Combined Compact Difference Scheme for the Grid System in Which the Boundary is Located between Regular GRID Points

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We propose a Combined Compact Difference (CCD) scheme for the grid system in which the boundary is located between regular grid points. We analyze the stability of the proposed CCD scheme for a 1-D advection diffusion problem by using the matrix method. The finite difference representation of the 1-D equation consists of the CCD scheme for the spatial derivatives and the 4th Runge-Kutta method for the time marching. It is shown that the new numerical method is stable for larger Courant number and diffusion number than those of the original method. We also show a numerical test of a 1-D advection diffusion simulation using this numerical method.

1. INTRODUCTION

Various phenomena with different spatial and temporal scales are found in many flows, turbulent fluid flows and aeroacoustic noise being common examples. Direct numerical simulations of these flows require high-resolution numerical methods. One candidate is the Compact Difference (sp-CD) scheme with spectral-like resolution proposed by Lele as a high-resolution finite difference method. CD schemes have been used in many studies. For example, Shang solved the time-dependent Maxwell equations, Ekaterinairis solved the Euler equations and Meitz and Fasel solved the Navier-Stokes equations using a CD scheme. However, the different numerical schemes must be used at a few points near the boundary.

The Combined Compact Difference (CCD) scheme was proposed by Chu and Fan and the coupled-derivative (C-D) scheme was proposed by Mahesh. These schemes are similar and higher derivatives at 3-point stencil are used. These schemes have higher resolution than CD schemes with the same accuracy. Nihei and Ishii developed the Combined Compact Difference (sp-CCD) scheme with spectral-like resolution for solving the shallow water equations. Nihei&Ishii also simulated the 3-D lid-driven cavity flow by using the sp-CCD scheme. We investigated the stability of a numerical method using the sp-CCD scheme for a 1-D advection diffusion problem in [9]. In order to improve the stability we proposed a new CCD scheme for nonperiodic boundary condition for the problem.

These schemes have been derived for uniform grid. For application of these schemes to problems with complex geometries and boundary conditions, the usual approach is to use a mapping from nonuniform grid to uniform grid and apply these schemes directly on the mapped coordinate. However, to solve problems with too complex geometries and boundary conditions, the use of body fitting grid system is difficult.
In this study, we extend a CCD scheme for the regular grid system and propose a CCD scheme for the irregular boundary condition in which the boundary is located between regular grid points. We also investigate the stability of the proposed scheme for a 1-D advection diffusion problem.

2. COMBINED COMPACT DIFFERENCE SCHEME FOR THE GRID SYSTEM IN WHICH THE BOUNDARY IS LOCATED BETWEEN REGULAR GRID POINTS

First we consider the regular grid system \( \{ x_i = i\Delta x \} \) which has uniform spacing \( \Delta x \) and the nodes are indexed by \( i (i = 0, 1, 2, \ldots, N) \). The left boundary is located at the distance \( k\Delta x \) from the inner boundary point \( x_i \) that is adjacent to the boundary as shown in Fig.1. The right boundary is located on the boundary point \( x_N \). Consider the numerical derivatives of a function \( f(x) \) at \( N \) grid points. Let \( f_i, f'_i, f''_i, f'''_i \) be the values of the function and its first, second and third derivatives at \( i \)-th grid point \( x_i \), respectively.

\[
\begin{array}{cccc}
  k\Delta x & \Delta x & \Delta x & \Delta x \\
  i = 0 & i = 1 & i = 2 & i = 3 & i = 4 \\
\end{array}
\]

Fig.1 Grid points near the boundary.

