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High Order Compact Scheme for Dirichlet Boundary Points

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Abstract: *In this paper, we introduce a new high order scheme for boundary points when calculating the derivative of smooth functions by Compact Scheme. The primitive function reconstruction method of ENO schemes is applied to obtain the conservative form of the Compact Scheme. Equations for approximating the derivatives around the boundary points* 1 *and* N *are determined for the Dirichlet boundary conditions. Numerical tests are presented to demonstrate the capabilities of this new scheme, and a comparison to the lower-order boundary scheme shows its advantages.*

1 Introduction

Throughout the years, compact schemes have been extensively used in the simulation of complex flow which requires high-order accurate numerical schemes with low dispersion and dissipation errors [1, 2, 3]. Due to the properties of the compact scheme, it is necessary to use high order equations also near the boundary. Most of the analyses of the order of schemes were concentrated on the inner points' equations, by either applying periodic boundary conditions or by using examples where the values near the boundary are never affected [4, 5, 7]. This kind of approach may not correctly define the *global* order of the scheme when non-periodic boundary conditions, such as Dirichlet or Neumann, are applied, or when the solution is dynamic near the boundary.

In this paper, a new high-order class of compact schemes for the boundary points is developed, namely sixth order (it will be called the "6-6-6" scheme throughout the paper). Equations of the interior and boundary points for the conservative formulation are derived, assuming Dirichlet boundary conditions are given. Their respective truncation errors are also determined. The scheme is applied to numerical examples to demonstrate its capabilities. Also, a comparison to the standard lower-order boundary compact scheme (called the "3-4-6-4-3" scheme), which uses third order equations at the boundary, fourth order equations near the boundary, and sixth order at the interior points, will be presented.

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2 Compact Scheme

2.1 Basic Formulation

A Padé-type compact scheme can be constructed based on the Hermite interpolation where both function and derivative at grid points are involved, e.g. a fourth order finite difference scheme can be constructed if both the function and first derivative are used at three grid points. Given the values of a function on a set of nodes, the finite difference approximation to the derivative of the function is expressed as a linear combination of the given function values. For a function f, we may write a compact scheme by using five grid points [6]:

$$\begin{aligned} &\beta_- f'_{j-2} + \alpha_- f'_{j-1} + f'_j + \alpha_+ f'_{j+1} + \beta_+ f'_{j+2} = \\ &= \tfrac{1}{h}\left(a f_{j-2} + b f_{j-1} + c f_j + d f_{j+1} + e f_{j+2}\right), \end{aligned} \tag{1}$$

where h is the mesh spacing.

Equation (1) can achieve up to 8th order of accuracy, depending on the values of the constants.

If we assume a symmetric and tri-diagonal system, by setting $\beta_- = \beta_+ = 0$, we obtain a one-parameter family of fourth-order compact schemes [6]:

$$\begin{aligned} &\alpha f'_{j-1} + f'_j + \alpha f'_{j+1} = \\ &= \frac{1}{h}\left[-\frac{4\alpha-1}{12} f_{j-2} - \frac{\alpha+2}{3} f_{j-1} + \frac{\alpha+2}{3} f_{j+1} + \frac{4\alpha-1}{12} f_{j+2}\right]. \end{aligned} \tag{2}$$

With $\alpha = \frac{1}{3}$, a sixth order compact scheme can be obtained:

$$\frac{1}{3} f'_{j-1} + f'_j + \frac{1}{3} f'_{j+1} = \frac{1}{h}\left[-\frac{1}{36} f_{j-2} - \frac{7}{9} f_{j-1} + \frac{7}{9} f_{j+1} + \frac{1}{36} f_{j+2}\right]. \tag{3}$$

2.2 Conservative property

It is important to maintain the conservation property of the scheme for shock wave capturing, as conservative numerical methods locate shocks correctly. Let us describe the conservative formulation to be applied in our scheme.

For 1-D conservation laws

$$u_t(x,t) + f_x(u(x,t)) = 0, \tag{4}$$

a semi-discrete conservative form of (4) can be determined when a conservative approximation to the spatial derivative f_x is applied [5]:

$$\frac{du_j}{dt} = -\frac{1}{h}(\hat{f}_{j+\frac{1}{2}} - \hat{f}_{j-\frac{1}{2}}), \tag{5}$$

where $f_j = \frac{1}{h}\int_{x_j-\frac{h}{2}}^{x_j+\frac{h}{2}} \hat{f}(\xi) d\xi$. $\hat{f}$ is the flux defined by the integration, which is an exact expression of the flux, but it is different from f.

