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Generalized Combined Compact Differencing Method

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Abstract: In this article a general class of highly accurate finite difference schemes of arbitrary order with minimal stencil size (three point), called generalized combined compact differencing method (GCCDM), is introduced. Details of the derivation of GCCDM for the uniform and non-uniform grid points are presented. The accuracy analysis of the GCCDM is performed using Fourier analysis and the results are compared with other high accurate finite difference methods such as super compact finite difference method (SCFDM). Accuracy analysis shows that the GCCDM in a uniform grid is more accurate than the SCFDM for a given order of accuracy. In addition, it is shown that the sixth-order and eighth-order combined compact differencing methods are special cases of the GCCDM.

Key-Words: Compact Finite Difference, Numerical Accuracy, High Resolution Schemes, Fourier Analysis

1 Introduction

In many numerical simulations of fluid dynamics problems, especially those possess a wide range of length and time scales, low-order schemes are not enough. The compact finite difference schemes, introduced as far back as the 1930s, have been found simple ways of reaching the objectives of high accuracy and low computational cost [1, 2, 3, 4, 5, 6]. Compared with the traditional explicit finite difference schemes of the same order, compact schemes have proved to be significantly more accurate with the added benefit of using smaller stencil sizes, which can be essential when treating non-periodic boundary conditions.

In the standard symmetric compact finite difference methods, such as Pade [4, 6] and super compact finite difference method (SCFDM) [7, 8] the formulation of the method for the approximation of the first derivative includes the function and its odd derivatives and in a similar manner, the formula of the method for the approximation of the second derivative includes the function and its even derivatives. But it is possible to derive another class of symmetric compact finite difference schemes that their formulation can be used to approximate the first and second derivatives simultaneously. Chu and Fan [9] in 1998, presented a three-point sixth-order (and also eighth-order) combined compact scheme and showed that their method has better resolution characteristics than other (compact and non-compact) schemes. A similar class of schemes was developed by Mahesh [10] which he called them coupled-derivative (C-D) methods.

In this article, the idea of using both odd and even derivatives as unknowns in the formulation of a compact finite difference scheme, is used to introduce a general class of highly accurate finite difference schemes of arbitrary order with minimal stencil size (three point) for the uniform and non-uniform grid points. Since the method can be considered as a generalized form of the current three-point combined compact methods, it is called Generalized Combined Compact Differencing Method (GCCDM).

This paper is organized as follows. Section 2 presents the details of the derivation of the GCCDM in uniform grid. The derivation of the method in non-uniform grid is described in section 3. Accuracy analysis of the GCCDM in uniform and non-uniform grid points is presented in section 4 and finally conclusions are given in section 5.

2 Derivation of the GCCDM in Uniform Grid

This section is devoted to the derivation of the GCCDM in uniform grid points. The GCCDM has two set of equations namely, basic equations and auxiliary equations. These equations are obtained using the Taylor series. A forward discrete Taylor series for an arbitrary function, f, in any direction, x, and in a uniform grid can be written as:

$$f_{j+1} = f_j + hf'_j + \frac{h^2}{2!}f''_j + \dots \tag{1}$$

where h is the grid spacing and the prime denotes the derivative. By defining a forward operator as $\delta_x^+ f_j = f_{j+1} - f_j$, equation (1) can be rewritten in the following form:

$$\delta_x^+ f_j = hf'_j + \frac{h^2}{2!}f''_j + \dots \tag{2}$$

Using the same procedure a similar equation for backward Taylor series can be obtained,

$$\delta_x^- f_j = hf'_j - \frac{h^2}{2!}f''_j + \dots \tag{3}$$

where $\delta_x^- f_j = f_j - f_{j-1}$. Two basic equations of the GCCDM are achieved by adding and subtracting equations (2) and (3) as bellow:

$$(\delta_x^+ + \delta_x^-)f_j = \frac{2}{1!}f_j^{<1>} + \frac{2}{3!}f_j^{<3>} + \dots + \frac{2}{(2M-1)!}f_j^{<2M-1>} \tag{4}$$

$$(\delta_x^+ - \delta_x^-)f_j = \frac{2}{2!}f_j^{<2>} + \frac{2}{4!}f_j^{<4>} + \dots + \frac{2}{(2M)!}f_j^{<2M>} \tag{5}$$

in which $f_j^{<k>} = h^k\left(\frac{\partial^k f}{\partial x^k}\right)_j$.

