + Af'_{i+1} + Bf'_{i+2} = a_1 \frac{f_{i+1} - f_{i-1}}{2h} + a_2 \frac{f_{i+2} - f_{i-2}}{4h} + a_3 \frac{f_{i+3} - f_{i-3}}{6h}, \tag{1}$$

where A, B, a_1, a_2, and a_3 are constants to be determined. To compute the constants, the first unmatched coefficients of Taylor series expansion are used to determine the formal truncation error. By doing so, we obtain

$$\text{2nd order} : a_1 + a_2 + a_3 = 2A + 2B + 1, \tag{2}$$

$$\text{4th order} : a_1 + 2^2 a_2 + 3^2 a_3 = 2\frac{3!}{2!}(2^2 B + A), \tag{3}$$

$$\text{6th order} : a_1 + 2^4 a_2 + 3^4 a_3 = 2\frac{5!}{4!}(2^4 B + A), \tag{4}$$

$$\text{8th order} : a_1 + 2^6 a_2 + 3^6 a_3 = 2\frac{7!}{6!}(2^6 B + A), \tag{5}$$

$$\text{10th order} : a_1 + 2^8 a_2 + 3^8 a_3 = 2\frac{9!}{8!}(2^8 B + A). \tag{6}$$

The preceding equations are solved to obtain up to 10th-order accurate compact finite difference schemes for the first derivative. Using (1), compact finite difference approximation for the first derivative can be written as

$$H_1 \mathbf{f}' = H_2 \mathbf{f}, \tag{7}$$

where $\mathbf{f}' = (f'_1, f'_2, \ldots, f'_N)^T$ and $\mathbf{f} = (f_1, f_2, \ldots, f_N)^T$. From (7), we get

$$\mathbf{f}' = D_x^{p,1} \mathbf{f}, \tag{8}$$

where $D_x^{p,1}$ is the desired differentiation matrix corresponding to the first derivative approximation. From 1, we have

$$H_1 = \begin{pmatrix} 1 & A & B & 0 & 0 & 0 & 0 & \dots & 0 & 0 & 0 & 0 & 0 & B & A \\ A & 1 & A & B & 0 & 0 & 0 & \dots & 0 & 0 & 0 & 0 & 0 & 0 & B \\ B & A & 1 & A & B & 0 & 0 & \dots & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & B & A & 1 & A & B & 0 & \dots & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \hdotsfor{15} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \dots & 0 & B & A & 1 & A & B & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \dots & 0 & 0 & B & A & 1 & A & B \\ B & 0 & 0 & 0 & 0 & 0 & 0 & \dots & 0 & 0 & 0 & B & A & 1 & A \\ A & B & 0 & 0 & 0 & 0 & 0 & \dots & 0 & 0 & 0 & 0 & B & A & 1 \end{pmatrix}, \tag{9}$$

$$H_2 = \begin{pmatrix} 0 & a_1' & a_2' & a_3' & 0 & 0 & 0 & 0 & \dots & 0 & 0 & 0 & 0 & 0 & -a_3' & -a_2' & -a_1' \\ -a_1' & 0 & a_1' & a_2' & a_3' & 0 & 0 & 0 & \dots & 0 & 0 & 0 & 0 & 0 & 0 & -a_3' & -a_2' \\ -a_2' & -a_1' & 0 & a_1' & a_2' & a_3' & 0 & 0 & \dots & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -a_3' \\ -a_3' & -a_2' & -a_1' & 0 & a_1' & a_2' & a_3' & 0 & \dots & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -a_3' & -a_2' & -a_1' & 0 & a_1' & a_2' & a_3' & \dots & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \hdotsfor{17} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \dots & -a_3' & -a_2' & -a_1' & 0 & a_1' & a_2' & a_3' & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \dots & 0 & -a_3' & -a_2' & -a_1' & 0 & a_1' & a_2' & a_3' \\ a_3' & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \dots & 0 & 0 & -a_3' & -a_2' & -a_1' & 0 & a_1' & a_2' \\ a_2' & a_3' & 0 & 0 & 0 & 0 & 0 & 0 & \dots & 0 & 0 & 0 & -a_3' & -a_2' & -a_1' & 0 & a_1' \\ a_1' & a_2' & a_3' & 0 & 0 & 0 & 0 & 0 & \dots & 0 & 0 & 0 & 0 & -a_3' & -a_2' & -a_1' & 0 \end{pmatrix}, \tag{10}$$

where $a_1' = \frac{a_1}{2h}$, $a_2' = \frac{a_2}{4h}$, and $a_3' = \frac{a_3}{6h}$ and a_1, a_2, a_3, A, and B are obtained from (2) through (6). We now discuss compact schemes with 4th-, 6th-, 8th-, and 10th-order accuracy for approximating first derivatives.

Fourth-order accurate compact approximation: For fourth-order accurate compact finite difference schemes, solving (2) and (3) gives $A = \frac{1}{4}$, $B = 0$, $a_3 = 0$, $a_2 = 0$, and $a_1 = \frac{3}{2}$ and (1) becomes

$$\frac{1}{4} f_{i-1}' + f_i' + \frac{1}{4} f_{i+1}' = \frac{3}{2} \frac{f_{i+1} - f_{i-1}}{2h}, \quad 1 \le i \le N.$$

Substituting these values into H_1 and H_2, given in (9) and (10), allows the formation of the required differentiation matrix $D_x^{p,1}$.

Sixth-order accurate compact approximation: For a sixth-order accurate compact finite difference scheme, solving (2) through (4) gives $A = \frac{1}{3}$, $B = 0$, $a_3 = 0$, $a_2 = \frac{1}{9}$, and $a_1 = \frac{14}{9}$ and (1) becomes

$$\frac{1}{3} f_{i-1}' + f_i' + \frac{1}{3} f_{i+1}' = \frac{14}{9} \frac{f_{i+1} - f_{i-1}}{2h} + \frac{1}{9} \frac{f_{i+2} - f_{i-2}}{4h}, \quad 1 \le i \le N.$$

Substituting these values into H_1 and H_2, given in (9) and (10), allows the formation of the required differentiation matrix $D_x^{p,1}$.

Eighth-order accurate compact approximation: For an eighth-order accurate compact finite difference scheme, solving (2) through (5) gives $A = \frac{4}{9}$, $B = \frac{1}{36}$, $a_3 = 0$, $a_2 = \frac{25}{54}$, and $a_1 = \frac{40}{27}$ and (1) becomes

$$\frac{1}{36} f_{i-2}' + \frac{4}{9} f_{i-1}' + f_i' + \frac{4}{9} f_{i+1}' + \frac{1}{36} f_{i+2}' = \frac{40}{27} \frac{f_{i+1} - f_{i-1}}{2h} + \frac{25}{54} \frac{f_{i+2} - f_{i-2}}{4h}, \quad 1 \le i \le N.$$

Substituting these values into H_1 and H_2, given in (9) and (10), allows the formation of the required differentiation matrix $D_x^{p,1}$.

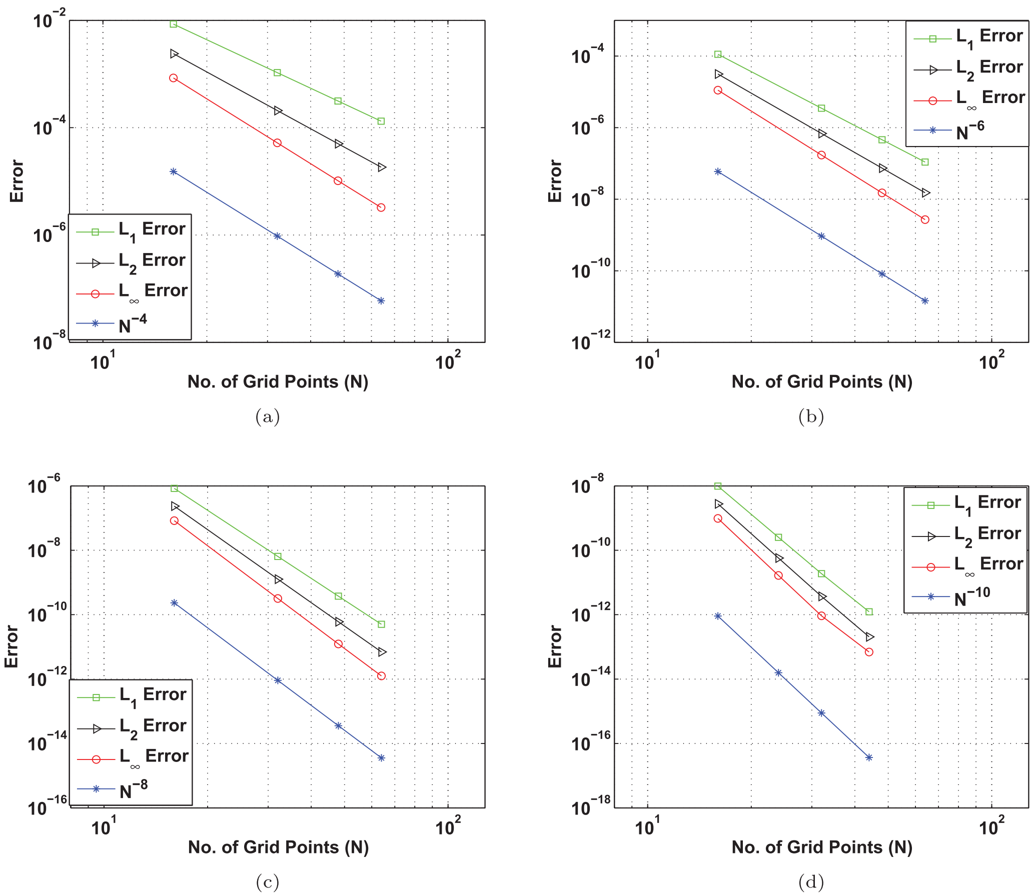


Fig. 1. First derivative approximations of $sin(2\pi x)$ on $[0, 1]$ using 4th-order accurate compact approximation (a), 6th-order accurate compact approximation (b), 8th-order accurate compact approximation (c), and 10th-order accurate compact approximation (d).

Tenth-order accurate compact approximation: For a 10th-order accurate compact finite difference scheme, solving (2) through (6) gives $A = \frac{1}{2}$, $B = \frac{1}{20}$, $a_3 = \frac{1}{100}$, $a_2 = \frac{101}{150}$, and $a_1 = \frac{17}{12}$ and (1) becomes

$$\frac{1}{20}f'_{i-2} + \frac{1}{2}f'_{i-1} + f'_i + \frac{1}{2}f'_{i+1} + \frac{1}{20}f'_{i+2} = \frac{17}{12}\frac{f_{i+1} - f_{i-1}}{2h} + \frac{101}{150}\frac{f_{i+2} - f_{i-2}}{4h} + \frac{1}{100}\frac{f_{i+3} - f_{i-3}}{6h}, \quad 1 \le i \le N.$$

Substituting these values into H_1 and H_2, given in (9) and (10), allows the formation of the required differentiation matrix $D_x^{p,1}$.

The preceding results were validated using the test function $f(x) = sin(2\pi x)$ on the interval $[0, 1]$. Error norms of the difference between the exact differential and the compact approximation were calculated and plotted in Figure 1. These confirm the order of accuracy of the various schemes. The function `compact_first_periodic.m` computes $D_x^{p,1}$ (see Section 1 in the accompanying User Manual for details).

Remark 1. By using (1), the most accurate compact schemes that we can obtain are 10th order. However, we can extend these schemes to higher order by increasing the stencil size on the left- and right-hand sides of (1).

2.1.2 Approximation of the Second Derivative. In this section, high-order compact finite difference approximations for second derivatives are discussed, and it is shown that up to 10th-order accurate compact approximations can be obtained. If f_i'' represents the second derivative of the function $f(x)$ at x_i, then an approximation of the second derivative may be written as

$$Bf_{i-2}'' + Af_{i-1}'' + f_i'' + Af_{i+1}'' + Bf_{i+2}'' = a_1\frac{f_{i+1} - 2f_i + f_{i-1}}{h^2} + a_2\frac{f_{i+2} - 2f_i + f_{i-2}}{4h^2} + a_3\frac{f_{i+3} - 2f_i + f_{i-3}}{9h^2}. \tag{11}$$

To compute the coefficients, we first use unmatched coefficients to determine the formal truncation error, giving

$$\text{2nd order}: a_1 + a_2 + a_3 = 2A + 2B + 1, \tag{12}$$

$$\text{4th order}: a_1 + 2^2a_2 + 3^2a_3 = \frac{4!}{2!}(2^2B + A), \tag{13}$$

$$\text{6th order}: a_1 + 2^4a_2 + 3^4a_3 = \frac{6!}{4!}(2^4B + A), \tag{14}$$

$$\text{8th order}: a_1 + 2^6a_2 + 3^6a_3 = \frac{8!}{6!}(2^6B + A), \tag{15}$$

$$\text{10th order}: a_1 + 2^8a_2 + 3^8a_3 = \frac{10!}{8!}(2^8B + A). \tag{16}$$

Using (11), a compact finite difference scheme for second derivatives may be written as

$$H_1\mathbf{f}'' = H_2\mathbf{f}, \tag{17}$$

where $\mathbf{f}'' = (f_1'', f_2'', \ldots, f_N'')^T$. From (17), we get

$$\mathbf{f}'' = D_{xx}^{p,1}\mathbf{f}, \tag{18}$$

where $D_{xx}^{p,1}$ is the desired differentiation matrix corresponding to the second derivative approximation. From 11, we have

$$H_1 = \begin{pmatrix} 1 & A & B & 0 & 0 & 0 & 0 & \ldots & 0 & 0 & 0 & 0 & 0 & B & A \\ A & 1 & A & B & 0 & 0 & 0 & \ldots & 0 & 0 & 0 & 0 & 0 & 0 & B \\ B & A & 1 & A & B & 0 & 0 & \ldots & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & B & A & 1 & A & B & 0 & \ldots & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \ldots & 0 & B & A & 1 & A & B & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \ldots & 0 & 0 & B & A & 1 & A & B \\ B & 0 & 0 & 0 & 0 & 0 & 0 & \ldots & 0 & 0 & 0 & B & A & 1 & A \\ A & B & 0 & 0 & 0 & 0 & 0 & \ldots & 0 & 0 & 0 & 0 & B & A & 1 \end{pmatrix}, \tag{19}$$

$$H_2 = \begin{pmatrix}
-2s' & a_1' & a_2' & a_3' & 0 & 0 & 0 & 0 & \dots & 0 & 0 & 0 & 0 & 0 & -a_3' & -a_2' & -a_1' \\
-a_1' & -2s' & a_1' & a_2' & a_3' & 0 & 0 & 0 & \dots & 0 & 0 & 0 & 0 & 0 & 0 & -a_3' & -a_2' \\
-a_2' & -a_1' & -2s' & a_1' & a_2' & a_3' & 0 & 0 & \dots & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -a_3' \\
-a_3' & -a_2' & -a_1' & -2s' & a_1' & a_2' & a_3' & 0 & \dots & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & -a_3' & -a_2' & -a_1' & -2s' & a_1' & a_2' & a_3' & \dots & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\hdotsfor{17} \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \dots & -a_3' & -a_2' & -a_1' & -2s' & a_1' & a_2' & a_3' & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \dots & 0 & -a_3' & -a_2' & -a_1' & -2s' & a_1' & a_2' & a_3' \\
a_3' & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \dots & 0 & 0 & -a_3' & -a_2' & -a_1' & -2s' & a_1' & a_2' \\
a_2' & a_3' & 0 & 0 & 0 & 0 & 0 & 0 & \dots & 0 & 0 & 0 & -a_3' & -a_2' & -a_1' & -2s' & a_1' \\
a_1' & a_2' & a_3' & 0 & 0 & 0 & 0 & 0 & \dots & 0 & 0 & 0 & 0 & -a_3' & -a_2' & -a_1' & -2s'
\end{pmatrix}, \tag{20}$$

where $a_1' = \frac{a_1}{h^2}$, $a_2' = \frac{a_2}{4h^2}$, $a_3' = \frac{a_3}{9h^2}$, and $s' = a_1' + a_2' + a_3'$. We now discuss compact schemes of 4th-, 6th-, 8th-, and 10th-order accuracy for the second derivative.