For the interior points \( x_i \) (\( 2 \leq i \leq N - 1 \)), we use the Combined Compact Difference (sp-CCD) scheme with spectral-like resolution proposed by Nihei&Ishii. The sp-CCD representation can be written as

\[
A \begin{pmatrix} f_{i+1}^s \\ f_i^s \\ f_{i-1}^s \end{pmatrix} + E \begin{pmatrix} f_{i+1}' \\ f_i' \\ f_{i-1}' \end{pmatrix} + B \begin{pmatrix} f_{i+1}'' \\ f_i'' \\ f_{i-1}'' \end{pmatrix} = g_i, \quad (2 \leq i \leq N - 1)
\]

where

\[
A = \begin{pmatrix}
  a_1 & -b_1 & c_1h^2 \\
  -a_2 \frac{h^2}{2} & b_2 & -c_1h \\
  a_3 \frac{h^2}{2} & -b_3 & c_3 \\
\end{pmatrix}, \quad E = \begin{pmatrix}
  1 & 0 & 0 \\
  0 & 1 & 0 \\
  0 & 0 & 1 \\
\end{pmatrix}, \quad B = \begin{pmatrix}
  a_1 & b_1\Delta x & c_1\Delta x^2 \\
  a_2 \frac{\Delta x^2}{2} & b_2 \Delta x & c_2 \Delta x \\
  a_3 \frac{\Delta x^2}{2} & b_3 & c_3 \\
\end{pmatrix}, \quad g_i = \begin{pmatrix}
  \frac{d_1}{\Delta x} (f_{i+1} - f_{i-1}) \\
  \frac{d_2}{\Delta x^2} (f_{i+1} - 2f_i + f_{i-1}) \\
  \frac{d_3}{\Delta x^3} (f_{i+1} - 2f_i + f_{i-1}) \\
\end{pmatrix}.
\]

The parameters \( a_1, b_1, c_1, d_1, a_2, b_2, c_2, d_2 \) and \( d_3 \) determine the formal accuracy of the scheme. The sp-CCD scheme whose parameters are given as

\[
a_1 = \frac{8d_3 + 195}{240}, \quad b_1 = \frac{-16d_3 + 255}{1200}, \quad c_1 = \frac{4d_3 + 45}{1800}, \quad d_1 = \frac{8d_3 + 315}{240},
\]

\[
a_2 = \frac{11d_3 - 15}{16}, \quad b_2 = \frac{-3d_3 - 7}{16}, \quad c_2 = \frac{d_2 - 3}{48}, \quad d_2 = 9.12992,
\]

\[
a_3 = d_3, \quad b_3 = \frac{8d_3 + 15}{20}, \quad c_3 = \frac{4d_3 + 15}{60}, \quad d_3 = \frac{165d_3 - 450}{28d_3 - 80}
\]

has eighth-order accuracy and high resolution for the first and second derivative and has forth-order accuracy for the third derivative, respectively.
For the point $x_i$ adjacent to the boundary, we propose the scheme as follows:

$$
E \left( \begin{array}{c}
\begin{array}{c}
 f_{i-1}' \\
 f_i'
\end{array}
\end{array} \right) + C \left( \begin{array}{c}
\begin{array}{c}
 f_{i-1}' \\
 f_i'
\end{array}
\end{array} \right) = g_i', \quad g_i' = \begin{bmatrix}
\frac{r_{11}}{\Delta x} \left( (k' + (1 - k) f_i) - f_{i-1} \right) \\
\frac{r_{12}}{\Delta x} \left( (k' + (1 - k) f_i) - f_{i-1} \right) \\
\frac{r_{13}}{\Delta x^2} \left( (k' + (1 - k) f_i) - f_{i-1} \right)
\end{bmatrix}, \quad C_i = \begin{bmatrix}
c_{i1} & c_{i2} & c_{i3} \\
\frac{c_{i1}}{\Delta x} & c_{i2} & c_{i3} \\
\frac{c_{i1}}{\Delta x^2} & \frac{c_{i2}}{\Delta x} & c_{i3}
\end{bmatrix}
$$

where $f'$ is the given value of the function $f(x)$ on the boundary. This boundary condition is the Dirichlet condition. This boundary scheme has fourth-order accuracy for the first derivative, third-order accuracy for the second derivative and second-order accuracy for the third derivative, respectively.