Equations (4) and (5) are the basic equations of the GCCDM method. It can be seen that the basic equations relate function f to the higher derivatives. In these equations the number of unknowns are much more than equations thus some additional equations i.e., the auxiliary equations are needed to close the system. The auxiliary equations are obtained similar to the basic equations. For each derivative of f (e.g. lth derivative) the forward and backward discrete Taylor series are written and then similar to the basic equations are added and subtracted. This procedure leads to two sets of auxiliary equations as follows:

$$f_{j+1}^{<l>} - f_{j-1}^{<l>} = \frac{2}{1!}f_j^{<l+1>} + \frac{2}{3!}f_j^{<l+3>} + \dots + \frac{2}{(2M-l)!}f_j^{<2M>} \tag{6}$$

$$f_{j+1}^{<l>} - 2f_j^{<l>} + f_{j-1}^{<l>} = \frac{2}{2!}f_j^{<l+2>} + \frac{2}{4!}f_j^{<l+4>} + \dots + \frac{2}{(2M)!}f_j^{<2M-1>} \tag{7}$$

where $l = 1, 2, 3, \dots, M-1$.

Equations (4)-(7) form a (three-point) closed system of equations which can simultaneously be used to approximate the first and second derivatives of f in a uniform grid with the accuracy of order $2M$. Different formulations of the method are derived by letting $M = 1, 2, 3, \dots$. It can be shown that the particular cases of the GCCDM are the second-order central (M=1), fourth-order compact (M=2), sixth-order combined compact (M=3) and eighth-order combined compact (M=4) methods. For example using $M = 3$ in equations (4)-(7) leads to the following sixth-order GCCDM relations:

$$\begin{aligned}
(\delta_x^+ + \delta_x^-)f_j &= \frac{2}{1!}f_j^{<1>} + \frac{2}{3!}f_j^{<3>} + \frac{2}{5!}f_j^{<5>} \\
(\delta_x^+ - \delta_x^-)f_j &= \frac{2}{2!}f_j^{<2>} + \frac{2}{4!}f_j^{<4>} + \frac{2}{6!}f_j^{<6>} \\
f_{j+1}^{<1>} - f_{j-1}^{<1>} &= \frac{2}{1!}f_j^{<2>} + \frac{2}{3!}f_j^{<4>} + \frac{2}{5!}f_j^{<6>} \\
f_{j+1}^{<1>} - 2f_j^{<1>} + f_{j-1}^{<1>} &= \frac{2}{2!}f_j^{<3>} + \frac{2}{4!}f_j^{<5>} \\
f_{j+1}^{<2>} - f_{j-1}^{<2>} &= \frac{2}{1!}f_j^{<3>} + \frac{2}{3!}f_j^{<5>} \\
f_{j+1}^{<2>} - 2f_j^{<2>} + f_{j-1}^{<2>} &= \frac{2}{2!}f_j^{<4>} + \frac{2}{4!}f_j^{<6>}
\end{aligned} \tag{8}$$