Fourth-order accurate compact approximation: For a fourth-order accurate compact finite difference scheme, solving (12) and (13) gives $A = \frac{1}{10}$, $B = 0$, $a_3 = 0$, $a_2 = 0$, and $a_1 = \frac{6}{5}$ and (11) becomes

$$\frac{1}{10} f''_{i-1} + f''_i + \frac{1}{10} f''_{i+1} = \frac{6}{5} \frac{f_{i+1} - 2f_i + f_{i-1}}{h^2}, \quad 1 \le i \le N.$$

Substituting these values into H_1 and H_2, given in (19) and (20), allows the formation of the required differentiation matrix $D_{xx}^{p,1}$.

Sixth-order accurate compact approximation: For a sixth-order accurate compact finite difference scheme, solving (12) through (14) gives $A = \frac{2}{11}$, $B = 0$, $a_3 = 0$, $a_2 = \frac{3}{11}$, and $a_1 = \frac{12}{11}$ and (11) becomes

$$\frac{2}{11} f''_{i-1} + f''_i + \frac{2}{11} f''_{i+1} = \frac{12}{11} \frac{f_{i+1} - 2f_i + f_{i-1}}{h^2} + \frac{3}{11} \frac{f_{i+2} - 2f_i + f_{i-2}}{4h^2}, \quad 1 \le i \le N.$$

Substituting these values into H_1 and H_2, given in (19) and (20), allows the formation of the required differentiation matrix $D_{xx}^{p,1}$.

Eighth-order accurate compact approximation: For an eighth-order accurate compact finite difference scheme, solving (12) through (15) gives $A = \frac{344}{1179}$, $B = \frac{2461}{252306}$, $a_3 = 0$, $a_2 = \frac{498238}{630765}$, and $a_1 = \frac{414417}{505791}$ and (11) becomes

$$\begin{aligned}\frac{2461}{252306} f''_{i-2} + \frac{344}{1179} f''_{i-1} + f''_i + \frac{344}{1179} f''_{i+1} + \frac{2461}{252306} f''_{i+2} = {} & \frac{414417}{505791} \frac{f_{i+1} - 2f_i + f_{i-1}}{h^2} \\ & + \frac{498238}{630765} \frac{f_{i+2} - 2f_i + f_{i-2}}{4h^2}, \\ & 1 \le i \le N.\end{aligned}$$

Substituting these values into H_1 and H_2, given in (19) and (20), allows the formation of the required differentiation matrix $D_{xx}^{p,1}$.

Tenth-order accurate compact approximation: For a 10th-order accurate compact finite difference scheme, solving (12) through (16) gives $A = \frac{334}{899}$, $B = \frac{43}{1798}$, $a_3 = \frac{79}{1798}$, $a_2 = \frac{1038}{899}$,

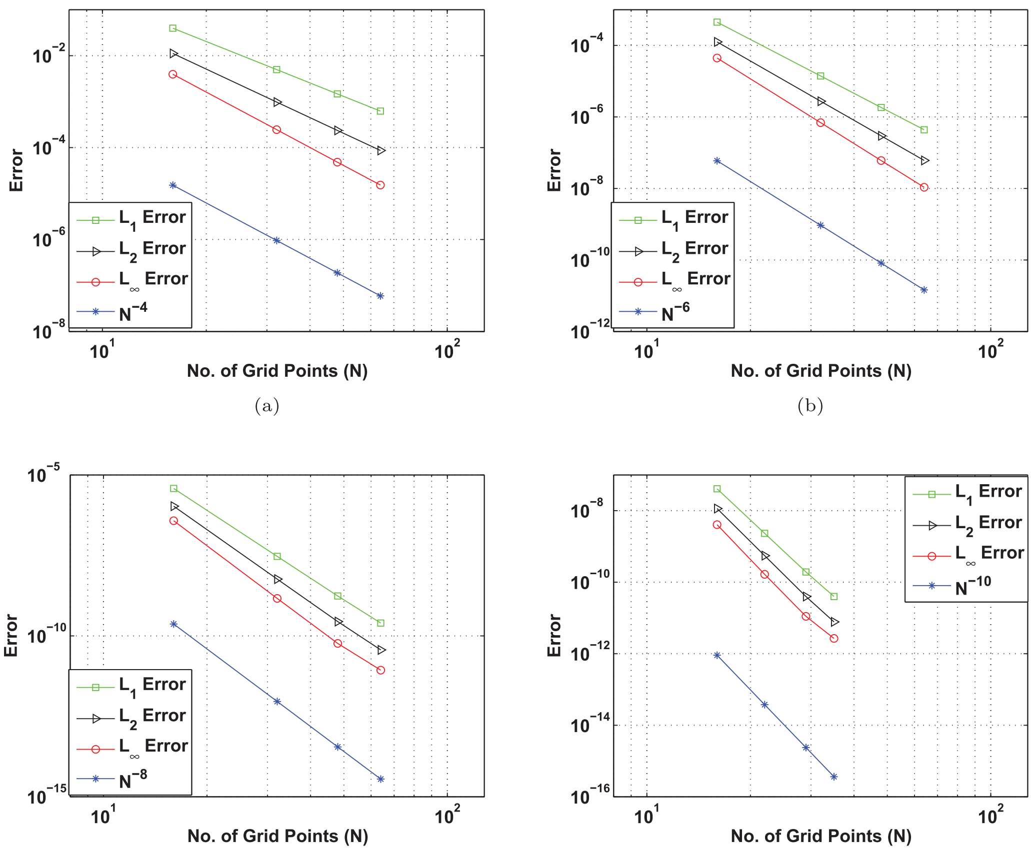


Fig. 2. Second derivative approximations of $sin(2\pi x)$ on $[0, 1]$ using 4th-order accurate compact approximation (a), 6th-order accurate compact approximation (b), 8th-order accurate compact approximation (c), and 10th-order accurate compact approximation (d).

and $a_1 = \frac{1065}{1798}$ and (11) becomes

$$\frac{43}{1798} f''_{i-2} + \frac{334}{899} f''_{i-1} + f''_i + \frac{334}{899} f''_{i+1} + \frac{43}{1798} f''_{i+2} = \frac{1065}{1798} \frac{f_{i+1} - 2f_i + f_{i-1}}{h^2} + \frac{1038}{899} \frac{f_{i+2} - 2f_i + f_{i-2}}{4h^2} + \frac{79}{1798} \frac{f_{i+3} - 2f_i + f_{i-3}}{9h^2}, \quad 1 \leq i \leq N.$$

Substituting these values into H_1 and H_2, given in (19) and (20), allows the formation of the required differentiation matrix $D_{xx}^{p,1}$.

The preceding results were validated using the test function $f(x) = sin(2\pi x)$ on the interval $[0, 1]$. Error plots given in Figure 2 confirm the order of accuracy of the schemes. The function `compact_second_periodic.m` computes $D_{xx}^{p,1}$ (see Section 2 of the accompanying User Manual for details).

2.1.3 *Approximation of the Third Derivative.* High-order compact finite difference approximations for the third derivative are discussed in this section, and we show that up to sixth-order accurate compact schemes for third derivatives may be obtained in a similar manner. Let f_i''' denotes the third derivative of the function f at grid points x_i, then approximation of the third derivative may be written as

$$Af_{i-1}''' + f_i''' + Af_{i+1}''' = a_1 \frac{f_{i+2} - 2f_{i+1} + 2f_{i-1} - f_{i-2}}{2h^3} + a_2 \frac{f_{i+3} - 3f_{i+1} + 3f_{i-1} - f_{i-3}}{8h^3}, \tag{21}$$

where A, a_1, and a_2 are constants to be determined. To compute the constants, the first unmatched coefficients of Taylor series expansion are used to determine the formal truncation error. Using (21), compact finite difference approximation for the third derivative may be written as

$$H_1 \mathbf{f}''' = H_2 \mathbf{f}, \tag{22}$$

where $\mathbf{f}''' = (f_1''', f_2''', \ldots, f_N''')^T$. From (22), we get

$$\mathbf{f}''' = D_{xxx}^{p,1} \mathbf{f}, \tag{23}$$

where $D_{xxx}^{p,1}$ is the desired differentiation matrix corresponding to the third derivative approximation. From 21, we have

$$H_1 = \begin{pmatrix} 1 & A & 0 & \ldots & 0 & 0 & A \\ A & 1 & A & \ldots & 0 & 0 & 0 \\ \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots \\ 0 & 0 & 0 & \ldots & A & 1 & A \\ A & 0 & 0 & \ldots & 0 & A & 1 \end{pmatrix}, \tag{24}$$

$$H_2 = \left(\begin{array}{ccccccccccccccc}
0 & -(2a_1' + 3a_2') & a_1' & a_2' & 0 & 0 & 0 & \ldots & 0 & 0 & 0 & 0 & -a_2' & -a_1' & (2a_1' + 3a_2') \\
(2a_1' + 3a_2') & 0 & -(2a_1' + 3a_2') & a_1' & a_2' & 0 & 0 & \ldots & 0 & 0 & 0 & 0 & 0 & -a_2' & -a_1' \\
-a_1' & (2a_1' + 3a_2') & 0 & -(2a_1' + 3a_2') & a_1' & a_2' & 0 & \ldots & 0 & 0 & 0 & 0 & 0 & 0 & -a_2' \\
-a_2' & -a_1' & (2a_1' + 3a_2') & 0 & -(2a_1' + 3a_2') & a_1' & a_2' & \ldots & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\multicolumn{15}{c}{\dotfill} \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & \ldots & -a_2' & -a_1' & (2a_1' + 3a_2') & 0 & -(2a_1' + 3a_2') & a_1' & a_2' \\
a_2' & 0 & 0 & 0 & 0 & 0 & 0 & \ldots & 0 & -a_2' & -a_1' & (2a_1' + 3a_2') & 0 & -(2a_1' + 3a_2') & a_1' \\
a_1' & a_2' & 0 & 0 & 0 & 0 & 0 & \ldots & 0 & 0 & -a_2' & -a_1' & (2a_1' + 3a_2') & 0 & -(2a_1' + 3a_2') \\
-(2a_1' + 3a_2') & a_1' & a_2' & 0 & 0 & 0 & 0 & \ldots & 0 & 0 & 0 & -a_2' & -a_1' & (2a_1' + 3a_2') & 0
\end{array}\right), \tag{25}$$

where $a_1' = \frac{a_1}{2h^3}$, $a_2' = \frac{a_2}{8h^3}$. We now discuss compact schemes of fourth- and sixth-order accuracy for the third derivative.

Fourth-order accurate compact approximation: For a fourth-order accurate compact finite difference scheme, we observe that $A = \frac{1}{2}$, $a_2 = 0$, and $a_1 = 2$ and (21) becomes

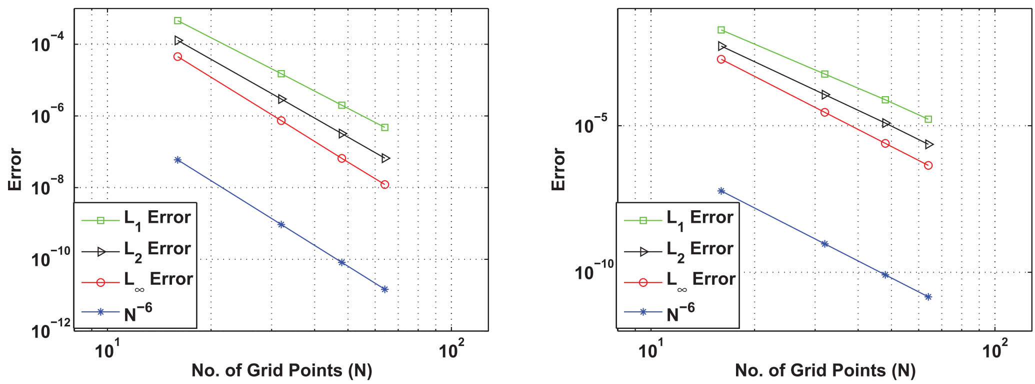
$$\frac{1}{2} f_{i-1}''' + f_i''' + \frac{1}{2} f_{i+1}''' = 2 \frac{f_{i+2} - 2f_{i+1} + 2f_{i-1} - f_{i-2}}{2h^3}, \quad 1 \le i \le N.$$

Substituting these values into H_1 and H_2, given in (24) and (25), allows the formation of the required differentiation matrix $D_{xxx}^{p,1}$.