For the boundary point $x_N$, we propose the scheme as follows:

$$
C_S \left( \begin{array}{c}
\begin{array}{c}
 f_{N-1}' \\
 f_N'
\end{array}
\end{array} \right) = g^*_N, \quad C_N = \begin{bmatrix}
\frac{4}{\Delta x} & \frac{1}{3} \frac{1}{\Delta x^2} \\
\frac{20}{\Delta x} & 5 & \frac{7}{3} \frac{1}{\Delta x} \\
\frac{36}{\Delta x^2} & 12 & 5
\end{bmatrix}, \quad g^*_N = \begin{bmatrix}
\frac{1}{\Delta x} \left( -\frac{9}{2} f_N + 4 f_{N-1} + \frac{1}{2} f_{N-2} \right) \\
\frac{1}{\Delta x^2} \left( 16 f_N - 12 f_{N-1} - 4 f_{N-2} \right) \\
\frac{1}{\Delta x^3} \left( -30 f_N + 24 f_{N-1} + 6 f_{N-2} \right)
\end{bmatrix}
$$

This boundary scheme has fifth-order accuracy for the first derivative, fourth-order accuracy for the second derivative and second-order accuracy for the third derivative, respectively.

Then, the systems of the sp-CCD equations are given as

$$
\begin{bmatrix}
E & C_1 & O & \cdots & O & O \\
A & E & B & O & O & X_1 \\
O & A & E & B & O & X_2 \\
\vdots & \ddots & \ddots & \ddots & \ddots & \vdots \\
O & O & A & E & B & X_{N-1} \\
O & O & \cdots & O & C_N & E & X_N
\end{bmatrix} \begin{bmatrix}
X_1 \\
X_2 \\
\vdots \\
X_{N-1} \\
X_N
\end{bmatrix} = \begin{bmatrix}
g^*_1 \\
g_2 \\
\vdots \\
g_{N-1} \\
g^*_N
\end{bmatrix}
$$

where $O$ is a null matrix and $X_i = (f_i', f''_i, f'''_i)^T$.

Finally, since $g_i$ is a linear simultaneous equation of $f$, we can express above systems as $PX = GF$, where $X = (X_1, X_2, \ldots, X_N)^T$ and $F = (f_1', f_2', \ldots, f_N')^T$.

When the left boundary is located on the boundary point $x_1$ and the right boundary is located at the distance $k\Delta x$ from the inner boundary point $x_i$ that is adjacent to the boundary, the scheme is formulated as follows,
at the point \( x_i \):

\[
\mathbf{E} \left( \begin{array}{c}
f_i^* \\
 f_i''^* \\
 f_i'''^* \\
 f_i''''^*
\end{array} \right) + \mathbf{C}_i \left( \begin{array}{c}
f_i^* \\
 f_i''^* \\
 f_i'''^* \\
 f_i''''^*
\end{array} \right) = \mathbf{g}^*_i, \quad \mathbf{C}_i = \left( \begin{array}{cccc}
4 & -\Delta x & 1/3 & \Delta x^2 \\
20/ \Delta x & 5 & -7/3 & \Delta x \\
36/ \Delta x^2 & -12/ \Delta x & 5 & \\
\end{array} \right), \quad \mathbf{g}^*_i = \left( \begin{array}{c}
1/ \Delta x \left( -9 f_i + 4 f_i + 1/2 f_i \right) \\
1/ \Delta x \left( 16 f_i - 12 f_i - 4 f_i \right) \\
1/ \Delta x \left( -30 f_i + 24 f_i + 6 f_i \right)
\end{array} \right).
\]

at the point \( x_N \):

\[
\mathbf{C}_N \left( \begin{array}{c}
f_N^* \\
 f_N''^* \\
 f_N'''^* \\
 f_N''''^*
\end{array} \right) + \mathbf{E} \left( \begin{array}{c}
f_N^* \\
 f_N''^* \\
 f_N'''^* \\
 f_N''''^*
\end{array} \right) = \mathbf{g}^*_N, \quad \mathbf{g}^*_N = \left( \begin{array}{c}
-\frac{r_{11}}{\Delta x} \left( kf_i^* + (1 - k) f_i \right) - f_{N-1}^* \\
-\frac{r_{12}}{\Delta x^2} \left( kf_i^* + (1 - k) f_i \right) - f_{N-1}^* \\
-\frac{r_{13}}{\Delta x^3} \left( kf_i^* + (1 - k) f_i \right) - f_{N-1}^* \\
\end{array} \right), \quad \mathbf{C}_N = \left( \begin{array}{ccc}
c_{11} & -c_{12} \Delta x & c_{14} \Delta x^2 \\
-c_{21} / \Delta x & c_{22} & -c_{23} \Delta x \\
c_{31} / \Delta x^2 & -c_{32} / \Delta x & c_{33}
\end{array} \right).
\]