In equations (8) it is possible to eliminate some of derivatives. Therefor, after bypassing some manipulations, the above set of equations can be written in the form

$$\begin{aligned}
\frac{7}{16}(f'_{j+1} &+ f'_{j-1}) + f'_j - \frac{h}{16}(f''_{j+1} - f''_{j-1}) = \\
&= \frac{15}{16h}(f_{j+1} - f'_{j-1}) \\
\frac{9}{8h}(f'_{j+1} &- f'_{j-1}) + f''_j - \frac{1}{8}(f''_{j+1} + f''_{j-1}) = \\
&= \frac{3}{h^2}(f_{j+1} - 2f'_j + f'_{j-1})
\end{aligned} \tag{9}$$

which are the sixth-order combined compact relations derived by Chu and Fan [9]. Equations (8) or (9) can be used to discretize a governing equation containing the first and second derivatives, in a uniform grid, with periodic boundary conditions. It is clear that using the second form of the equations (9) needs less computational cost.

In general, when the GCCDM relations are used to discretize a problem with periodic boundary conditions, additional relations are not needed. Application of the GCCDM scheme to problems with non-periodic boundary conditions, needs forward and backward equations in boundaries. These two-point relations (with the same order of the accuracy of the central equations) are derived similar to those obtained for the super compact finite difference method (SCFDM) [8]. It should be noted that these forward and backward relations only can be used with the original form of the GCCDM relations [i.e. equations (4)-(7)]. The boundary relations for the second form of the scheme, e.g. sixth-order equations (9), in non-periodic domains can be determined by following the procedure given by Chu and Fan [9]. These boundary equations has less order of accuracy than the central relations.

3 Derivation of the GCCDM in Non-uniform Grid

In this section a more general form the GCCDM relations in non-uniform grids is presented. These equations can be derived similar to the uniform equations by using the Taylor series in a non-uniform grid. The forward and backward discrete Taylor series can be written as

$$\delta_x^+ f_j = h_j f_j' + \frac{h_j^2}{2!} f_j'' + \dots$$
$$\delta_x^- f_j = h_{j-1} f_j' - \frac{h_{j-1}^2}{2!} f_j'' + \dots$$

in which $h_j = x_{j+1} - x_j$.

Therefor, the basic equations of the GCCDM in non-uniform grid can be derived as

$$\delta_x^\circ f_j = (1+\sigma_j) f_j^{<1>} + \frac{1}{2!}(1-\sigma_j^2) f_j^{<2>} + \dots + \frac{1}{N!}[1+(-1)^{N+1}\sigma_j^N] f_j^{<N>} \quad (10)$$

$$\delta_x^2 f_j = (1-\sigma_j) f_j^{<1>} + \frac{1}{2!}(1+\sigma_j^2) f_j^{<2>} + \dots + \frac{1}{N!}[1+(-1)^{N}\sigma_j^N] f_j^{<N>} \quad (11)$$

and the auxiliary equations can be found as bellow

$$\delta_x^\circ f_j^{<l>} = (1+\sigma_j) f_j^{<l+1>} + \frac{1}{2!}(1-\sigma_j^2) f_j^{<l+2>} + \dots + \frac{1}{(N-1)!}[1+(-1)^{N}\sigma_j^{N-1}] f_j^{<N>} \quad (12)$$

$$\delta_x^2 f_j^{<l>} = (1-\sigma_j) f_j^{<l+1>} + \frac{1}{2!}(1+\sigma_j^2) f_j^{<l+2>} + \dots + \frac{1}{(N-1)!}[1+(-1)^{N-1}\sigma_j^{N-1}] f_j^{<N>} \quad (13)$$

where $l = 1, 2, 3, \dots, N/2 - 1$ and

$$\delta_x^2 = \delta_x^+ \delta_x^- = \delta_x^- \delta_x^+, \ \delta_x^\circ = \delta_x^+ + \delta_x^-$$
$$\sigma_j = \frac{h_{j-1}}{h_j}, f_j^{<k>} = h_j^k \left(\frac{\partial^k f}{\partial x^k}\right)_j$$

Equations (10)-(13) form the general formulation of the GCCDM in a non-uniform grid for the approximation of the first and second derivatives with the accuracy of order N.