Sixth-order accurate compact approximation: For a sixth-order accurate compact finite difference scheme, we observe that $A = \frac{7}{16}$, $a_2 = \frac{-1}{8}$, and $a_1 = 2$ and (21) becomes

$$\frac{7}{16} f_{i-1}''' + f_i''' + \frac{7}{16} f_{i+1}''' = 2 \frac{f_{i+2} - 2f_{i+1} + 2f_{i-1} - f_{i-2}}{2h^3} - \frac{1}{8} \frac{f_{i+3} - 3f_{i+1} + 3f_{i-1} - f_{i-3}}{8h^3}, \quad 1 \le i \le N.$$

Substituting these values into H_1 and H_2, given in (24) and (25), allows the formation of the required differentiation matrix $D_{xxx}^{p,1}$.



(a) (b)

Fig. 3. (a) Sixth-order accurate third derivative approximation of $sin(2\pi x)$ on $[0, 1]$. (b) Sixth-order accurate fourth derivative approximation of $sin(2\pi x)$ on $[0, 1]$.

The preceding results were validated using the test function $f(x) = sin(2\pi x)$ on the interval $[0, 1]$. The error plot given in Figure 3(a) confirms the order of accuracy of the scheme. The function `compact_third_periodic.m` computes $D^{p,1}_{xxx}$ (see Section 3 of the accompanying User Manual for details).

Remark 2. By using (21), the most accurate compact schemes that we can obtain for third derivatives are sixth order. However, we can extend these schemes to higher order by increasing the stencil size on the left- and right-hand sides of (21).

2.1.4 Approximation of the Fourth Derivative. High-order compact finite difference approximations for the fourth derivative are discussed now, and we show that compact schemes of up to sixth order can be obtained. Let f_i'''' denotes the fourth derivative of the function f at grid points x_i, then approximation of the fourth derivative may be written as

$$\begin{aligned} Af_{i-1}'''' + f_i'''' + Af_{i+1}'''' = a_1 \frac{f_{i+2} - 4f_{i+1} + 6f_i - 4f_{i-1} + f_{i-2}}{h^4} \\ + a_2 \frac{f_{i+3} - 9f_{i+1} + 16f_i - 9f_{i-1} + f_{i-3}}{6h^4}, \quad 1 \le i \le N, \end{aligned} \tag{26}$$

where A, a_1, and a_2 are constants to be determined. To compute the constants, the first unmatched coefficients of Taylor series expansion are used to determine the formal truncation error. Using (26), compact finite difference approximation for the fourth derivative can be written as

$$H_1 \mathbf{f}'''' = H_2 \mathbf{f}, \tag{27}$$

where $\mathbf{f}'''' = (f_1'''', f_2'''', \ldots, f_N'''')^T$. From (27), we get

$$\mathbf{f}'''' = D^{p,1}_{xxxx} \mathbf{f}, \tag{28}$$

where $D^{p,1}_{xxxx}$ is the desired differentiation matrix corresponding to the fourth derivative approximation. We have

$$H_1 = \begin{pmatrix} 1 & A & 0 & \ldots & 0 & 0 & A \\ A & 1 & A & \ldots & 0 & 0 & 0 \\ \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots \\ 0 & 0 & 0 & \ldots & A & 1 & A \\ A & 0 & 0 & \ldots & 0 & A & 1 \end{pmatrix}, \tag{29}$$

$$H_2 = \begin{pmatrix} 6a_1' + 16a_2' & -(4a_1' + 9a_2') & a_1' & a_2' & 0 & 0 & 0 & \dots & 0 & 0 & 0 & 0 & a_2' & a_1' & -(4a_1' + 9a_2') \\ -(4a_1' + 9a_2') & 6a_1' + 16a_2' & -(4a_1' + 9a_2') & a_1' & a_2' & 0 & 0 & \dots & 0 & 0 & 0 & 0 & 0 & a_2' & a_1' \\ a_1' & -(4a_1' + 9a_2') & 6a_1' + 16a_2' & -(4a_1' + 9a_2') & a_1' & a_2' & 0 & \dots & 0 & 0 & 0 & 0 & 0 & 0 & a_2' \\ a_2' & a_1' & -(4a_1' + 9a_2') & 6a_1' + 16a_2' & -(4a_1' + 9a_2') & a_1' & a_2' & \dots & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & & & \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \dots & a_2' & a_1' & -(4a_1' + 9a_2') & 6a_1' + 16a_2' & -(4a_1' + 9a_2') & a_1' & a_2' \\ a_2' & 0 & 0 & 0 & 0 & 0 & 0 & \dots & 0 & a_2' & a_1' & -(4a_1' + 9a_2') & 6a_1' + 16a_2' & -(4a_1' + 9a_2') & a_1' \\ a_1' & a_2' & 0 & 0 & 0 & 0 & 0 & \dots & 0 & 0 & a_2' & a_1' & -(4a_1' + 9a_2') & 6a_1' + 16a_2' & -(4a_1' + 9a_2') \\ -(4a_1' + 9a_2') & a_1' & a_2' & 0 & 0 & 0 & 0 & \dots & 0 & 0 & 0 & a_2' & a_1' & -(4a_1' + 9a_2') & 6a_1' + 16a_2' \end{pmatrix}, \tag{30}$$

where $a_1' = \frac{a_1}{h^4}$, $a_2' = \frac{a_2}{6h^4}$. We now discuss compact schemes of fourth- and sixth-order accuracy for the fourth derivative.

Fourth-order accurate compact approximation: For a fourth-order accurate compact finite difference scheme, we obtain $A = \frac{1}{4}$, $a_2 = 0$, and $a_1 = \frac{3}{2}$ and (26) becomes

$$\frac{1}{4} f_{i-1}'''' + f_i'''' + \frac{1}{4} f_{i+1}'''' = \frac{3}{2} \frac{f_{i+2} - 4f_{i+1} + 6f_i - 4f_{i-1} + f_{i-2}}{h^4}, \quad 1 \leq i \leq N.$$

Substituting these values into H_1 and H_2, given in (29) and (30), allows the formation of the required differentiation matrix $D_{xxxx}^{p,1}$.

Sixth-order accurate compact approximation: For a sixth-order accurate compact finite difference scheme, we obtain $A = \frac{7}{26}$, $a_2 = \frac{1}{13}$, and $a_1 = \frac{19}{13}$ and (26) becomes

$$\begin{aligned} \frac{7}{26} f_{i-1}'''' + f_i'''' + \frac{7}{26} f_{i+1}'''' = {} & \frac{19}{13} \frac{f_{i+2} - 4f_{i+1} + 6f_i - 4f_{i-1} + f_{i-2}}{h^4} \\ & + \frac{1}{13} \frac{f_{i+3} - 9f_{i+1} + 16f_i - 9f_{i-1} + f_{i-3}}{6h^4}, \quad 1 \leq i \leq N. \end{aligned}$$

Substituting these values into H_1 and H_2, given in (29) and (30), allows the formation of the required differentiation matrix $D_{xxxx}^{p,1}$.

The preceding results were validated using the test function $f(x) = sin(2\pi x)$ on the interval $[0, 1]$. The error plot given in Figure 3(b) confirms the order of accuracy of the scheme. The function `compact_fourth_periodic.m` computes $D_{xxxx}^{p,1}$ (see Section 4 of the accompanying User Manual for details).

Remark 3. We restrict ourselves to fourth derivative approximation in this article. However, high-order compact finite difference schemes for fifth and higher derivatives can be constructed in an analogous way as discussed in Section 2.1.

2.2 High-Order Compact Finite Difference Schemes in Two Dimensions with Periodic Boundary Conditions

High-order compact finite difference approximations for partial derivative are discussed in this section, and it is shown that up to 10th-order accurate compact approximations can be obtained. We represent the unknown function $f_{i,j} = f(x_i, y_j)$ in vector form where $1 \leq i \leq N_x + 1$ and $1 \leq j \leq N_y + 1$. For simplicity, we take $N_x = N_y = N$ in this article, hence $\mathbf{f} = (f_{1,1}, f_{2,1}, \dots, f_{N,1}, f_{1,2}, \dots, f_{N,N})^T$. In the case of function of two variables, the differentiation matrix will be of order N^2.

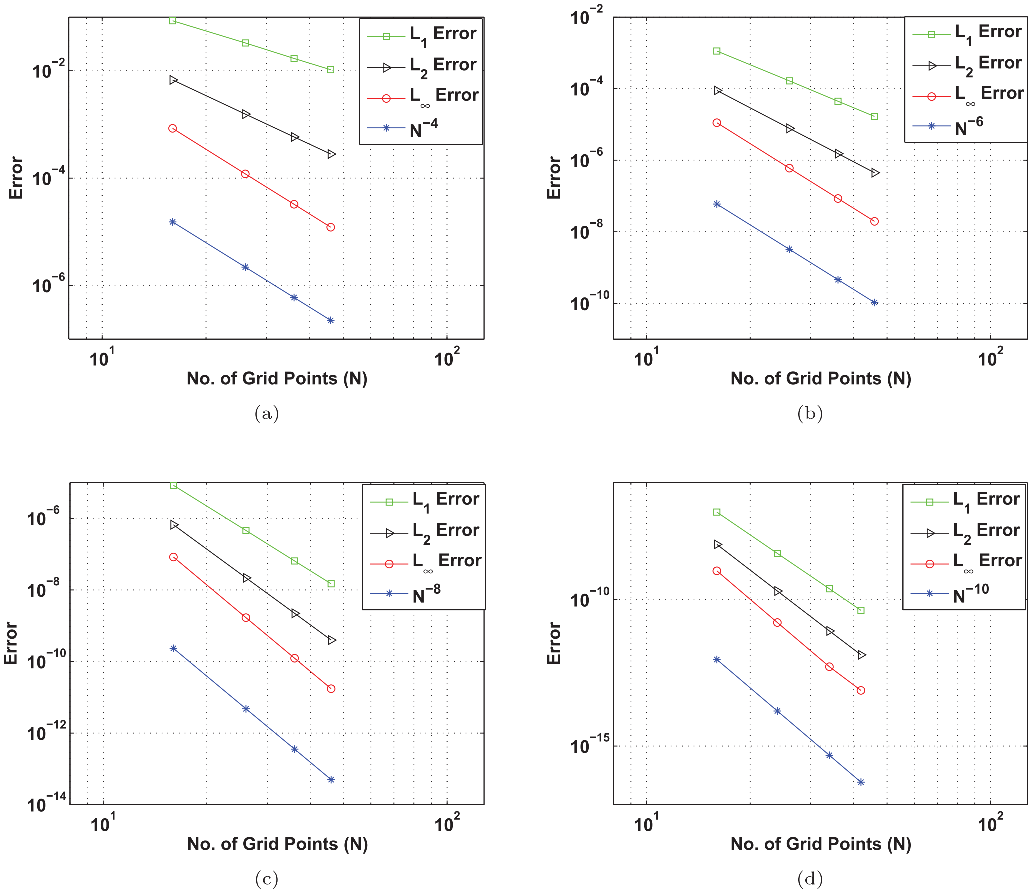


Fig. 4. Partial derivative ($\frac{\partial}{\partial x}$) approximations of $sin(2\pi x)cos(2\pi y)$ on $[0,1] \times [0,1]$ using 4th-order accurate compact approximation (a), 6th-order accurate compact approximation (b), 8th-order accurate compact approximation (c), and 10th-order accurate compact approximation (d).

2.2.1 Approximation of $\frac{\partial}{\partial x}$. If $D_x^{p,2}$ represents the differentiation matrix corresponding to the $\frac{\partial}{\partial x}$, then

$$D_x^{p,2} = \begin{pmatrix} D_x^{p,1} & 0 & 0\,0\ldots 0\,0 & 0 & 0 \\ 0 & D_x^{p,1} & 0\,0\ldots 0\,0 & 0 & 0 \\ \ldots\ldots & \ldots & \ldots\ldots & & \\ 0 & 0 & 0\,0\ldots 0\,0 & D_x^{p,1} & 0 \\ 0 & 0 & 0\,0\ldots 0\,0 & 0 & D_x^{p,1} \end{pmatrix}, \tag{31}$$

where $D_x^{p,1}$ is the differentiation matrix corresponding to the first derivative approximation obtained from Section 2.1.1. We use 4th-, 6th-, 8th-, and 10th-order accurate $D_x^{p,1}$ to obtain 4th, 6th, 8th-, and 10th-order accurate approximation for $D_x^{p,2}$, respectively. The above results were validated using the test function $sin(2\pi x)cos(2\pi y)$. Error plots given in Figure 4 confirm the order of accuracy of the schemes. The function `compact_first_periodic_2dx.m` computes $D_x^{p,2}$ (see Section 5 of the accompanying User Manual for details).

ALGORITHM 1: Algorithm for Approximation of $\frac{\partial}{\partial y}$

$m = 1$
for $k = 1, 2, \ldots, N$
    $g = 1$
    for $i = 1 : N$
        for $j = 1 : N$
            $D_y^{p,2}(m, N(j-1)+g) = D_x^{p,2}(k, j)$
        end
        $m = m + 1$
        $g = g + 1$
    end
end

2.2.2 Approximation of $\frac{\partial}{\partial y}$. We followed the approach of Shukla et al. (2007) to obtain the differentiation matrix corresponding to $\frac{\partial}{\partial y}$ from $D_x^{p,2}$. The differentiation matrix corresponding to $\frac{\partial}{\partial y}$ ($D_y^{p,2}$) may be obtained by using Algorithm 1. Results were validated using the test function $sin(2\pi x)cos(2\pi y)$. Error plots given in Figure 5 confirm the order of accuracy of the schemes. The function `compact_first_periodic_2dy.m` computes $D_y^{p,2}$ (see Section 6 of the accompanying User Manual for details).

2.2.3 Approximation of $\frac{\partial^2}{\partial x^2}$. If $D_{xx}^{p,2}$ represents the differentiation matrix corresponding to the $\frac{\partial^2}{\partial x^2}$, then

$$D_{xx}^{p,2} = \begin{pmatrix} D_{xx}^{p,1} & 0 & 0\,0 \ldots 0\,0 & 0 & 0 \\ 0 & D_{xx}^{p,1} & 0\,0 \ldots 0\,0 & 0 & 0 \\ \ldots\ldots & \ldots\ldots & \ldots\ldots\ldots & & \\ 0 & 0 & 0\,0 \ldots 0\,0 & D_{xx}^{p,1} & 0 \\ 0 & 0 & 0\,0 \ldots 0\,0 & 0 & D_{xx}^{p,1} \end{pmatrix}, \tag{32}$$

where $D_{xx}^{p,1}$ is differentiation matrix corresponding to the second derivative approximation discussed in Section 2.1.2. Results were validated using the test function $sin(2\pi x)cos(2\pi y)$. Error plots given in Figure 6 confirm the order of accuracy of the schemes. The function `compact_first_periodic_2dxx.m` computes $D_{xx}^{p,2}$ (see Section 7 of the accompanying User Manual for details).