If we define H as the primitive function of $\hat{f}$,

$$H\left(x_{j+1/2}\right) = \int_{-\infty}^{x_j+\frac{h}{2}} \hat{f}(\xi)d\xi = \sum_{i=-\infty}^{j} \int_{x_i-\frac{h}{2}}^{x_i+\frac{h}{2}} \hat{f}(\xi)d\xi = h\sum_{i=-\infty}^{j} f_i, \tag{6}$$

then H is easy to be calculated.

The numerical flux $\hat{f}$ at the cell interfaces is the derivative of its primitive function H, i.e.,

$$\hat{f}_{j+\frac{1}{2}} = H'_{j+\frac{1}{2}}. \tag{7}$$

All equations given above are exact without approximations. However, the primitive function H is a discrete data set and we must use a numerical method to obtain the derivatives of H, which will introduce numerical errors, or in other words, order of accuracy.

This procedure, $f \to H \to \hat{f} \to f'$, is called *reconstruction*, introduced by Shu & Osher [8, 9], and the application of the numerical scheme to the primitive function instead of the function itself ensures that the conservative property is attained.

There is only one problem left for the numerical method, which is how to determine (7), or how to obtain accurate derivatives, for a discrete data set.

3 Obtaining the derivatives

Consider a uniformly spaced mesh where the nodes are indexed by i, and the independent variable at the nodes is $x_i = a + h(i-1)$ for $1 \le i \le N$, with $a \le x_i \le b$, then $h = \frac{b-a}{N-1}$ is the mesh spacing. The function values at the nodes, $f_i = f(x_i)$, are given. To determine the approximations to the derivatives f'_i, $i = 1, 2, \ldots, N$, where $i = 1$ and $i = N$ are respectively the left and right boundary points, we must first calculate the derivatives of the primitive function $H_{j+1/2}$, $H'_{j+1/2}$, for $j = 0, 1, 2, \ldots, N$. For this, we define two sets of points: the interior points $j = 2, \ldots, N-2$ and the boundary points $j = 0, 1$ and $j = N-1, N$.

3.1 Interior points

Let us determine the relationship between H and H' for the interior points $j = 2, 3, \ldots, N-2$, by using the compact scheme formulation.

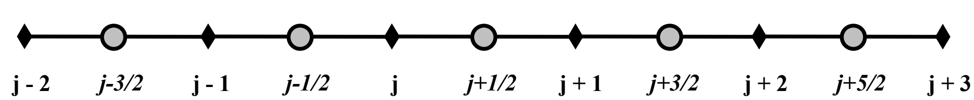


Figure 1: Compact Scheme formulation

Our objective is to obtain a sixth order compact scheme centered at $j+1/2$ (see Figure 1);

then, by using 5 function values and 3 derivatives, we obtain

$$\frac{1}{3}H'_{j-\frac{1}{2}} + H'_{j+\frac{1}{2}} + \frac{1}{3}H'_{j+\frac{3}{2}} = \\ = \frac{1}{h}\left(-\frac{1}{36}H_{j-\frac{3}{2}} - \frac{7}{9}H_{j-\frac{1}{2}} + \frac{7}{9}H_{j+\frac{3}{2}} + \frac{1}{36}H_{j+\frac{5}{2}}\right). \tag{8}$$

The truncation error of equation (8) can be found by using a Taylor expansion around $j+1/2$,

$$\frac{1}{3}H'_{j-\frac{1}{2}} + H'_{j+\frac{1}{2}} + \frac{1}{3}H'_{j+\frac{3}{2}} - \frac{1}{h}\left(-\frac{1}{36}H_{j-\frac{3}{2}} - \frac{7}{9}H_{j-\frac{1}{2}} + \frac{7}{9}H_{j+\frac{3}{2}} + \frac{1}{36}H_{j+\frac{5}{2}}\right) = \\ = -\frac{1}{1260}h^6 H^{(7)}_{j+\frac{1}{2}} - \frac{1}{15120}h^8 H^{(9)}_{j+\frac{1}{2}} + \dots,$$

which shows that a sixth order of accuracy is obtained for the formula of the interior points.