3. STABILITY ANALYSIS

We use the method which we used in [9] in order to analyze the stability of the proposed CCD scheme. We consider the initial value problem of a 1-D advection diffusion equation

\[
\frac{\partial \phi}{\partial t} = v \frac{\partial \phi}{\partial x} - c \frac{\partial \phi}{\partial x},
\]

where \( v \) and \( c \) are real constants and \( \phi = \phi(x,t) \) is a scalar function.

For simplicity consider a uniformly spaced mesh where the nodes are indexed by \( i \). The coordinate values at the nodes are \( x_i = (i-1) \Delta x \) for \( 1 \leq i \leq N \) and the function values at the nodes \( \phi_i = \phi(x_i) \) are given. Using the spatial 1st difference operator \( \mathbf{C} \) and the spatial 2nd difference operator \( \mathbf{D} \), the semi-discrete equation is given by

\[
\frac{\partial \tilde{\phi}}{\partial t} = \frac{1}{\Delta t} \left( \sigma \mathbf{D} \tilde{\phi} - \sigma \mathbf{C} \tilde{\phi} \right) = \frac{1}{\Delta t} \mathbf{S} \tilde{\phi}
\]

where \( \tilde{\phi} = (\phi_1, \phi_2, \ldots, \phi_N) \), \( \sigma = c \Delta t / \Delta x \) is the Courant number, \( \sigma_d = v \Delta t / \Delta x^2 \) is the diffusion number and \( \mathbf{S} = \sigma \mathbf{D} - \sigma \mathbf{C} \) is an \( N \times N \) constant matrix. We discuss the stability of the linear dynamical system. There are many definitions of stability in the literature of Computational Fluid Dynamics. In the present work, we consider the notions of Lyapunov and asymptotic stability in [9].

3.1. Stability Region of the Runge-Kutta method

We use the explicit RK method for the time marching and analyze the stability with various \( \sigma \) and \( \sigma_d \). The discrete dynamical system of Eq.(1) is

\[
\tilde{\phi}^{n+1} = RK_l(\sigma \mathbf{D} - \sigma \mathbf{C}) \tilde{\phi}^n,
\]

(2)

Here \( RK_l(\sigma \mathbf{D} - \sigma \mathbf{C}) \), \( l \in N \) is the \( l \)-th RK operator, which corresponds to the \( l \)-th truncated series of the exponential of \( (\sigma \mathbf{D} - \sigma \mathbf{C}) \), that is,

\[
RK_l(\sigma \mathbf{D} - \sigma \mathbf{C}) = id + (\sigma \mathbf{D} - \sigma \mathbf{C}) + \cdots + \frac{1}{l!}(\sigma \mathbf{D} - \sigma \mathbf{C})^l, \quad l \in N,
\]

where \( id \) is the identity operator.
We follow a set of eigenvalues of \( S \) i.e. \( S_\nu = \{ \lambda \in C : (\sigma_j^D - \sigma_j^C)\mathbf{\bar{\nu}} = \lambda \mathbf{\bar{\nu}} \} \) and the stability region of the \( l \)-th RK method i.e. \( S_l = \{ \lambda \in C : |R(l)\lambda| \leq 1 \} \) where \( C \) is a complex number. The fully discrete algorithm (Eq.(2)) is stable if \( S_\nu \subset S_l \).

The stability region in the upper half complex plane is shown in Fig.2 for the first-, second-, third-, fourth-, sixth- and eighth-order explicit RK methods. Kobayashi(11) discussed the properties of the stability region for the advection equation which Eq.(1) corresponds to by giving \( \sigma_d = 0 \). Any centered method for the advection equation with periodic boundary condition is unstable for the first- and second-order RK methods, since the stability curve for the first- and second-order RK methods is tangent to the imaginary axis in the negative real region. On the other hand, the stability curve of the higher-order RK method is tangent to imaginary axis in the positive real region. Also, for centered methods the fourth-order RK method provides an improved stability as compared to the sixth-order RK method. Thus, we use the fourth-order RK method.