2.2.4 Approximation of $\frac{\partial^2}{\partial y^2}$. The differentiation matrix corresponding to $\frac{\partial^2}{\partial y^2}$ ($D_{yy}^{p,2}$) may be obtained by using Algorithm 2. Results were validated using the test function $sin(2\pi x)cos(2\pi y)$. Error plots given in Figure 7 confirm the order of accuracy of the schemes. The function `compact_first_periodic_2dyy.m` computes $D_{yy}^{p,2}$ (see Section 8 of the accompanying User Manual for details).

2.2.5 Approximation of $\frac{\partial^2}{\partial x \partial y}$. If $D_{xy}^{p,2}$ represents the differentiation matrix corresponding to the $\frac{\partial^2}{\partial x \partial y}$, then

$$D_{xy}^{p,2} = kron\left(D_x^{p,1}, D_y^{p,1}\right), \tag{33}$$

where matrix $D_x^{p,1}$ is discussed in Section 2.1.1 and $D_y^{p,1}$ is the differentiation matrix for first derivative in the y direction. Here, *kron* is a built in Matlab function, which computes the tensor prod-

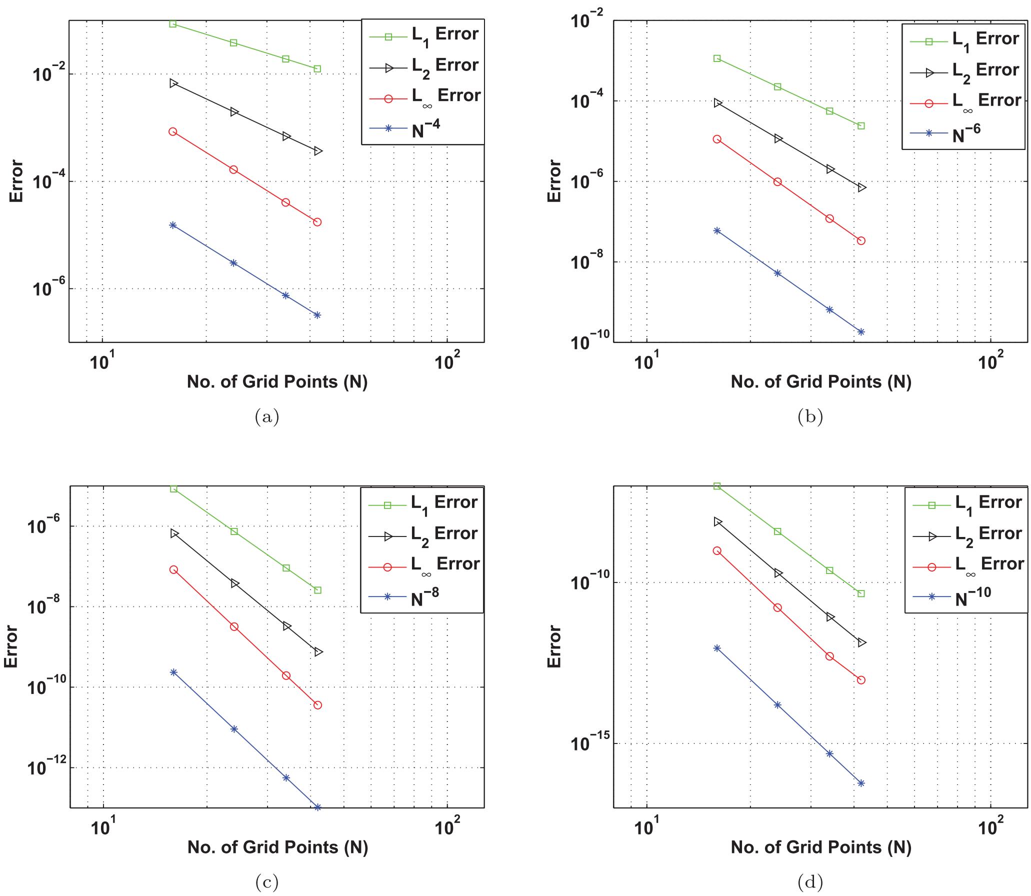


Fig. 5. Partial derivative ($\frac{\partial}{\partial y}$) approximations of $sin(2\pi x)cos(2\pi y)$ on $[0,1] \times [0,1]$ using 4th-order accurate compact approximation (a), 6th-order accurate compact approximation (b), 8th-order accurate compact approximation (c), and 10th-order accurate compact approximation (d).

uct of two matrices. In this case, results were validated with the test function $sin(2\pi x)cos(2\pi y)$. Error plots given in Figure 8 confirm the order of accuracy of the schemes. The function `compact_first_periodic_2dxy.m` computes $D_{xy}^{p,2}$ (see Section 9 of the accompanying User Manual for details).

2.3 Fourier Analysis of Compact Finite Difference Schemes

Fourier analysis is a classical technique for comparing two difference schemes in numerical analysis. An extensive study of the use of Fourier analysis on compact finite difference schemes may be found in Lele (1992). Fourier analysis of a finite difference scheme quantifies the resolution characteristics of the difference approximation. Here we provide a glimpse of Fourier analysis for first, second, third, and fourth derivative approximation; for more details about Fourier analysis, see Lele (1992).

Fourier analysis for first derivative approximation: If we denote the wave number by ω whose domain is $[0, \pi]$ and denote a modified wave number for first derivative approximation by

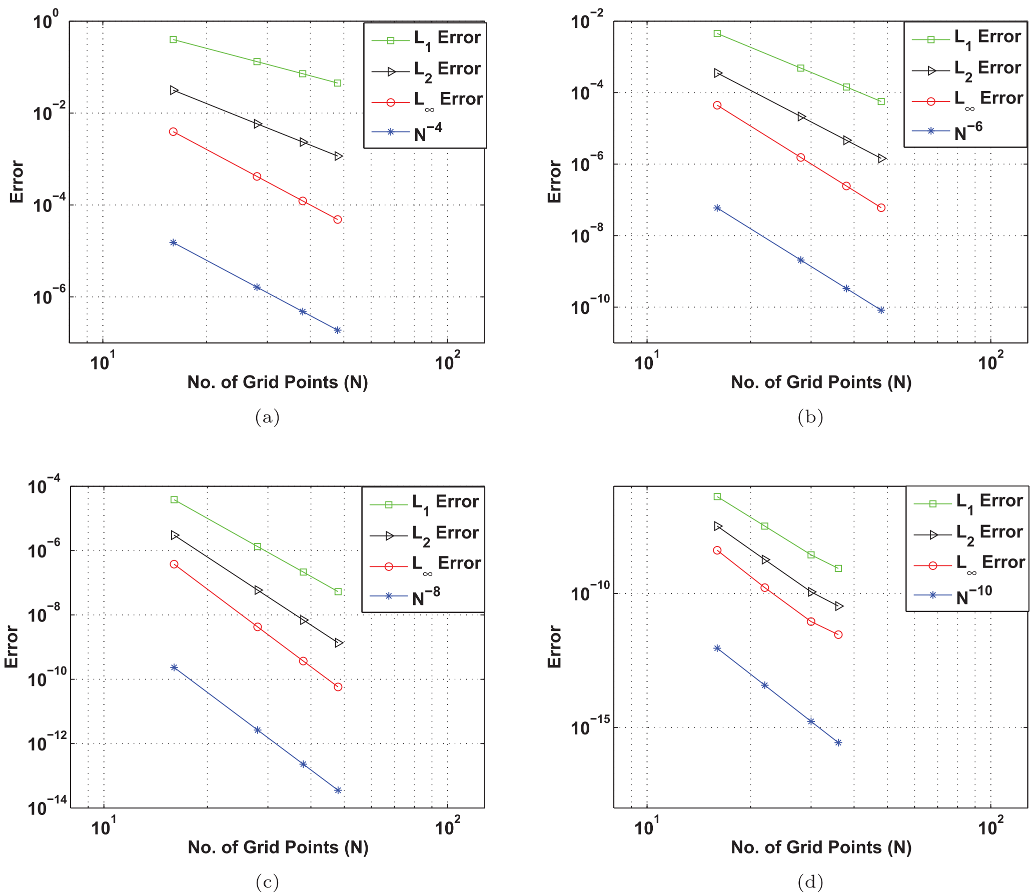


Fig. 6. Partial derivative ($\frac{\partial^2}{\partial x^2}$) approximations of $sin(2\pi x)cos(2\pi y)$ on $[0,1]\times[0,1]$ using 4th-order accurate compact approximation(a), 6th-order accurate compact approximation (b), 8th-order accurate compact approximation (c), and 10th-order accurate compact approximation (d).

ω', then by (1) they can be related by

$$\omega' = \frac{a_1 sin(\omega) + (a_2/2)sin(2\omega) + (a_3/3)sin(3\omega)}{1 + 2Acos(\omega) + 2Bcos(2\omega)}.$$

Fourier analysis for second derivative approximation: The wave number ω and modified wave number ω'' for second derivative approximation may be related via (11) to give

$$\omega'' = \frac{2a_1(1 - cos(\omega)) + (a_2/2)(1 - cos(2\omega)) + (2a_3/9)(1 - cos(3\omega))}{1 + 2Acos(\omega) + 2Bcos(2\omega)}.$$

Fourier analysis for third derivative approximation: The wave number ω and modified wave number ω''' for third derivative approximation may be related via (21) to give

$$\omega''' = \frac{a_1(2sin(\omega) - sin(2\omega)) + (a_2/4)(3sin(\omega) - sin(3\omega))}{1 + 2Acos(\omega)}.$$

ALGORITHM 2: Algorithm for Approximation of $\frac{\partial^2}{\partial y^2}$

$m = 1$
for $k = 1, 2, \ldots, N$
  $g = 1$
  for $i = 1 : N$
    for $j = 1 : N$
      $D_{yy}^{p,2}(m, N(j-1)+g) = D_{xx}^{p,2}(k, j)$
    end
    $m = m + 1$
    $g = g + 1$
  end
end

Fourier analysis for fourth derivative approximation: The wave number ω and modified wave number ω'''' for fourth derivative approximation may be related via (26) to give

$$\omega'''' = \frac{2a_1(cos(2\omega) - 4cos(\omega) + 3) + (a_2/3)(cos(3\omega) - 9cos(\omega) + 8)}{1 + 2Acos(\omega)}.$$

In Figure 9, modified wave numbers versus wave numbers are plotted for various difference schemes for first, second, third and fourth derivatives, respectively. These plots clearly shows that compact finite difference approximations have better resolution characteristics when compared to classical finite difference approximations. As a special case, we see the abnormal behavior of a fourth-order accurate compact scheme for the third derivative approximation in Figure 9(c). This is because the fourth-order accurate compact scheme becomes singular as $\omega \to \pi$ (Lele 1992). This can be avoided by using a sixth-order compact finite difference scheme for the third derivative approximation.

3 HIGH-ORDER COMPACT FINITE DIFFERENCE SCHEMES FOR DIRICHLET BOUNDARY CONDITIONS

In this section, high-order compact finite difference schemes are discussed for first and second derivative approximations for arbitrary functions of one and two variables with Dirichlet boundary conditions.

3.1 High-Order Compact Finite Difference Schemes for One Dimension with Dirichlet Boundary Conditions

In this case, uniform grid $x_i = x_{min} + h(i-1), \ \ 1 \le i \le N$, is assumed and the differentiation matrix will be of order N. We know that if boundary conditions are not periodic, one-sided compact finite difference schemes are needed at the boundary grid points x_1, x_2, x_{N-1} and x_N. For the interior grid points (x_3 to x_{N-2}), we use the compact finite difference schemes discussed in Section 2.1.

3.1.1 Approximation to the First Derivative. High-order compact schemes for first derivative approximation are discussed in this section, and it is shown that these schemes are up to sixth-order accurate. One-sided compact finite difference schemes at the boundary grid points are obtained as follows.

Boundary formulation at $i = 1$: The one-sided compact approximation for the first derivative at grid point x_1 may be written as

$$f_1' + Af_2' = \frac{1}{h}(a_1 f_1 + a_2 f_2 + a_3 f_3 + a_4 f_4 + a_5 f_5 + a_6 f_6 + a_7 f_7 + a_8 f_8), \tag{34}$$

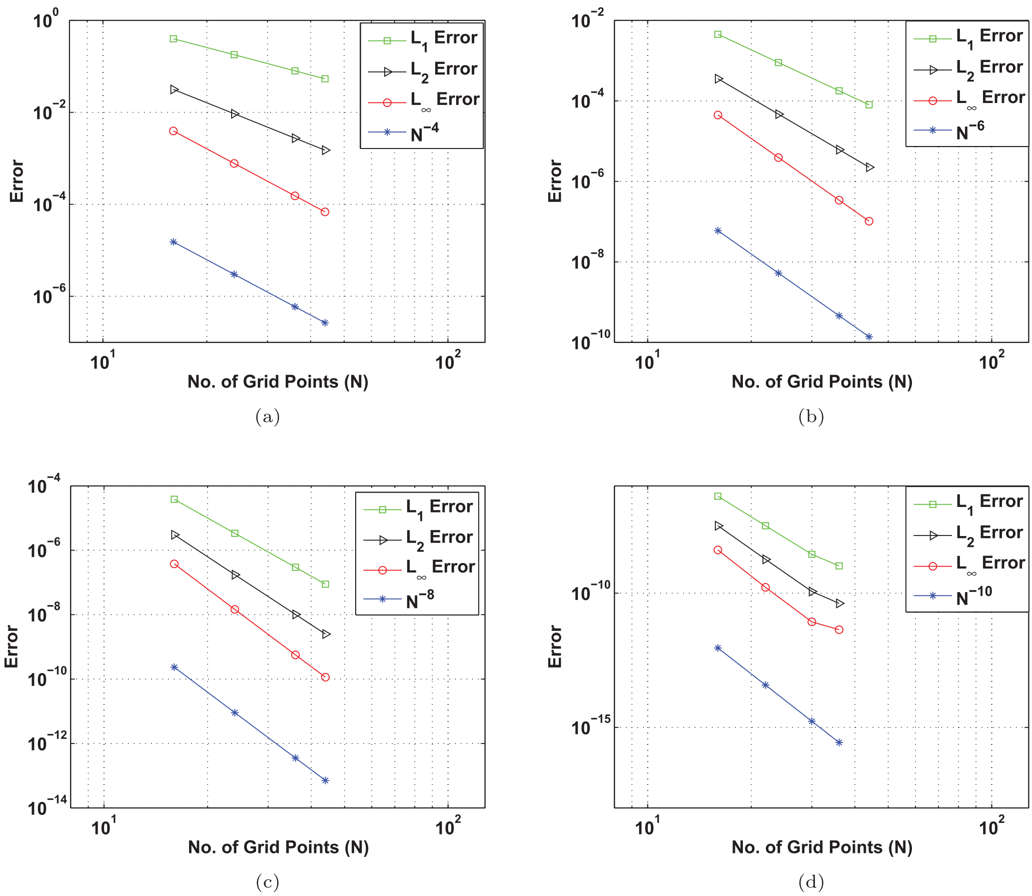


Fig. 7. Partial derivative ($\frac{\partial^2}{\partial y^2}$) approximations of $sin(2\pi x)cos(2\pi y)$ on $[0,1] \times [0,1]$ using 4th-order accurate compact approximation (a), 6th-order accurate compact approximation (b), 8th-order accurate compact approximation (c), and 10th-order accurate compact approximation (d).