Introducing the vectors

$$\mathbf{F} = \left\{ f^{<1>}, f^{<2>}, f^{<3>}, \dots, f^{<N>} \right\}^T,$$
$$\mathbf{E} = \left\{ \delta_x^\circ, \delta_x^2, 0, 0, \dots, 0 \right\}^T$$

and the matrices

$$\mathcal{Q} = \begin{pmatrix} \frac{1+\sigma}{1!} & \frac{1-\sigma^2}{2!} & \dots & \frac{1+(-1)^{N+1}\sigma^N}{N!} \\ \frac{1-\sigma}{1!} & \frac{1+\sigma^2}{2!} & \dots & \frac{1+(-1)^{N}\sigma^N}{N!} \\ 0 & \frac{1+\sigma}{1!} & \dots & \frac{1+(-1)^{N}\sigma^{N-1}}{(N-1)!} \\ 0 & \frac{1-\sigma}{1!} & \dots & \frac{1+(-1)^{N-1}\sigma^{N-1}}{(N-1)!} \\ 0 & 0 & \dots & \frac{1+(-1)^{N-1}\sigma^{N-2}}{(N-2)!} \\ 0 & 0 & \dots & \frac{1+(-1)^{N-2}\sigma^{N-2}}{(N-2)!} \\ 0 & 0 & 0 & \dots \end{pmatrix},$$

$$\mathcal{L} = \begin{pmatrix} 0 & 0 & \dots & 0 \\ 0 & 0 & \dots & 0 \\ -\delta_x^\circ & 0 & \dots & 0 \\ -\delta_x^2 & 0 & \dots & 0 \\ 0 & -\delta_x^\circ & \dots & 0 \\ 0 & -\delta_x^2 & \dots & 0 \\ 0 & 0 & \dots & 0 \\ 0 & 0 & \dots & 0 \end{pmatrix}$$

Equations (10)-(13) can be rewritten into a vector form and the following relation is achieved

$$(\mathcal{Q} + \mathcal{L})\mathbf{F}_j = \mathbf{E} f_j \quad (14)$$

$\mathcal{L}$ and $\mathcal{Q}$ are $N \times N$ matrices and $\mathbf{F}$ and $\mathbf{E}$ are N dimensional vectors. It is clear that by choosing $\sigma_j = 1$ and doing some modifications, equation (14) will transform to the vector form of the GCCDM in uniform grid.

4 Accuracy Analysis

In this section the results of the accuracy analysis of different orders of the GCCDM relations as well as the comparison with other high accurate finite difference methods such as SCFDM, is presented. The accuracy analysis in uniform and non-uniform grids is performed using the Fourier analysis [6, 11]. A single Fourier mode is chosen for the Fourier analysis

$$f_j = \exp(i\omega s), \qquad s = \frac{x_j}{h_j}, \quad i = \sqrt{-1} \quad (15)$$

where ω is the wave number.

In the present paper only the results of the Fourier are given, the details of the application of the Fourier analysis in uniform and non-uniform grids can be found in references [6, 11] and [12].

Figures 1 and 2 present the comparison of the modified wave numbers of the first and second derivative approximations for different orders of the GCCDM and SCFDM in a uniform grid. Accuracy analysis shows that the GCCDM in a uniform grid is more accurate than the SCFDM for a given order of accuracy and also has better resolution characteristics. Better accuracy of the GCCDM respect to the SCFDM shows that the GCCDM can perform better resolution characteristic than any current (three-point compact and non-compact) schemes.