**Fig. 2 Stability region for the RK methods of order 1, 2, 3, 4, 6 and 8.**

### 3.2. Stability Analysis

Using the \( N \times 3 \) projection matrices

\[
\begin{align*}
R_1 &= \begin{pmatrix}
1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0
\end{pmatrix}, & R_2 &= \begin{pmatrix}
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 1 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0
\end{pmatrix},
\end{align*}
\]

the matrix representations of first and second derivatives in the CCD scheme are

\[
F' = R_1 X = R_1 P^{-1} G F, \quad F'' = R_2 X = R_2 P^{-1} G F
\]  

\[\text{(3)}\]

where \( P^{-1} \) is obtained by using LU factorization and

\[
X = \begin{pmatrix}
X_1 \\
X_2 \\
\vdots \\
X_N
\end{pmatrix}, \quad F = \begin{pmatrix}
f_1 \\
f_2 \\
\vdots \\
f_N
\end{pmatrix}, \quad F' = \begin{pmatrix}
f'_1 \\
f'_2 \\
\vdots \\
f'_N
\end{pmatrix}, \quad F'' = \begin{pmatrix}
f''_1 \\
f''_2 \\
\vdots \\
f''_N
\end{pmatrix}
\]
Substituting Eq. (3) to the semi-discrete equation (Eq. (1)), we obtain
\[
\frac{\partial \phi}{\partial t} = \frac{1}{\Delta t} \left( \sigma_d R \phi - \sigma_c \phi \right) P G \phi = \frac{1}{\Delta t} S \phi,
\]
where \( S = (\sigma_d R \phi - \sigma_c \phi) P G \phi \) is a \( N \times N \) matrix. To investigate the stability we compute eigenvalues of the matrix \( S \) with different values of \( \sigma_c \) and \( \sigma_d \).

Fig.3 shows the stability region on the \( \sigma_c - \sigma_d \) plane for the periodic boundary condition in [9]. In this study, we use five values of \( \sigma_c \) and \( \sigma_d \) that had been used in [9]. These values are listed in Table.1. When \( \sigma_d = 0 \), Eq.(1) corresponds to the advection equation. When \( \sigma_c = 0 \), Eq.(1) corresponds to the diffusion equation.

![Fig.3 The stability region on \( \sigma_c - \sigma_d \) plane for the sp-CCD scheme for periodic boundary condition.](image)

<table>
<thead>
<tr>
<th>Table.1</th>
<th>Combinations of ( \sigma_c ) and ( \sigma_d ).</th>
</tr>
</thead>
<tbody>
<tr>
<td>CASE</td>
<td>(1)</td>
</tr>
<tr>
<td>( \sigma_c )</td>
<td>1.0991</td>
</tr>
<tr>
<td>( \sigma_d )</td>
<td>0</td>
</tr>
</tbody>
</table>

Fig.4 shows the sets of eigenvalues \( S_\phi \) (N=256) for four cases of \( k=1/4, 1/2, 3/4 \) and 1. All eigenvalues exist in \( S_\phi \). This means that the proposed scheme is stable for the 1-D advection diffusion equation when using \( \sigma_c \) and \( \sigma_d \) listed in Table.1. The stability region for \( k=1/2 \) on the \( \sigma_c - \sigma_d \) plane is shown in Fig.5. The stability region for \( k \geq 2^{-12} \) on the \( \sigma_c - \sigma_d \) plane is similar to the case of \( k=1/4 \). However, we can not find any eigenvalues including \( S_\phi \) for \( k \leq 2^{-13} \). The CFL stability limit for pure advection \( \sigma_{c,max} = 1.0991 \) can be used when \( \sigma_d \leq 0.09851 \). When \( \sigma_c \leq 0.7502 \), the diffusion stability limit maintains \( \sigma_{d,max} = 0.2706 \).