where constants A and a_i, $1 \leq i \leq 8$ are to be determined. From Taylor series expansion of (34), we can write

$$\text{Zeroth order} : a_1 + a_2 + a_3 + a_4 + a_5 + a_6 + a_7 + a_8 = 0, \tag{35}$$

$$\text{First order} : a_2 + 2a_3 + 3a_4 + 4a_5 + 5a_6 + 6a_7 + 7a_8 = A + 1, \tag{36}$$

$$\text{Second order} : a_2 + 2^2 a_3 + 3^2 a_4 + 4^2 a_5 + 5^2 a_6 + 6^2 a_7 + 7^2 a_8 = \frac{2!}{1!} A, \tag{37}$$

$$\text{Third order} : a_2 + 2^3 a_3 + 3^3 a_4 + 4^3 a_5 + 5^3 a_6 + 6^3 a_7 + 7^3 a_8 = \frac{3!}{2!} A, \tag{38}$$

$$\text{Fourth order} : a_2 + 2^4 a_3 + 3^4 a_4 + 4^4 a_5 + 5^4 a_6 + 6^4 a_7 + 7^4 a_8 = \frac{4!}{3!} A, \tag{39}$$

$$\text{Fifth order} : a_2 + 2^5 a_3 + 3^5 a_4 + 4^5 a_5 + 5^5 a_6 + 6^5 a_7 + 7^5 a_8 = \frac{5!}{4!} A, \tag{40}$$

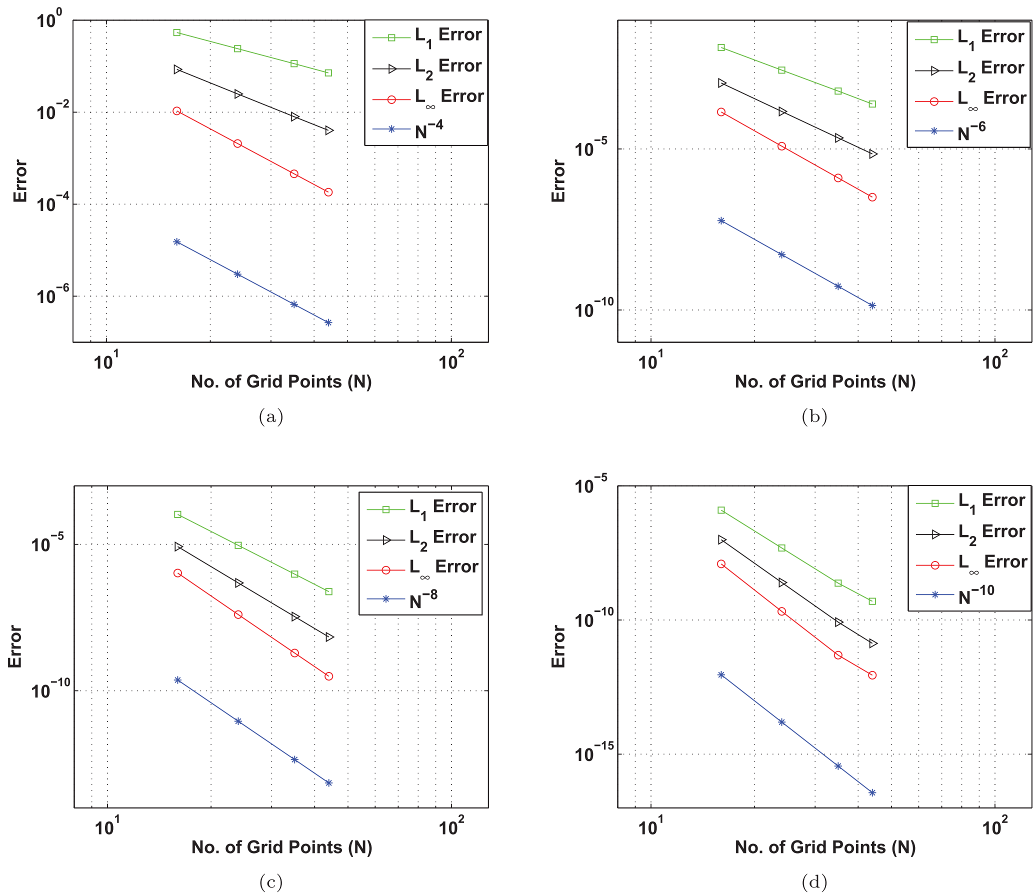


Fig. 8. Partial derivative ($\frac{\partial^2}{\partial x \partial y}$) approximations of $sin(2\pi x)cos(2\pi y)$ on $[0, 1] \times [0, 1]$ using 4th-order accurate compact approximation (a), 6th-order accurate compact approximation (b), 8th-order accurate compact approximation (c), and 10th-order accurate compact approximation (d).

$$\text{Sixth order}: a_2 + 2^6 a_3 + 3^6 a_4 + 4^6 a_5 + 5^6 a_6 + 6^6 a_7 + 7^6 a_8 = \frac{6!}{5!}A, \tag{41}$$

$$\text{Seventh order}: a_2 + 2^7 a_3 + 3^7 a_4 + 4^7 a_5 + 5^7 a_6 + 6^7 a_7 + 7^7 a_8 = \frac{7!}{6!}A, \tag{42}$$

$$\text{Eighth order}: a_2 + 2^8 a_3 + 3^8 a_4 + 4^8 a_5 + 5^8 a_6 + 6^8 a_7 + 7^8 a_8 = \frac{8!}{7!}A. \tag{43}$$

By solving (35) through (43), we can obtain the one-sided compact approximation for the first derivative at the grid point x_1.

Boundary formulation at $i = N$: The one-sided compact approximation for the first derivative at grid point x_N may be written as

$$f'_N + Af'_{N-1} = \frac{1}{h}(c_1 f_N + c_2 f_{N-1} + c_3 f_{N-2} + c_4 f_{N-3} + c_5 f_{N-4} + c_6 f_{N-5} + c_7 f_{N-6} + c_8 f_{N-7}), \tag{44}$$

where $c_i = -a_i$ for $1 \leq i \leq 8$ and a_i, A are obtained from (35) through (43).

Boundary formulation at $i = 2$: The one-sided compact approximation for the first derivative at grid point x_2 may be written as

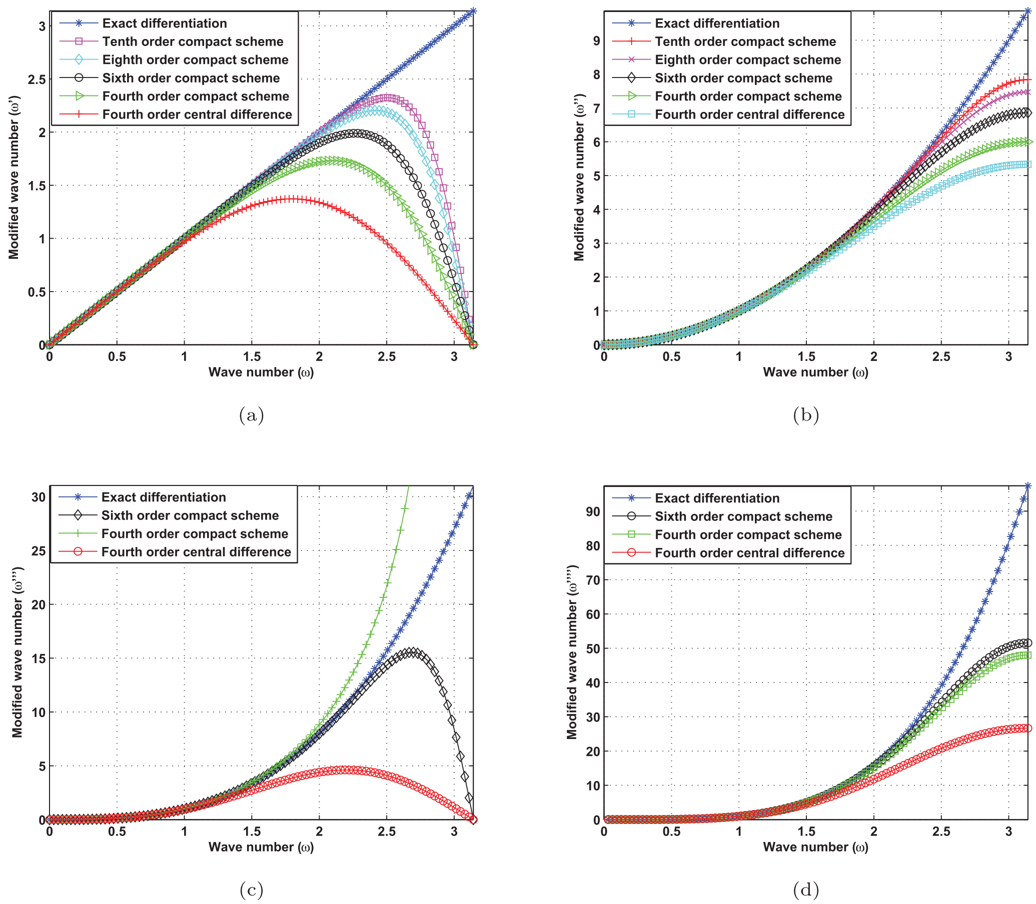


Fig. 9. Wave number and modified wave number for first derivative approximation (a), second derivative approximation (b), third derivative approximation (c), and fourth derivative approximation (d).

$$Af_1' + f_2' + Af_3' = \frac{1}{h}(a_1f_1 + a_2f_2 + a_3f_3 + a_4f_4 + a_5f_5 + a_6f_6 + a_7f_7 + a_8f_8), \tag{45}$$

where constants A and $a_i, 1 \leq i \leq 8$ are to be determined. From Taylor series expansion of (45), we can write

$$\text{Zeroth order}: a_1 + a_2 + a_3 + a_4 + a_5 + a_6 + a_7 + a_8 = 0, \tag{46}$$

$$\text{First order}: a_2 + 2a_3 + 3a_4 + 4a_5 + 5a_6 + 6a_7 + 7a_8 = 2A + 1, \tag{47}$$

$$\text{Second order}: a_2 + 2^2a_3 + 3^2a_4 + 4^2a_5 + 5^2a_6 + 6^2a_7 + 7^2a_8 = \frac{2!}{1!}(2A + 1), \tag{48}$$

$$\text{Third order}: a_2 + 2^3a_3 + 3^3a_4 + 4^3a_5 + 5^3a_6 + 6^3a_7 + 7^3a_8 = \frac{3!}{2!}(2^2A + 1), \tag{49}$$

$$\text{Fourth order}: a_2 + 2^4a_3 + 3^4a_4 + 4^4a_5 + 5^4a_6 + 6^4a_7 + 7^4a_8 = \frac{4!}{3!}(2^3A + 1), \tag{50}$$

$$\text{Fifth order}: a_2 + 2^5a_3 + 3^5a_4 + 4^5a_5 + 5^5a_6 + 6^5a_7 + 7^5a_8 = \frac{5!}{4!}(2^4A + 1), \tag{51}$$

$$\text{Sixth order}: a_2 + 2^6 a_3 + 3^6 a_4 + 4^6 a_5 + 5^6 a_6 + 6^6 a_7 + 7^6 a_8 = \frac{6!}{5!}(2^5 A + 1), \tag{52}$$

$$\text{Seventh order}: a_2 + 2^7 a_3 + 3^7 a_4 + 4^7 a_5 + 5^7 a_6 + 6^7 a_7 + 7^7 a_8 = \frac{7!}{6!}(2^6 A + 1), \tag{53}$$

$$\text{Eighth order}: a_2 + 2^8 a_3 + 3^8 a_4 + 4^8 a_5 + 5^8 a_6 + 6^8 a_7 + 7^8 a_8 = \frac{8!}{7!}(2^7 A + 1). \tag{54}$$

By solving (46) through (54), we can obtain the one-sided compact approximation for the first derivative at the grid point x_2.

Boundary formulation at $i = N - 1$: The one-sided compact approximation for the first derivative at grid point x_{N-1} may be written as

$$\begin{aligned} Af'_{N-2} + f'_{N-1} + Af'_N = {} & \frac{1}{h}(c_1 f_N + c_2 f_{N-1} + c_3 f_{N-2} + c_4 f_{N-3} + c_5 f_{N-4}) \\ & + \frac{1}{h}(c_6 f_{N-5} + c_7 f_{N-6} + c_8 f_{N-7}), \end{aligned} \tag{55}$$

where, $c_i = -a_i$ for $1 \le i \le 8$ and a_i, A are obtained from (46) through (54).