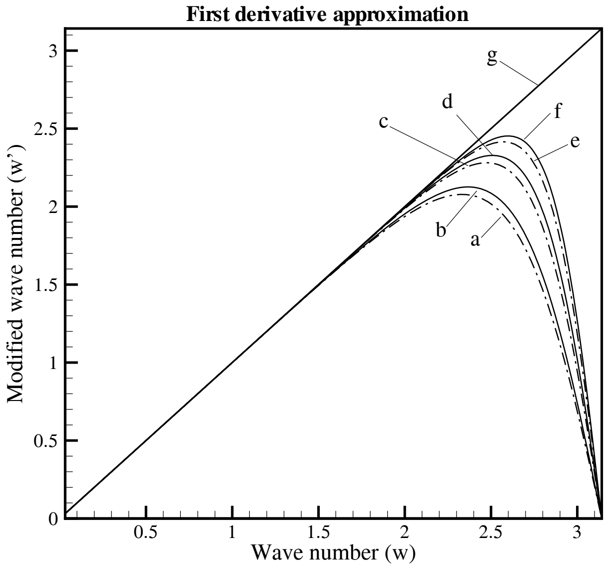

Figure 1: The modified wave number of the first derivative approximation in a uniform grid: (a) sixth-order SCFDM, (b) sixth-order GCCDM, (c) eighth-order SCFDM (d) eighth-order GCCDM, (e) tenth-order SCFDM, (f) tenth-order GCCDM, (g) exact differentiation.

The comparison of the modified wave numbers of the first and second derivative approximations of the sixth-order formulation of the GCCDM and SCFDM schemes in a non-uniform grid for different grid aspect ratios ($k = h_j/h_{j-1} = 1/\sigma_j$) are given in figures 3 and 4. Figures 3 and 4 show that the GCCDM is more accurate than the SCFDM in non-uniform grid points. Furthermore, this accuracy analysis of the GCCDM in a non-uniform grid shows that the GCCDM is less sensitive to the grid aspect ratio respect to the SCFDM and produces less errors especially for the large wave numbers.

As numerical examples the GCCDM has been applied to spatial differencing of some prototype linear and nonlinear geophysical fluid dynamics problems (e.g. the shallow water equations) and the results show that the GCCDM offers a promising compact finite difference method to implement in numerical simulation of fluid dynamics problems. Because of the page limits, these results are not presented in this article and will be reported elsewhere.

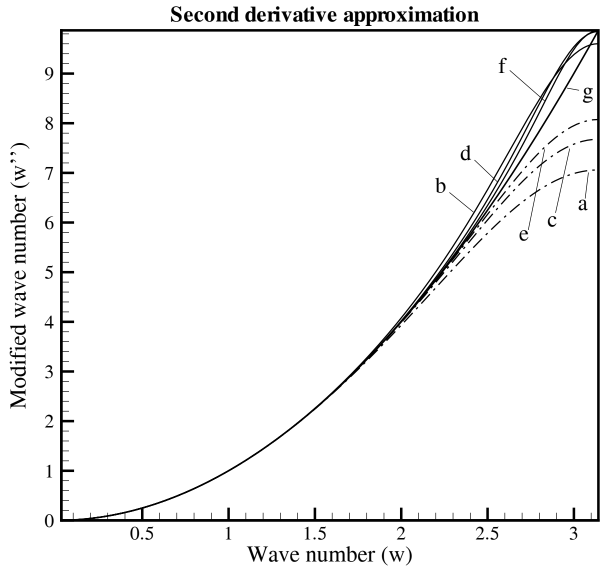

Figure 2: The modified wave number of the second derivative approximation in a uniform grid: (a) sixth-order SCFDM, (b) sixth-order GCCDM, (c) eighth-order SCFDM (d) eighth-order GCCDM, (e) tenth-order SCFDM, (f) tenth-order GCCDM, (g) exact differentiation.