3.2 Boundary points

In the previous subsection we have determined the formula to be applied for the interior points $j = 2, 3, \dots, N-2$. Now, let us determine the equations for the points near the boundaries at $j = 0, 1$ and $j = N-1, N$.

The equations for the boundary points will be different from the equations of the interior points, since there are no left or right nodes which could be used next to the left boundary or right boundary points, respectively. Depending on how many nodes we use, we can derive different order schemes for the boundary points.

The Dirichlet boundary conditions given in this case are $f(a) = A$ and $f(b) = B$.

In order to maintain the tri-diagonal nature of the schemes, we are using two point derivatives instead of three for the first point $j = 0$ and last point $j = N$.

a) For $j = 0$, we can use two derivatives and six points to obtain a 6th order scheme approximating the value of $H'_{\frac{1}{2}}$:

$$H'_{\frac{1}{2}} + 5H'_{\frac{3}{2}} = \\ = \frac{1}{h}\left(-\frac{197}{60}H_{\frac{1}{2}} - \frac{5}{12}H_{\frac{3}{2}} + 5H_{\frac{5}{2}} - \frac{5}{3}H_{\frac{7}{2}} + \frac{5}{12}H_{\frac{9}{2}} - \frac{1}{20}H_{\frac{11}{2}}\right). \tag{9}$$

The truncation error of equation (9) can be found by using Taylor expansion:

$$H'_{\frac{1}{2}} + 5H'_{\frac{3}{2}} - \frac{1}{h}\left(-\frac{197}{60}H_{\frac{1}{2}} - \frac{5}{12}H_{\frac{3}{2}} + 5H_{\frac{5}{2}} - \frac{5}{3}H_{\frac{7}{2}} + \frac{5}{12}H_{\frac{9}{2}} - \frac{1}{20}H_{\frac{11}{2}}\right) = \\ = \frac{1}{42}h^6 H^{(7)}_{\frac{1}{2}} + \frac{1}{21}h^7 H^{(8)}_{\frac{1}{2}} + \frac{13}{252}h^8 H^{(9)}_{\frac{1}{2}} + \dots$$

b) Similarly, for $j = N$, we can also use two derivatives and six points to obtain a 6$^{\text{th}}$ order scheme approximating the value of $H'_{N+\frac{1}{2}}$:

$$5H'_{N-\frac{1}{2}} + H'_{N+\frac{1}{2}} = \frac{1}{h}\left(\frac{197}{60}H_{N+\frac{1}{2}} + \right. \\ \left. + \frac{5}{12}H_{N-\frac{1}{2}} - 5H_{N-\frac{3}{2}} + \frac{5}{3}H_{N-\frac{5}{2}} - \frac{5}{12}H_{N-\frac{7}{2}} + \frac{1}{20}H_{N-\frac{9}{2}}\right). \tag{10}$$

The truncation error of equation (10) will be:

$$5H'_{N-\frac{1}{2}}+H'_{N+\frac{1}{2}}-\frac{1}{h}\left(\frac{197}{60}H_{N+\frac{1}{2}}+\frac{5}{12}H_{N-\frac{1}{2}}-5H_{N-\frac{3}{2}}+\frac{5}{3}H_{N-\frac{5}{2}}+\right.$$
$$\left.-\frac{5}{12}H_{N-\frac{7}{2}}+\frac{1}{20}H_{N-\frac{9}{2}}\right)=\frac{1}{42}h^6H^{(7)}_{N+\frac{1}{2}}-\frac{1}{21}h^7H^{(8)}_{N+\frac{1}{2}}+\frac{13}{252}h^8H^{(9)}_{N+\frac{1}{2}}+\dots$$

c) For $j=1$, three derivatives and five points are used to obtain the sixth order scheme approximating the value of $H'_{\frac{3}{2}}$:

$$\frac{1}{8}H'_{\frac{1}{2}}+H'_{\frac{3}{2}}+\frac{3}{4}H'_{\frac{5}{2}}=\frac{1}{h}\left(-\frac{43}{96}H_{\frac{1}{2}}-\frac{5}{6}H_{\frac{3}{2}}+\frac{9}{8}H_{\frac{5}{2}}+\frac{1}{6}H_{\frac{7}{2}}-\frac{1}{96}H_{\frac{9}{2}}\right). \quad (11)$$