Fourth-order accurate compact approximation: Fourth-order accurate compact approximations are required at $i = 1$ and $i = N$. For this, (35) through (39) are solved to give $A = 3$, $a_1 = \frac{-17}{6}$, $a_2 = \frac{3}{2}$, $a_3 = \frac{3}{2}$, and $a_4 = \frac{-1}{6}$, and other a_i are zero. Hence, we can write

$$\begin{aligned} f'_1 + 3f'_2 &= -\frac{17}{6h} f_1 + \frac{3}{2h} f_2 + \frac{3}{2h} f_3 - \frac{1}{6h} f_4, \quad i = 1, \\ \frac{1}{4} f'_{i-1} + f'_i + \frac{1}{4} f'_{i+1} &= \frac{3}{2} \frac{f_{i+1} - f_{i-1}}{2h}, \quad 2 \le i \le N-1, \\ f'_N + 3f'_{N-1} &= \frac{17}{6h} f_N - \frac{3}{2h} f_{N-1} - \frac{3}{2h} f_{N-2} + \frac{1}{6h} f_{N-3}, \quad i = N. \end{aligned}$$

The fourth-order accurate compact approximation for the first derivative in matrix form can be written as

$$\mathbf{f}' = D_x^{d,1} \mathbf{f}, \tag{56}$$

where $D_x^{d,1}$ is the desired differentiation matrix with

$$H_1 = \begin{pmatrix} 1 & 3 & 0 & 0 & \dots & 0 & 0 & 0 & 0 \\ \frac{1}{4} & 1 & \frac{1}{4} & 0 & \dots & 0 & 0 & 0 & 0 \\ \dots & \dots & \dots & \dots & \dots & & & & \\ 0 & 0 & 0 & 0 & \dots & 0 & \frac{1}{4} & 1 & \frac{1}{4} \\ 0 & 0 & 0 & 0 & \dots & 0 & 0 & 3 & 1 \end{pmatrix},$$

$$H_2 = \frac{1}{h} \begin{pmatrix} -\frac{17}{6} & \frac{3}{2} & \frac{3}{2} & -\frac{1}{6} & \dots & 0 & 0 & 0 & 0 \\ -\frac{3}{4} & 0 & \frac{3}{4} & 0 & \dots & 0 & 0 & 0 & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots & & \\ 0 & 0 & 0 & 0 & \dots & 0 & -\frac{3}{4} & 0 & \frac{3}{4} \\ 0 & 0 & 0 & 0 & \dots & \frac{1}{6} & -\frac{3}{2} & -\frac{3}{2} & \frac{17}{6} \end{pmatrix}.$$

Sixth-order accurate compact approximation: Sixth-order accurate compact approximations are required at $i = 1$, $i = 2$, $i = N - 1$, and $i = N$. For $i = 1$, solving (35) through (41) gives $A = 5$, $a_1 = \frac{-197}{60}$, $a_2 = \frac{-5}{12}$, $a_3 = 5$, $a_4 = \frac{-5}{3}$, $a_5 = \frac{5}{12}$, and $a_6 = \frac{-1}{20}$, and other a_i are zero. For $i = 2$, solving (46) through (52) gives $A = \frac{2}{11}$, $a_1 = \frac{-20}{33}$, $a_2 = \frac{-35}{132}$, $a_3 = \frac{34}{33}$, $a_4 = \frac{-7}{33}$, $a_5 = \frac{2}{33}$, and $a_6 = \frac{-1}{132}$, and other a_i are zero. Hence, the sixth-order compact finite difference scheme may be written as

$$\begin{aligned}
f_1' + 5f_2' &= -\frac{197}{60h}f_1 - \frac{5}{12h}f_2 + \frac{5}{h}f_3 - \frac{5}{3h}f_4 + \frac{5}{12h}f_5 - \frac{1}{20h}f_6, \quad i = 1,\\
\frac{2}{11}f_1' + f_2' + \frac{2}{11}f_3' &= -\frac{20}{33h}f_1 - \frac{35}{132h}f_2 + \frac{34}{33}f_3 - \frac{7}{33h}f_4 + \frac{2}{33h}f_5 - \frac{1}{132h}f_6, \quad i = 2,\\
\frac{1}{3}f_{i-1}' + f_i' + \frac{1}{3}f_{i+1}' &= \frac{14}{9}\frac{f_{i+1} - f_{i-1}}{2h} + \frac{1}{9}\frac{f_{i+2} - f_{i-2}}{4h}, \quad 3 \le i \le N-2,\\
\frac{2}{11}f_{N-2}' + f_{N-1}' + \frac{2}{11}f_N' &= \frac{20}{33h}f_N + \frac{35}{132h}f_{N-1} - \frac{34}{33}f_{N-2} + \frac{7}{33h}f_{N-3} - \frac{2}{33h}f_{N-4}\\
&\quad + \frac{1}{132h}f_{N-5}, \quad i = N-1,\\
f_N' + 5f_{N-1}' &= \frac{197}{60h}f_N + \frac{5}{12h}f_{N-1} - \frac{5}{h}f_{N-2} + \frac{5}{3h}f_{N-3} - \frac{5}{12h}f_{N-4}\\
&\quad + \frac{1}{20h}f_{N-5}, \quad i = N.
\end{aligned}$$

For the sixth-order accurate compact approximation for the first derivative, H_1 and H_2 may be written as

$$H_1 = \begin{pmatrix}
1 & 5 & 0 & 0 & \dots & 0 & 0 & 0 & 0\\
\frac{2}{11} & 1 & \frac{2}{11} & 0 & \dots & 0 & 0 & 0 & 0\\
0 & \frac{1}{3} & 1 & \frac{1}{3} & \dots & 0 & 0 & 0 & 0\\
\dots & \dots & \dots & \dots & & & & & \\
0 & 0 & 0 & 0 & \dots & \frac{1}{3} & 1 & \frac{1}{3} & 0\\
0 & 0 & 0 & 0 & \dots & 0 & \frac{2}{11} & 1 & \frac{2}{11}\\
0 & 0 & 0 & 0 & \dots & 0 & 0 & 5 & 1
\end{pmatrix},$$

$$H_2 = \frac{1}{h}\begin{pmatrix}
-\frac{197}{60} & \frac{5}{12} & 5 & -\frac{5}{3} & \frac{5}{12} & -\frac{1}{20} & \dots & 0 & 0 & 0 & 0 & 0 & 0\\
-\frac{20}{33} & -\frac{35}{132} & \frac{34}{33} & -\frac{7}{33} & \frac{2}{33} & -\frac{1}{132} & \dots & 0 & 0 & 0 & 0 & 0 & 0\\
-\frac{1}{36} & -\frac{14}{18} & 0 & \frac{14}{18} & \frac{1}{36} & 0 & \dots & 0 & 0 & 0 & 0 & 0 & 0\\
\dots & \dots & \dots & \dots & \dots & \dots & & & & & & & \\
0 & 0 & 0 & 0 & 0 & 0 & \dots & 0 & -\frac{1}{36} & -\frac{14}{18} & 0 & \frac{14}{18} & \frac{1}{36}\\
0 & 0 & 0 & 0 & 0 & 0 & \dots & \frac{1}{132} & -\frac{2}{33} & \frac{7}{33} & -\frac{34}{33} & \frac{35}{132} & \frac{20}{33}\\
0 & 0 & 0 & 0 & 0 & 0 & \dots & \frac{1}{20} & -\frac{5}{12} & \frac{5}{3} & -5 & -\frac{5}{12} & \frac{197}{60}
\end{pmatrix}.$$

The preceding results were validated using the test function $sin(x)$ on the interval $[0, 1]$. Error plots given in Figure 10 confirm the order of accuracy of the schemes. The function `first_compact_dirichlet.m` computes $D_x^{d,1}$ (see Section 10 of the accompanying User Manual for details).

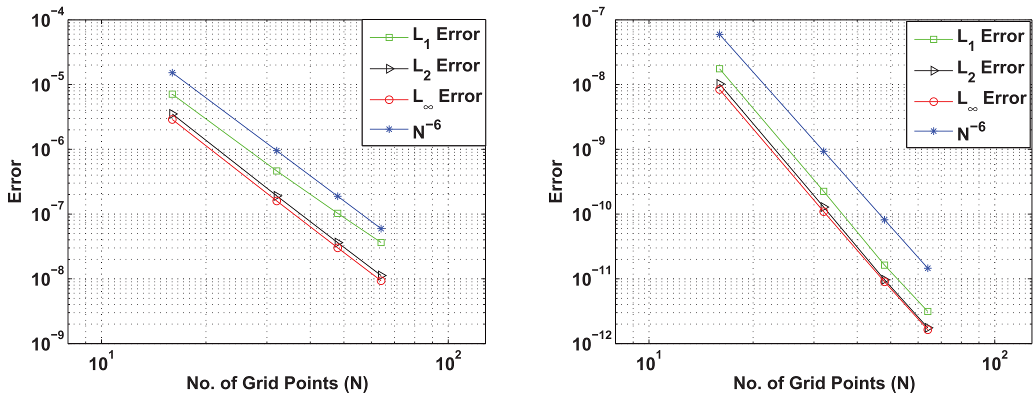
Remark 4. We restrict ourselves to sixth-order accurate compact finite difference schemes for derivative approximations with Dirichlet boundary conditions in this article. However, higher-order schemes may be developed in an analogous way.

3.1.2 Approximation to the Second Derivative. For this case as well, we obtain compact finite difference schemes at the boundary grid points x_1, x_2, x_{N-1}, and x_N.

Boundary formulation at $i = 1$:

$$f_1'' + Af_2'' = \frac{1}{h^2}\left(a_1f_1 + a_2f_2 + a_3f_3 + a_4f_4 + a_5f_5 + a_6f_6 + a_7f_7 + a_8f_8 + a_9f_9\right) \tag{57}$$

From (57), we have



(a) (b)

Fig. 10. First derivative approximations of $sin(x)$ on $[0, 1]$ with Dirichlet boundary conditions using fourth-order accurate compact approximations (a) and sixth-order accurate compact approximations (b).

$$(-1)^{th} \text{ order} : a_1 + a_2 + a_3 + a_4 + a_5 + a_6 + a_7 + a_8 + a_9 = 0, \tag{58}$$

$$\text{Zeroth order} : a_2 + 2a_3 + 3a_4 + 4a_5 + 5a_6 + 6a_7 + 7a_8 + 8a_9 = 0, \tag{59}$$

$$\text{First order} : a_2 + 2^2a_3 + 3^2a_4 + 4^2a_5 + 5^2a_6 + 6^2a_7 + 7^2a_8 + 8^2a_9 = \frac{2!}{1!}(1 + A), \tag{60}$$

$$\text{Second order} : a_2 + 2^3a_3 + 3^3a_4 + 4^3a_5 + 5^3a_6 + 6^3a_7 + 7^3a_8 + 8^3a_9 = \frac{3!}{1!}A, \tag{61}$$

$$\text{Third order} : a_2 + 2^4a_3 + 3^4a_4 + 4^4a_5 + 5^4a_6 + 6^4a_7 + 7^4a_8 + 8^4a_9 = \frac{4!}{2!}A, \tag{62}$$

$$\text{Fourth order} : a_2 + 2^5a_3 + 3^5a_4 + 4^5a_5 + 5^5a_6 + 6^5a_7 + 7^5a_8 + 8^5a_9 = \frac{5!}{3!}A, \tag{63}$$

$$\text{Fifth order} : a_2 + 2^6a_3 + 3^6a_4 + 4^6a_5 + 5^6a_6 + 6^6a_7 + 7^6a_8 + 8^6a_9 = \frac{6!}{4!}A, \tag{64}$$

$$\text{Sixth order} : a_2 + 2^7a_3 + 3^7a_4 + 4^7a_5 + 5^7a_6 + 6^7a_7 + 7^7a_8 + 8^7a_9 = \frac{7!}{5!}A, \tag{65}$$

$$\text{Seventh order} : a_2 + 2^8a_3 + 3^8a_4 + 4^8a_5 + 5^8a_6 + 6^8a_7 + 7^8a_8 + 8^8a_9 = \frac{8!}{6!}A, \tag{66}$$

$$\text{Eighth order} : a_2 + 2^9a_3 + 3^9a_4 + 4^9a_5 + 5^9a_6 + 6^9a_7 + 7^9a_8 + 8^9a_9 = \frac{9!}{7!}A. \tag{67}$$

By solving (58) through (67), we can obtain the one-sided compact approximation for the second derivative at the grid point x_1.

Boundary formulation at $i = N$:

$$\begin{aligned} f''_N + Af''_{N-1} = {} & \frac{1}{h^2}\left(c_1 f_N + c_2 f_{N-1} + c_3 f_{N-2} + c_4 f_{N-3} + c_5 f_{N-4} + c_6 f_{N-5}\right) \\ & + \frac{1}{h^2}(c_7 f_{N-6} + c_8 f_{N-7} + c_9 f_{N-8}), \end{aligned} \tag{68}$$

where, $c_i = a_i$ for $1 \le i \le 9$ and a_i, A are obtained from (58) through (67).

Boundary formulation at $i = 2$:

$$Af_1'' + f_2'' + Af_3'' = \frac{1}{h^2}\left(a_1 f_1 + a_2 f_2 + a_3 f_3 + a_4 f_4 + a_5 f_5 + a_6 f_6 + a_7 f_7 + a_8 f_8 + a_9 f_9\right) \tag{69}$$

From (69), we have

$$(-1)^{th} \text{ order}: a_1 + a_2 + a_3 + a_4 + a_5 + a_6 + a_7 + a_8 + a_9 = 0, \tag{70}$$

$$\text{Zeroth order}: a_2 + 2a_3 + 3a_4 + 4a_5 + 5a_6 + 6a_7 + 7a_8 + 8a_9 = 0, \tag{71}$$

$$\text{First order}: a_2 + 2^2 a_3 + 3^2 a_4 + 4^2 a_5 + 5^2 a_6 + 6^2 a_7 + 7^2 a_8 + 8^2 a_9 = \frac{2!}{1!}(2A+1), \tag{72}$$

$$\text{Second order}: a_2 + 2^3 a_3 + 3^3 a_4 + 4^3 a_5 + 5^3 a_6 + 6^3 a_7 + 7^3 a_8 + 8^3 a_9 = \frac{3!}{1!}(2A+1), \tag{73}$$

$$\text{Third order}: a_2 + 2^4 a_3 + 3^4 a_4 + 4^4 a_5 + 5^4 a_6 + 6^4 a_7 + 7^4 a_8 + 8^4 a_9 = \frac{4!}{2!}(2^2A+1), \tag{74}$$

$$\text{Fourth order}: a_2 + 2^5 a_3 + 3^5 a_4 + 4^5 a_5 + 5^5 a_6 + 6^5 a_7 + 7^5 a_8 + 8^5 a_9 = \frac{5!}{3!}(2^3A+1), \tag{75}$$

$$\text{Fifth order}: a_2 + 2^6 a_3 + 3^6 a_4 + 4^6 a_5 + 5^6 a_6 + 6^6 a_7 + 7^6 a_8 + 8^6 a_9 = \frac{6!}{4!}(2^4A+1), \tag{76}$$

$$\text{Sixth order}: a_2 + 2^7 a_3 + 3^7 a_4 + 4^7 a_5 + 5^7 a_6 + 6^7 a_7 + 7^7 a_8 + 8^7 a_9 = \frac{7!}{5!}(2^5A+1), \tag{77}$$

$$\text{Seventh order}: a_2 + 2^8 a_3 + 3^8 a_4 + 4^8 a_5 + 5^8 a_6 + 6^8 a_7 + 7^8 a_8 + 8^8 a_9 = \frac{8!}{6!}(2^6A+1), \tag{78}$$

$$\text{Eighth order}: a_2 + 2^9 a_3 + 3^9 a_4 + 4^9 a_5 + 5^9 a_6 + 6^9 a_7 + 7^9 a_8 + 8^9 a_9 = \frac{9!}{7!}(2^7A+1). \tag{79}$$

Solving (70) through (79), we can obtain one-sided compact approximation for the second derivative at the grid point x_2.