We illustrate the stability region on \( \sigma_c - \sigma_d \) plane for the CCD scheme (red) and the sp-CCD scheme for periodic boundary condition (green) and for nonperiodic boundary condition (blue) in Fig.6. It shows that the stability region for the proposed CCD scheme is larger than the previous CCD scheme for periodic boundary condition and similar to one of the original CCD scheme for nonperiodic boundary condition.
Fig. 4 Sets of eigenvalue (N=256): ‘red’ $S_1$, ‘green’ case(1), ‘blue’ case(2), purple’ case(3), ‘Carolina blue’ case(4) and ‘brown’ case(5).

Fig. 5 The region of $\sigma_\tau$ and $\sigma_\nu$ where the CCD scheme is stable.
Fig. 6 The stability region on the $\sigma_c$-$\sigma_d$ plane for the proposed CCD scheme (red) and the sp-CCD scheme for periodic boundary condition (green) and for nonperiodic boundary condition (blue).

4. NUMERICAL TEST

We test the proposed scheme for a 1-D advection diffusion problem [10]

$$\frac{\partial u}{\partial t} = v \frac{\partial^2 u}{\partial x^2} - c \frac{\partial u}{\partial x},$$

where $v = 1$, $c = 10$ and $u = u(x,t)$ is a scalar function. The analytical solution of this equation is $u_{ke}(x,t) = u_0 \exp[-(x-ct)^2 / 4\nu t] / 2\sqrt{\pi \nu t}$. The computational domain is $0 \leq x \leq 5$, the initial condition is $u(x,0) = \exp[-(x-1.15-c t_0)^2 / 4\nu t_0] / 2\sqrt{\pi \nu t_0}$, where $t_0 = 10^{-3}$ and $\sigma_c = 0.001$. The boundary condition is given by $f(t) = u(0,t) = \exp[-(1.15-c(t+t_0))^2 / 4\nu(t+t_0)] / 2\sqrt{\pi \nu(t+t_0)}$. The computational result (points) and the analytical solution (line) for $N=32$, $k=1/2$, $t=0.0$, $0.1$ and $0.2$ are plotted in Fig. 7. It shows that the proposed scheme computed the solution without divergence and that the wave propagation is computed correctly even though there is no grid point on the peak at $t = 0$. Fig. 8 shows the average values of the absolute errors of the result for $N=16, 32, 64$, $t = 0.2$. The average value of the absolute errors is $\sum |u_{ke} - u_{num}| / N$, where $u_{num}$ is the numerical solution. The errors decrease rapidly.

We solve the 1-D advection diffusion equation in the case of $v = 13/63$, $c = 10$, $N=32$, $\sigma_c = 1.0$, $\sigma_d = 0.13$, $v t_0 = 0.01$. The $\sigma_c$ and $\sigma_d$ are more close to the stability limit than the above test. The results are shown in Fig. 9. Fig. 9 shows that the numerical solution is computed correctly except for the solution on the peak at $t=0.1$ is damped a little.

5. CONCLUSION

We proposed a Combined Compact Difference (CCD) scheme for the grid system in which the boundary is located between regular grid points and investigated the stability of a numerical method using the proposed CCD scheme and the 4th order RK method for the 1-D advection diffusion equation. We analyzed the stability region of the CCD scheme on the $\sigma_c$-$\sigma_d$ plane. The region for the new CCD scheme with $k \geq 2^{-12}$ is larger than one of the original CCD scheme for periodic boundary condition and similar to one of the original CCD scheme for nonperiodic boundary condition. We also showed that numerical error of a 1-D advection diffusion problem using this numerical method is
small. In this paper, we discussed the stability of CCD scheme with Dirichlet boundary conditions. We can get similar CCD schemes with Neumann boundary conditions and/or the mixed boundary conditions. The stability analyses of them are the future works.

**Fig. 7** Computational result (points) and analytical solution (line) at $t=0.0$ (red), $t=0.1$ (green) and $t=0.2$ (blue).

**Fig. 8** the averages values of the absolute errors of the computational result in $N=16, 32, 64, t=0.2$.

**Fig. 9** Computational result (points) and analytical solution (line) at $t=0.0$ (red), $t=0.1$ (green) and $t=0.2$ (blue) with $v/t_0 = 0.01$. 
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REFERENCE