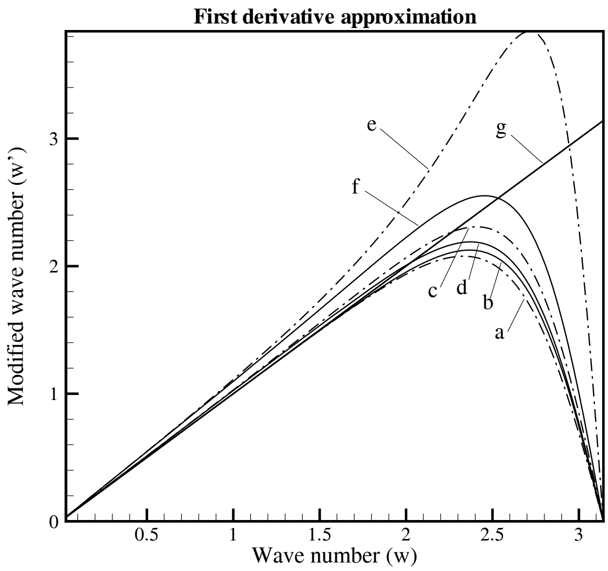

Figure 3: The modified wave number of sixth-order approximation of the first derivative in a non-uniform grid: (a) SCFDM in uniform grid ($k = 1$), (b) GCCDM in uniform grid ($k = 1$), (c) SCFDM in non-uniform grid with $k = 1.05$, (d) GCCDM in non-uniform grid with $k = 1.05$, (e) SCFDM in non-uniform grid with $k = 1.2$, (f) GCCDM in non-uniform grid with $k = 1.2$, (g) exact differentiation.

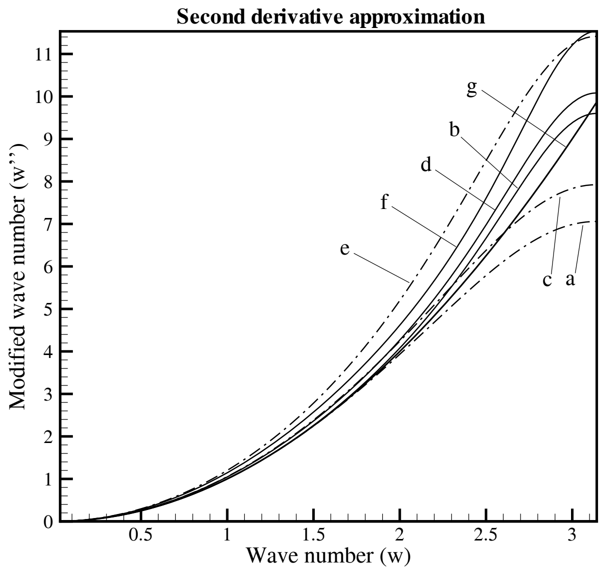

Figure 4: The modified wave number of sixth-order approximation of the second derivatives in a non-uniform grid: (a) SCFDM in uniform grid ($k = 1$), (b) GCCDM in uniform grid ($k = 1$), (c) SCFDM in non-uniform grid with $k = 1.05$, (d) GCCDM in non-uniform grid with $k = 1.05$, (e) SCFDM in non-uniform grid with $k = 1.2$, (f) GCCDM in non-uniform grid with $k = 1.2$, (g) exact differentiation.

5 Conclusion

The formulation of a three-point highly accurate finite difference method, called generalized combined compact differencing method has been presented. The method can be used for the approximation of the first and second derivatives as well as using for the solution (discretization) of fluid dynamics problems, with any order of the accuracy in uniform and non-uniform grid points. The idea of the GCCDM and its derivation procedure can be used to obtain the corresponding relations for the staggered grids (which have not been presented in this article).

Fourier analysis indicates that the GCCDM is more accurate and has better resolution characteristics than any current three-point scheme, such as the SCFDM, with the same order of the accuracy. In addition the Fourier analysis of the method shows that the GCCDM is less sensitive to the grid aspect ratio than the SCFDM, in non-uniform grids.

What is certain is that the GCCDM offers a promising finite-difference method to implement in numerical simulations of the fluid dynamics (and other branches) problems. It combines high accuracy over a great part of spectral space with low cost and minimal stencil size. It involves only inverting block three-diagonal matrices whose computational cost depends linearly on spatial resolution.

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