The truncation error of (11) is given below:

$$\frac{1}{8}H'_{\frac{1}{2}}+H'_{\frac{3}{2}}+\frac{3}{4}H'_{\frac{5}{2}}-\frac{1}{h}\left(-\frac{43}{96}H_{\frac{1}{2}}-\frac{5}{6}H_{\frac{3}{2}}+\frac{9}{8}H_{\frac{5}{2}}+\frac{1}{6}H_{\frac{7}{2}}-\frac{1}{96}H_{\frac{9}{2}}\right)=$$
$$=\frac{1}{840}h^6H^{(7)}_{\frac{3}{2}}+\frac{1}{1344}h^7H^{(8)}_{\frac{3}{2}}+\frac{1}{2880}h^8H^{(9)}_{\frac{3}{2}}+\dots$$

d) Similarly, for $j=N-1$, we use three derivatives and five points to obtain the 6th order scheme approximating the value of $H'_{N-\frac{1}{2}}$:

$$\frac{3}{4}H'_{N-\frac{3}{2}}+H'_{N-\frac{1}{2}}+\frac{1}{8}H'_{N+\frac{1}{2}}=$$
$$=\frac{1}{h}\left(\frac{43}{96}H_{N+\frac{1}{2}}+\frac{5}{6}H_{N-\frac{1}{2}}-\frac{9}{8}H_{N-\frac{3}{2}}-\frac{1}{6}H_{N-\frac{5}{2}}+\frac{1}{96}H_{N-\frac{7}{2}}\right). \quad (12)$$

The truncation error of (12) will be:

$$\frac{3}{4}H'_{N-\frac{3}{2}}+H'_{N-\frac{1}{2}}+\frac{1}{8}H'_{N+\frac{1}{2}}+$$
$$-\frac{1}{h}\left(\frac{43}{96}H_{N+\frac{1}{2}}+\frac{5}{6}H_{N-\frac{1}{2}}-\frac{9}{8}H_{N-\frac{3}{2}}-\frac{1}{6}H_{N-\frac{5}{2}}+\frac{1}{96}H_{N-\frac{7}{2}}\right)=$$
$$=\frac{1}{840}h^6H^{(7)}_{N-\frac{1}{2}}-\frac{1}{1344}h^7H^{(8)}_{N-\frac{1}{2}}+\frac{1}{2880}h^8H^{(9)}_{N-\frac{1}{2}}+\dots$$

The equations (8)-(12) are then used to create a symmetric tri-diagonal implicit system of $N+1$ equations that is solved to determine the derivatives $H'_{j+1/2}$, $j=0,1,2,\dots,N$.

4 Numerical Results

We will first demonstrate that the newly developed sixth order scheme (6-6-6) can actually achieve sixth order by using Dirichlet boundary conditions, for different smooth functions, and then we compare the results of the Dirichlet boundary conditions to the previous scheme with lower order equations at the boundaries (3-4-6-4-3).

4.1 6-6-6 Scheme for Dirichlet boundary conditions

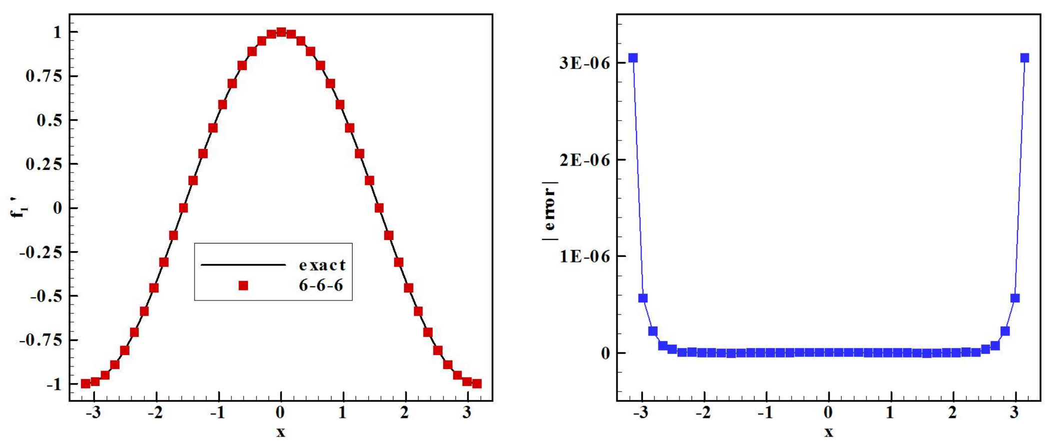
We first test the functions $f_1(x)=\sin(x)$, $f_2(x)=\sin(8x)$ and $f_3(x)=\sin(3x)+\cos(2x)$, $x\in[-\pi,\pi]$, with corresponding Dirichlet boundary conditions $f_1(-\pi)=0$, $f_1(\pi)=0$;