Boundary formulation at $i = N - 1$:

$$\begin{aligned} Af_{N-2}'' + f_{N-1}'' + Af_N'' = {} & \frac{1}{h^2}\left(c_1 f_N + c_2 f_{N-1} + c_3 f_{N-2} + c_4 f_{N-3} + c_5 f_{N-4}\right) \\ & + \frac{1}{h^2}\left(c_6 f_{N-5} + c_7 f_{N-6} + c_8 f_{N-7} + c_9 f_{N-8}\right), \end{aligned} \tag{80}$$

where $c_i = a_i$ for $1 \le i \le 9$ and a_i, A are obtained from (70) through (79).

Fourth-order accurate compact approximation: Fourth-order accurate compact approximations are required at $i = 1$ and $i = N$. Solving (58) through (63), we obtain $A = 10$, $a_1 = \frac{145}{12}$, $a_2 = \frac{-76}{3}$, $a_3 = \frac{29}{2}$, $a_4 = \frac{-4}{3}$, and $a_5 = \frac{1}{12}$, and all other a_i are zero. Hence, we have

$$\begin{aligned} f_1'' + 10 f_2'' &= \frac{145}{12h^2} f_1 - \frac{76}{3h^2} f_2 + \frac{29}{2h^2} f_3 - \frac{4}{3h^2} f_4 + \frac{1}{12h^2} f_5, \quad i = 1, \\ \frac{1}{10} f_{i-1}'' + f_i'' + \frac{1}{10} f_{i+1}'' &= \frac{6}{5}\frac{f_{i+1} - 2f_i + f_{i-1}}{h^2}, \quad 2 \le i \le N-1, \\ f_N'' + 10 f_{N-1}'' &= \frac{145}{12h^2} f_N - \frac{76}{3h^2} f_{N-1} + \frac{29}{2h^2} f_{N-2} - \frac{4}{3h^2} f_{N-3} + \frac{1}{12h^2} f_{N-4}. \\ & \quad i = N. \end{aligned}$$

The fourth-order compact approximation for the second derivative in matrix form can be written as

$$\mathbf{f}'' = D_{xx}^{d,1}\mathbf{f}, \tag{81}$$

where $D_{xx}^{d,1}$ is required differentiation matrix and

$$H_1 = \begin{pmatrix} 1 & 10 & 0 & 0 \dots 0 & 0 & 0 & 0 \\ \frac{1}{10} & 1 & \frac{1}{10} & 0 \dots 0 & 0 & 0 & 0 \\ \dots \dots \dots \dots \\ 0 & 0 & 0 & 0 \dots 0 & \frac{1}{10} & 1 & \frac{1}{10} \\ 0 & 0 & 0 & 0 \dots 0 & 0 & 10 & 1 \end{pmatrix},$$

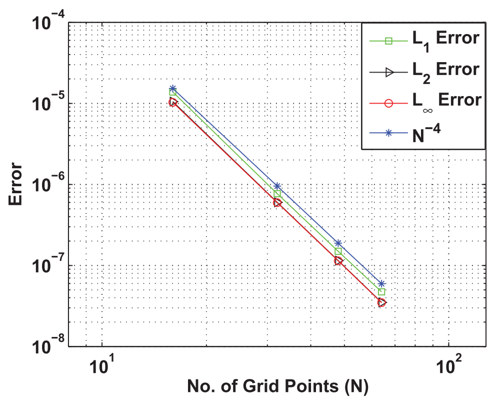
$$H_2 = \frac{1}{h^2} \begin{pmatrix} \frac{145}{12} & \frac{-76}{3} & \frac{29}{2} & -\frac{4}{3} & \frac{1}{12} & \dots & 0 & 0 & 0 & 0 & 0 \\ \frac{6}{5} & -\frac{12}{5} & \frac{6}{5} & 0 & 0 & \dots & 0 & 0 & 0 & 0 & 0 \\ \dots \dots \dots \dots \\ 0 & 0 & 0 & 0 & 0 & \dots & 0 & 0 & \frac{6}{5} & -\frac{12}{5} & \frac{6}{5} \\ 0 & 0 & 0 & 0 & 0 & \dots & \frac{1}{12} & -\frac{4}{3} & \frac{29}{2} & -\frac{76}{3} & \frac{145}{12} \end{pmatrix}.$$

Sixth-order accurate compact approximation: Sixth-order accurate compact approximations are required at $i = 1$, $i = 2$, $i = N - 1$, and $i = N$. For $i = 1$, solving (58) through (65) gives $A = \frac{126}{11}$, $a_1 = \frac{2077}{157}$, $a_2 = -\frac{2943}{110}$, $a_3 = \frac{573}{44}$, $a_4 = \frac{167}{99}$, $a_5 = -\frac{18}{11}$, $a_6 = \frac{57}{110}$, and $a_7 = -\frac{131}{1980}$, and other a_i are zero. For $i = 2$, solving (70) through (77) gives $A = \frac{11}{128}$, $a_1 = \frac{585}{512}$, $a_2 = -\frac{141}{64}$, $a_3 = \frac{459}{512}$, $a_4 = \frac{9}{32}$, $a_5 = -\frac{81}{512}$, $a_6 = \frac{3}{64}$, and $a_7 = \frac{-3}{512}$, and other a_i are zero. Hence, we have

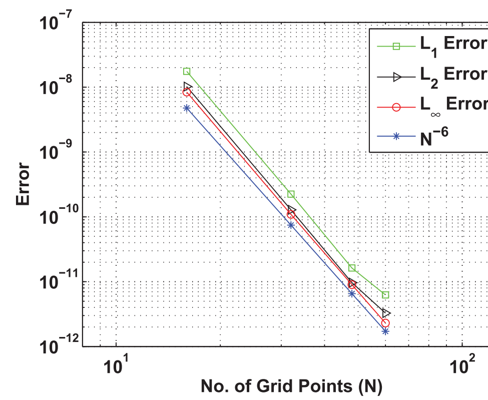
$$\begin{aligned} f_1'' + \frac{126}{11} f_2'' &= \frac{2077}{157h^2} f_1 - \frac{2943}{110h^2} f_2 + \frac{573}{44h^2} f_3 + \frac{167}{99h^2} f_4 - \frac{18}{11h^2} f_5 \\ &\quad + \frac{57}{110h^2} f_6 - \frac{131}{1980h^2} f_7, \quad i = 1, \\ \frac{11}{128} f_1'' + f_2'' + \frac{11}{128} f_3'' &= \frac{585}{512h^2} f_1 - \frac{141}{64h^2} f_2 + \frac{459}{512h^2} f_3 + \frac{9}{32h^2} f_4 \\ &\quad - \frac{81}{512h^2} f_5 + \frac{3}{64h^2} f_6 - \frac{3}{512} f_7, \quad i = 2, \\ \frac{2}{11} f_{i-1}'' + f_i'' + \frac{2}{11} f_{i+1}'' &= \frac{12}{11} \frac{f_{i+1} - 2f_i + f_{i-1}}{h^2} + \frac{3}{11} \frac{f_{i+2} - 2f_i + f_{i-2}}{4h^2}, \quad 3 \le i \le N-2, \\ \frac{11}{128} f_{N-2}'' + f_{N-1}'' + \frac{11}{128} f_N'' &= \frac{585}{512h^2} f_N - \frac{141}{64h^2} f_{N-1} + \frac{459}{512h^2} f_{N-2} + \frac{9}{32h^2} f_{N-3} \\ &\quad - \frac{81}{512h^2} f_{N-4} + \frac{3}{64h^2} f_{N-5} - \frac{3}{512} f_{N-6}, \quad i = N-1, \\ f_N'' + \frac{126}{11} f_{N-1}'' &= \frac{2077}{157h^2} f_N - \frac{2943}{110h^2} f_{N-1} + \frac{573}{44h^2} f_{N-2} + \frac{167}{99h^2} f_{N-3} \\ &\quad - \frac{18}{11h^2} f_{N-4} + \frac{57}{110h^2} f_{N-5} - \frac{131}{1980h^2} f_{N-6}, \quad i = N. \end{aligned}$$

For the sixth-order compact approximation for the second derivative, H_1 and H_2 may be written as

$$H_1 = \begin{pmatrix} 1 & \frac{126}{11} & 0 & 0 & \dots & 0 & 0 & 0 & 0 \\ \frac{11}{128} & 1 & \frac{11}{128} & 0 & \dots & 0 & 0 & 0 & 0 \\ 0 & \frac{2}{11} & 1 & \frac{2}{11} & \dots & 0 & 0 & 0 & 0 \\ \dots \dots \dots \dots \\ 0 & 0 & 0 & 0 & \dots & \frac{2}{11} & 1 & \frac{2}{11} & 0 \\ 0 & 0 & 0 & 0 & \dots & 0 & \frac{11}{128} & 1 & \frac{11}{128} \\ 0 & 0 & 0 & 0 & \dots & 0 & 0 & \frac{126}{11} & 1 \end{pmatrix},$$



(a)



(b)

Fig. 11. Second derivative approximations of $sin(x)$ on $[0, 1]$ with Dirichlet boundary conditions using fourth-order accurate compact approximations (a) and sixth-order accurate compact approximations (b).

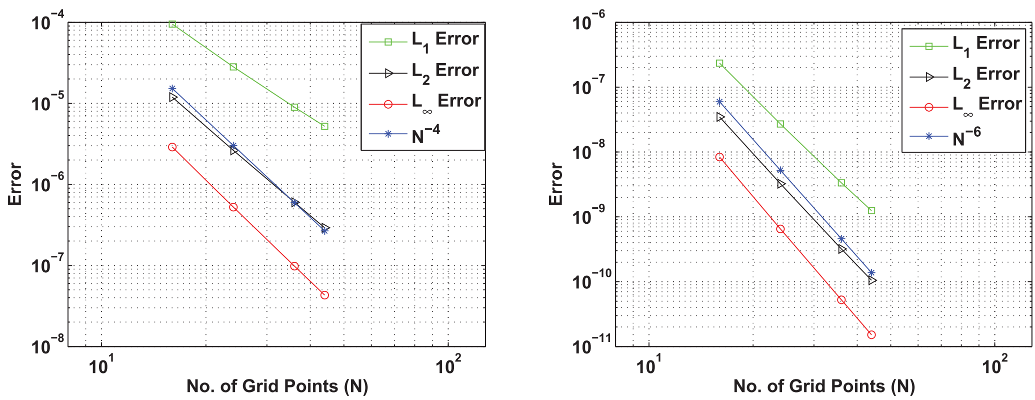
$$H_2 = \frac{1}{h^2}\begin{pmatrix} \frac{2077}{157} & -\frac{2943}{110} & \frac{573}{44} & \frac{167}{99} & \frac{18}{11} & \frac{57}{110} & -\frac{131}{1980} & \dots & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{585}{512} & -\frac{141}{64} & \frac{459}{512} & \frac{9}{32} & -\frac{81}{512} & \frac{3}{64} & -\frac{3}{512} & \dots & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -\frac{3}{44} & -\frac{12}{11} & -\frac{51}{22} & \frac{12}{11} & \frac{3}{44} & 0 & 0 & \dots & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \dots & \dots & \dots & \dots & \dots & & & & & & & & & & \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \dots & 0 & 0 & \frac{3}{44} & \frac{12}{11} & -\frac{51}{22} & -\frac{12}{11} & -\frac{3}{44} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \dots & -\frac{3}{512} & \frac{3}{64} & -\frac{81}{512} & \frac{9}{32} & \frac{459}{512} & -\frac{141}{64} & \frac{585}{512} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \dots & -\frac{131}{1980} & \frac{57}{110} & \frac{18}{11} & \frac{167}{99} & \frac{573}{44} & -\frac{2943}{110} & \frac{2077}{157} \end{pmatrix}.$$

The preceding results were validated using the test function $sin(x)$ on the interval $[0, 1]$. The error plot given in Figure 11 confirms the order of accuracy of the scheme. The function `second_compact_dirichlet.m` computes $D_{xx}^{d,1}$ (see Section 11 of the accompanying User Manual for details).

Remark 5. In the case of Dirichlet boundary conditions, we restrict ourselves to second derivative approximation in this article. However, compact schemes for the approximation of third and higher derivatives may be developed in an analogous way. Moreover, Fourier analysis of these boundary schemes may be performed in the similar way to Section 2.3.

3.2 High-Order Compact Finite Difference Schemes in Two Dimensions with Dirichlet Boundary Conditions

High-order compact finite difference approximations for partial derivatives are discussed in this section, and we derive up to sixth-order accurate compact schemes. We represent the unknown function $f_{i,j} = f(x_i, y_j)$ in vector form where $1 \le i \le N$ and $1 \le j \le N$. Hence, $\mathbf{f} = (f_{1,1}, f_{2,1}, \dots, f_{N,1}, f_{1,2}, \dots, f_{N,N})^T$ and the differentiation matrix will be of order N^2.



(a) (b)

Fig. 12. Partial derivative ($\frac{\partial}{\partial x}$) approximations of $sin(x)cos(y)$ on $[0, 1] \times [0, 1]$ with Dirichlet boundary conditions using fourth-order accurate compact approximation (a) and sixth-order accurate compact approximation (b).