$f_2(-\pi) = 0$, $f_2(\pi) = 0$;$f_3(-\pi) = 1$, $f_3(\pi) = 1$. All these test functions have analytic derivatives, $f_1'(x) = \cos(x)$, $f_2'(x) = 8\cos(8x)$, and $f_3'(x) = 3\cos(3x) - 2\sin(2x)$.

(a) For the function $f_1(x) = \sin(x)$, $x \in [-\pi, \pi]$, we obtain the L_1, L_2, and L_∞ errors and their corresponding orders for various values of N (Table 1). Note that N includes the right boundary point, and so the number of spatial subdivisions is $N - 1$. The comparison of the exact and the numerical solution for the derivative, $f_1'(x) = \cos(x)$, with $N = 41$, is shown in Figure 2(a), and the numerical error at each point is shown in Figure 2(b). We can observe that the largest absolute values of the errors appear near the boundary points.

N	L_1 Error	L_1 Order	L_2 Error	L_2 Order	L_∞ Error	L_∞ Order
11	2.50E-02	-	1.39E-02	-	9.65E-03	-
21	4.86E-04	5.69	2.68E-04	5.70	1.86E-04	5.70
41	8.06E-06	5.91	4.40E-06	5.93	3.05E-06	5.93
81	1.30E-07	5.95	6.97E-08	5.98	4.83E-08	5.98
161	8.54E-09	5.93	1.09E-09	6.00	7.57E-10	6.00
321	1.41E-10	3.92	1.96E-11	5.80	1.19E-11	5.99

Table 1: Errors of the numerical solution for $f_1(x) = \sin(x)$



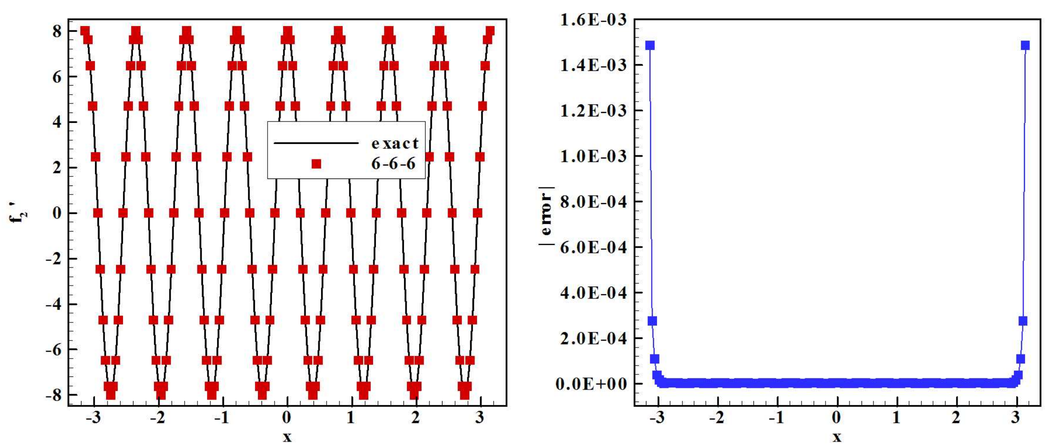
(a) (b)

Figure 2: (a) Derivatives and (b) Numerical errors for f_1 with $N = 41$

(b) We repeat the analysis for a different function, $f_2(x) = \sin(8x)$, $x \in [-\pi, \pi]$. The L_1, L_2, and L_∞ errors and their corresponding orders for various values of N were calculated and are displayed in Table 2. The comparison of the exact and the numerical solution for the derivative, $f_2'(x) = 8\cos(8x)$, with $N = 161$, is shown in Figure 3(a), and the numerical error at each point is shown in Figure 3(b). We can observe that, with this function, the largest absolute values of the errors are also located close to the boundary points.

N	L_1 Error	L_1 Order	L_2 Error	L_2 Order	L_∞ Error	L_∞ Order
41	4.57	-	2.40	-	1.68	-
81	2.10E-01	4.44	1.11E-01	4.44	7.70E-02	4.45
161	4.22E-03	5.64	2.14E-03	5.69	1.49E-03	5.70
321	7.47E-05	5.82	3.52E-05	5.93	2.44E-05	5.93
641	1.36E-06	5.78	5.58E-07	5.98	3.86E-07	5.98
1281	2.69E-08	5.66	8.71E-09	6.00	6.03E-09	6.00

Table 2: Errors of the numerical solution for $f_2(x) = \sin(8x)$



(a) (b)

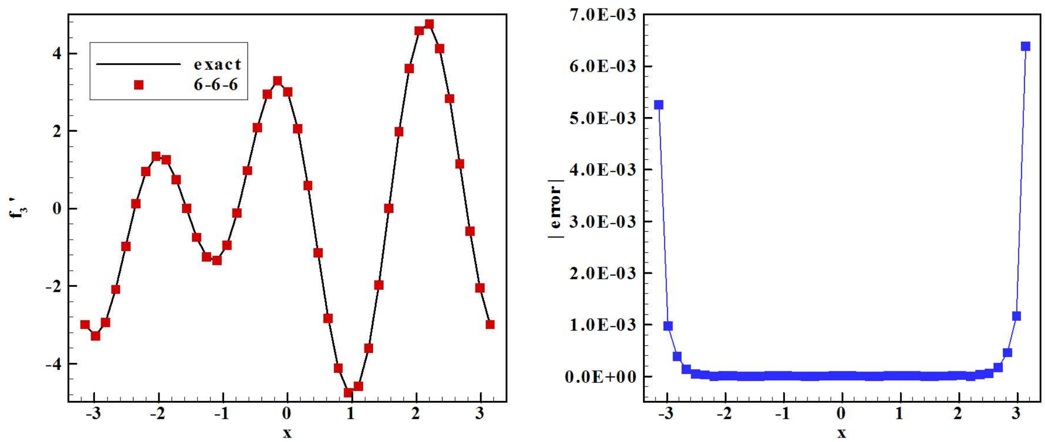
Figure 3: (a) Derivatives and (b) Numerical errors for f_2 with $N = 161$

(c) Once again, the analysis is repeated for the function $f_3(x) = \sin(3x) + \cos(2x)$, $x \in [-\pi, \pi]$. The L_1, L_2, and L_∞ errors and their corresponding orders for various values of N were calculated and are displayed in Table 3. The comparison of the exact and the numerical solution for the derivative, $f_3'(x) = 3\cos(3x) - 2\sin(2x)$, with $N = 41$, is shown in Figure 4(a), and the numerical error at each point is shown in Figure 4(b). A similar behavior for the numerical error can be observed for this function.

The investigation performed on the three functions shows that the scheme 6-6-6 is capable of achieving sixth-order accuracy for the whole interval when Dirichlet boundary conditions are applied.

N	L_1 Error	L_1 Order	L_2 Error	L_2 Order	L_∞ Error	L_∞ Order
11	7.07	-	3.48	-	2.71	-
21	5.78E-01	3.61	3.20E-01	3.44	2.31E-01	3.56
41	1.54E-03	5.23	8.44E-03	5.25	6.38E-03	5.17
81	2.77E-04	5.80	1.50E-04	5.81	1.22E-04	5.70
161	4.63E-06	5.90	2.55E-06	5.88	2.30E-06	5.73
321	7.88E-08	5.87	4.78E-08	5.74	4.66E-08	5.63

Table 3: Errors of the numerical solution for $f_3(x) = \sin(3x) + \cos(2x)$



(a) (b)

Figure 4: (a) Derivatives and (b) Numerical errors for f_3 with $N = 41$

4.2 Comparison of 6-6-6 Scheme with 3-4-6-4-3 Scheme

The results obtained in the previous subsection were obtained by using the new scheme 6-6-6, which guarantees that sixth global order of accuracy can be achieved for smooth functions, as shown. Now, we compare the results from the scheme 6-6-6 with the results obtained from the traditional scheme 3-4-6-4-3, with the function $f(x) = \sin(x)$, $x \in [-\pi, \pi]$, and with Dirichlet boundary conditions $f(-\pi) = 0$ and $f(\pi) = 0$.