3.2.1 Approximation of $\frac{\partial}{\partial x}$. If $D_x^{d,2}$ represents the differentiation matrix corresponding to the $\frac{\partial}{\partial x}$, then

$$D_x^{d,2} = \begin{pmatrix} D_x^{d,1} & 0 & 0\;0\;\ldots\;0\;0 & 0 & 0 \\ 0 & D_x^{d,1} & 0\;0\;\ldots\;0\;0 & 0 & 0 \\ \ldots\ldots\ldots\ldots\ldots\ldots & & & & \\ 0 & 0 & 0\;0\;\ldots\;0\;0 & D_x^{d,1} & 0 \\ 0 & 0 & 0\;0\;\ldots\;0\;0 & 0 & D_x^{d,1} \end{pmatrix}, \tag{82}$$

where $D_x^{d,1}$ is the differentiation matrix corresponding to the first derivative discussed in Section 3.1.1. We use fourth- or sixth-order accurate $D_x^{d,1}$ to obtain fourth- or sixth-order accurate approximation for $D_x^{d,2}$, respectively.

The preceding results were validated using the test function $sin(x)cos(y)$ on $[0, 1] \times [0, 1]$. Error plots given in Figure 12 confirm the order of accuracy of the scheme. The function `first_compact_dirichlet_2dx.m` computes $D_x^{d,2}$ (see Section 12 of the accompanying User Manual for details).

3.2.2 Approximation of $\frac{\partial}{\partial y}$. The differentiation matrix for $\frac{\partial}{\partial y}$ can be obtained by using $D_x^{d,2}$ given by (82). If $D_y^{d,2}$ represents the differentiation matrix corresponding to $\frac{\partial}{\partial y}$, then Algorithm 3 may be used to obtain $D_y^{d,2}$.

The preceding results were validated using the test function $sin(x)cos(y)$ on $[0, 1] \times [0, 1]$. Error plots given in Figure 13 confirm the order of accuracy of the scheme. The function `first_compact_dirichlet_2dy.m` computes $D_y^{d,2}$ (see Section 13 of the accompanying User Manual for details).

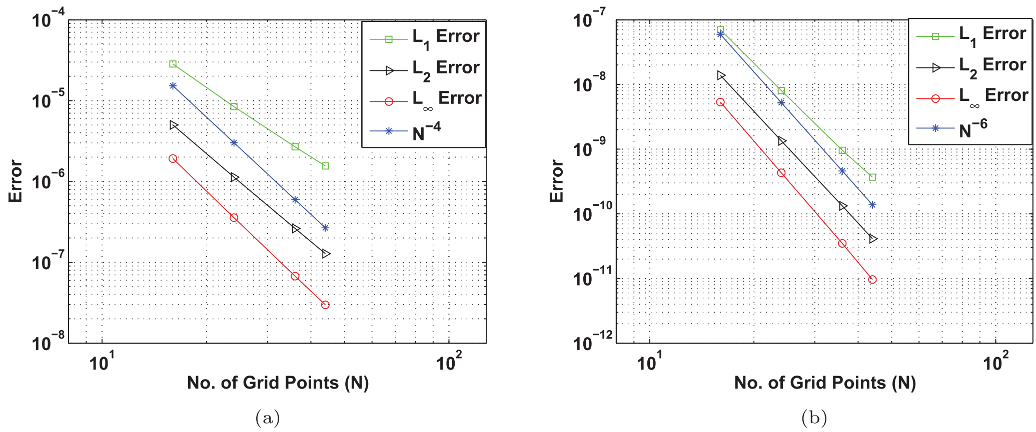


Fig. 13. Partial derivative ($\frac{\partial}{\partial y}$) approximations of $sin(x)cos(y)$ on $[0, 1] \times [0, 1]$ with Dirichlet boundary conditions using fourth-order accurate compact approximation (a) and sixth-order accurate compact approximation (b).

ALGORITHM 3: Algorithm for Approximation of $\frac{\partial}{\partial y}$

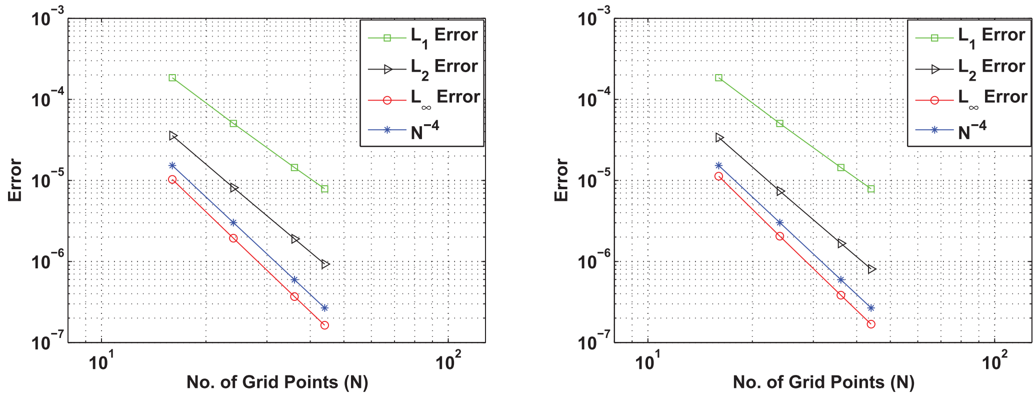
$m = 1$
for $k = 1, 2, \ldots, N$
  $g = 1$
  for $i = 1 : N$
    for $j = 1 : N$
      $D_y^{d,2}(m, N(j-1) + g) = D_x^{d,2}(k, j)$
    end
    $m = m + 1$
    $g = g + 1$
  end
end

3.2.3 *Approximation of* $\frac{\partial^2}{\partial x^2}$. If $D_{xx}^{d,2}$ represents the differentiation matrix corresponding to $\frac{\partial^2}{\partial x^2}$, then

$$D_{xx}^{d,2} = \begin{pmatrix} D_{xx}^{d,1} & 0 & 0\ 0 \ldots 0\ 0 & 0 & 0 \\ 0 & D_{xx}^{d,1} & 0\ 0 \ldots 0\ 0 & 0 & 0 \\ \ldots\ldots & \ldots\ldots & \ldots\ldots \\ 0 & 0 & 0\ 0 \ldots 0\ 0 & D_{xx}^{d,1} & 0 \\ 0 & 0 & 0\ 0 \ldots 0\ 0 & 0 & D_{xx}^{d,1} \end{pmatrix}, \tag{83}$$

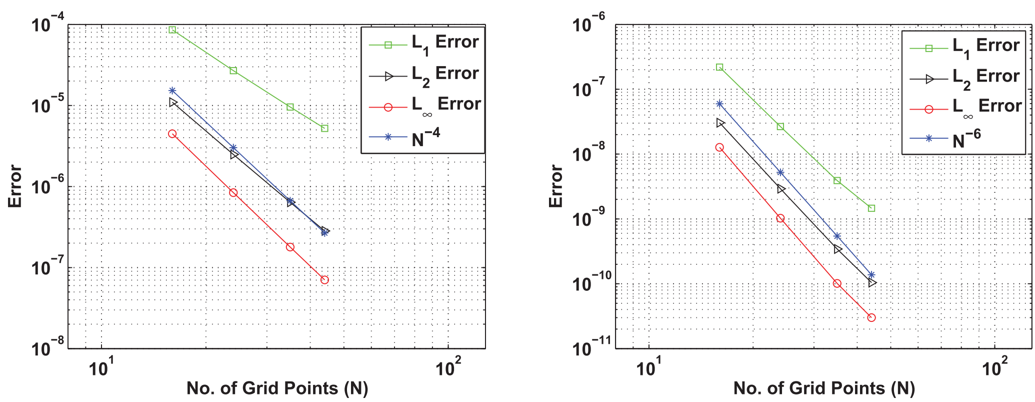
where $D_{xx}^{d,1}$ is the differentiation matrix corresponding to the second derivative discussed in Section 3.1.2.

The preceding results were validated using the test function $sin(x)cos(y)$ on $[0, 1] \times [0, 1]$. Error plots given in Figure 14(b) confirm the order of accuracy of the scheme. The function `second_compact_dirichlet_2dxx.m` computes $D_{xx}^{d,2}$ (see Section 14 of the accompanying User Manual for details).



(a) (b)

Fig. 14. Fourth-order accurate partial derivative approximation of $sin(x)cos(y)$ on $[0, 1] \times [0, 1]$ with Dirichlet boundary conditions ($\frac{\partial^2}{\partial x^2}$) approximation (a) and ($\frac{\partial^2}{\partial y^2}$) approximation (b).



(a) (b)

Fig. 15. Mixed derivative $\frac{\partial^2}{\partial x \partial y}$ approximation of $sin(x)cos(y)$ on $[0, 1] \times [0, 1]$ with Dirichlet boundary conditions using fourth-order accurate compact approximation (a) and sixth-order accurate compact approximation (b).

3.2.4 Approximation of $\frac{\partial^2}{\partial y^2}$. If $D_{yy}^{d,2}$ represents the differentiation matrix corresponding to $\frac{\partial^2}{\partial y^2}$, then Algorithm 4 may used to obtain the $D_{yy}^{d,2}$. The preceding results were validated using the test function $sin(x)cos(y)$ on $[0, 1] \times [0, 1]$. Error plots given in Figure 15 confirm the order of accuracy of the scheme. The function `second_compact_dirichlet_2dyy.m` computes $D_{yy}^{d,2}$ (see Section 15 of the accompanying User Manual for details).

3.2.5 Approximation of Mixed Derivatives With Dirichlet Boundary Conditions. In this section, high-order compact finite difference schemes for mixed derivatives are discussed. For more details on compact schemes for mixed derivatives, see Sen (2013, 2016). Approximation to $\frac{\partial^2}{\partial x \partial y}$ may be obtained by using $D_x^{d,1}$ and $D_y^{d,1}$ from (56). If $D_{xy}^{d,2}$ represents the differentiation matrix correspond-

ALGORITHM 4: Algorithm for Approximation of $\frac{\partial^2}{\partial y^2}$

$m = 1$
for $k = 1, 2, \ldots, N$
  $g = 1$
  for $i = 1 : N$
    for $j = 1 : N$
      $D_{yy}^{d,2}(m, N(j-1)+g) = D_{xx}^{d,2}(k, j)$
    end
    $m = m + 1$
    $g = g + 1$
  end
end

ing to the $\frac{\partial^2}{\partial x \partial y}$, then

$$D_{xy}^{d,2} = kron\left(D_x^{d,1}, D_y^{d,1}\right), \tag{84}$$

where matrix $D_y^{d,1}$ is obtained from (56) in the y direction. Here, $kron$ is a built in Matlab function, which returns the tensor product of two matrices.

The preceding results were validated using the test function $sin(x)cos(y)$ on $[0,1] \times [0,1]$. Error plots given in Figure 15 confirm the order of accuracy of the scheme. The function `mixed_compact_dirichlet_2dxy.m` computes $D_{xy}^{d,2}$ (see Section 16 of the accompanying User Manual for details).

4 HIGH-ORDER COMPACT SCHEMES FOR NEUMANN BOUNDARY CONDITIONS

In this section, a fourth-order accurate compact scheme for second derivative approximation with Neumann boundary conditions is discussed. In this case, Neumann boundary conditions are given as $f_x(x_1) = g_1$ and $f_x(x_N) = g_2$. For interior points, the fourth-order compact finite difference scheme from Section 2.1.2 may be written as

$$\frac{1}{10} f''_{i-1} + f''_i + \frac{1}{10} f''_{i+1} = \frac{6}{5} \frac{f_{i+1} - 2f_i + f_{i-1}}{h^2}, \quad 2 \le i \le N-1. \tag{85}$$

To incorporate the Neumann boundary conditions, fourth-order accurate compact relations are needed at the boundary points (i.e., $i = 1$ and N).

Boundary formulation for $i = 1$ and N: Compact fourth-order accurate relations at $i = 1$ and $i = N$ can be written as (Zhao et al. 2007)

$$\frac{11}{6} f''_1 - \frac{1}{3} f''_2 = -\frac{g_1}{h} + \frac{f_2 - f_1}{h^2}, \quad i = 1, \tag{86}$$

$$\frac{11}{6} f''_N - \frac{1}{3} f''_{N-1} = \frac{g_2}{h} + \frac{f_{N-1} - f_N}{h^2}, \quad i = N. \tag{87}$$

Now, (85) through (87) give a complete fourth-order scheme in the case of Neumann boundary conditions. Thus, the fourth-order compact approximation for the second derivative may be written in matrix form as

$$H_1 \mathbf{f}'' = -\frac{2}{h^2} H_2 \mathbf{f} + 12\mathbf{g},$$

where

$$H_1 = \begin{pmatrix} 22 & -4 & 0 & 0 & \dots & 0 & 0 & 0 & 0 \\ 1 & 10 & 1 & 0 & \dots & 0 & 0 & 0 & 0 \\ \dots & \dots & \dots & \dots & & & & & \\ 0 & 0 & 0 & 0 & \dots & 0 & 1 & 10 & 1 \\ 0 & 0 & 0 & 0 & \dots & 0 & 0 & -4 & 22 \end{pmatrix},$$

$$H_2 = \begin{pmatrix} 6 & -6 & 0 & 0 & \dots & 0 & 0 & 0 & 0 \\ -6 & 12 & -6 & 0 & \dots & 0 & 0 & 0 & 0 \\ \dots & \dots & \dots & \dots & & & & & \\ 0 & 0 & 0 & 0 & \dots & 0 & -6 & 12 & -6 \\ 0 & 0 & 0 & 0 & \dots & 0 & 0 & -6 & 6 \end{pmatrix},$$

and $\mathbf{g} = (-\frac{g_1}{h}, 0, \dots, 0, \frac{g_2}{h})^T$. For more details about the compact schemes with Neumann boundary conditions, see Zhao et al. (2007). The function `compact_second_neumann.m` computes the differentiation matrix corresponding to the second derivative approximation of a function with Neumann boundary conditions (see Section 17 of the accompanying User Manual for details).

5 CONCLUSION

A procedure for numerical differentiation of the functions is presented using compact finite difference schemes. Compact finite difference schemes of the 10th order for first and second derivative approximations and compact schemes of the 6th order for third and fourth derivative approximations are discussed for the functions with periodic boundary conditions. Compact finite difference schemes are compared to classical finite difference schemes using Fourier analysis, and it is observed that these schemes have better resolution characteristics. Moreover, derivative approximations for the functions with Dirichlet and Neumann boundary conditions are also obtained. Compact schemes are also discussed for the functions with two independent variables. We have validated the results using the test functions. The presented work can be used for solving partial differential equations in one and two dimensions.

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