The 3-4-6-4-3 scheme, which combines 3$^{\text{rd}}$ order schemes for points $j = 0, N$, 4$^{\text{th}}$ order schemes for $j = 1, N-1$, and sixth order schemes for the interior points $j = 2, 3, \ldots, N-2$, generates L_1, L_2, and L_∞errors and respective orders shown in Table 4. We found that the highest order achieved is second order, even though the lowest order formula used is of 3$^{\text{rd}}$ order. Comparing with the results from the 6-6-6 scheme (Table 1 is repeated in Table 5), we note a great improvement obtained by the new scheme 6-6-6, with significantly smaller errors. Figure 5(a) compares the derivatives calculated with $N = 81$ near the left boundary, while Figure 5(b) shows the profiles for the absolute values of the numerical errors for both schemes.

N	L_1 Error	L_1 Order	L_2 Error	L_2 Order	L_∞ Error	L_∞ Order
11	2.57E-01	-	1.30E-01	-	8.74E-02	-
21	6.83E-02	1.91	3.43E-02	1.92	2.31E-02	1.92
41	1.73E-02	1.98	8.68E-03	1.98	5.84E-03	1.98
81	4.35E-03	1.99	2.18E-03	2.00	1.47E-03	2.00
161	1.09E-03	2.00	5.45E-04	2.00	3.67E-04	2.00
321	2.72E-04	2.00	1.36E-04	2.00	9.17E-05	2.00

Table 4: Errors of the numerical solution for $f(x) = \sin(x)$ - Scheme 3-4-6-4-3

N	L_1 Error	L_1 Order	L_2 Error	L_2 Order	L_∞ Error	L_∞ Order
11	2.50E-02	-	1.39E-02	-	9.65E-03	-
21	4.86E-04	5.69	2.68E-04	5.70	1.86E-04	5.70
41	8.06E-06	5.91	4.40E-06	5.93	3.05E-06	5.93
81	1.30E-07	5.95	6.97E-08	5.98	4.83E-08	5.98
161	8.54E-09	5.93	1.09E-09	6.00	7.57E-10	6.00
321	1.41E-10	3.92	1.96E-11	5.80	1.19E-11	5.99

Table 5: Table 1 repeated - Errors of the numerical solution - Scheme 6-6-6

5 Conclusion

The traditional 3-4-6 order compact scheme can only obtain second order global accuracy even for a smooth function. The new 6-6-6 order compact scheme we developed can get sixth order global accuracy fully recovered for smooth functions. According to the analysis above, we have derived a sixth order general algorithm for boundary points which can be used for solving the derivative with Dirichlet boundary conditions. The conservative Compact Scheme developed in this work has been successfully applied to several one dimensional functions. High order accuracy is achieved by using the new boundary point scheme.

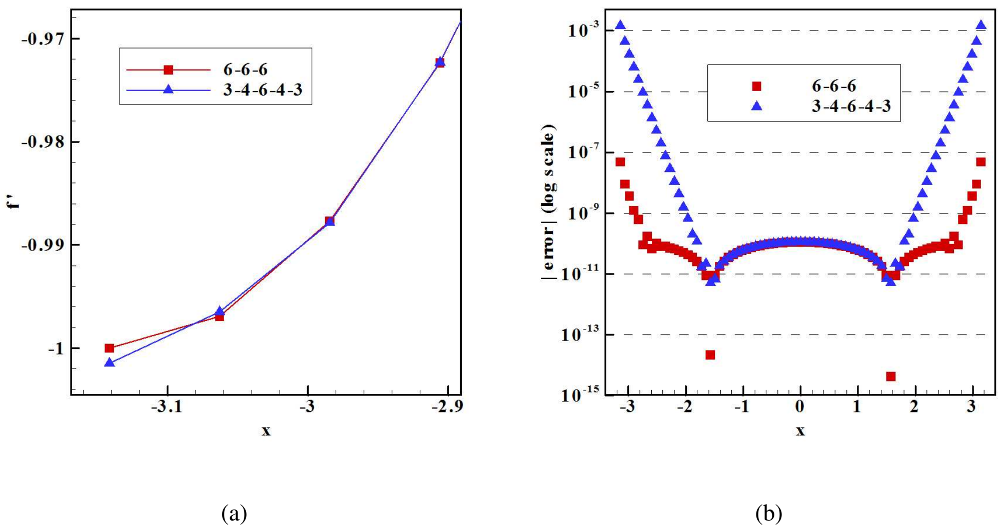


Figure 5: Comparison of (a) derivatives and (b) numerical errors for f with $N = 81$

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