High-order compact MacCormack scheme for two-dimensional compressible and non-hydrostatic equations of the atmosphere

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Abstract

This study is devoted to application of the fourth-order compact MacCormack scheme to spatial differencing of the conservative form of two-dimensional and non-hydrostatic equation of a dry atmosphere. To advance the solution in time a four-stage Runge-Kutta method is used. To perform the simulations, two test cases including evolution of a warm bubble and a cold bubble in a neutral atmosphere with open and rigid boundaries are employed. In addition, the second-order MacCormack and the standard fourth-order compact MacCormack schemes are used to perform the simulations. Qualitative and quantitative assessment of the numerical results for different test cases exhibit the superiority of the fourth-order compact MacCormack scheme on the second-order method.

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1. Introduction

Increasing the accuracy of numerical schemes used for simulation of fluid dynamics problems, particularly the geophysical fluid dynamics problems (atmospheric and oceanic), has been the subject of many research works. Recently, due to the increasing computing power of computers, the advantage of high-resolution numerical methods for numerical simulation of the governing equations of fluid flow is further emphasized.

The idea of compact finite difference methods originates from some works conducted in the 1920s and 1940s (Numerov, 1924; Fox and Goodwin, 1949). However, the pioneering works presented by Kreiss and Oliger (1972), Hirsh (1975) and Lele (1992) made these methods popular and showed that compact finite difference methods can be used as a powerful tool for numerical simulation of fluid dynamics problems appearing in different branches of science. Compact finite difference schemes have been developed that are able to provide a simple way to reach to main objectives in development of numerical algorithms, i.e., having in one hand a low cost and in other hand a highly accurate computational method.

These methods have also been used for numerical simulation of some geophysical fluid dynamics problems (for example, Navon and Riphagen, 1979; Chang and Shirer, 1985; Esfahani et al., 2005; Mohebalhojeh and Dritschel, 2007; Ghader et al., 2009; Golshahy et al., 2011; Ghader and Nordström, 2015).

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Most of the compact finite difference methods are symmetric (usually with 3 or 5 point stencil) and finding each derivative requires a matrix inversion. However, by splitting the derivative operator of a central compact method into one-sided forward and backward operators, a family of compact MacCormack-type schemes can be derived (Hixon and Turkel, 2000). While these classes of compact methods are as accurate as the original central compact methods used to derive the one-sided forward and backward operators, they need less computational work per point.

In addition, the one-sided nature of the MacCormack method is an advantage of the method especially when severe gradients are present (e.g., Mendez-Nunez and Carroll, 1993; Tolstykh, 1994). These two features (i.e., high accuracy and low computational cost) make the compact MacCormack-type scheme an attractive candidate for numerical modeling of the atmosphere and oceans. The compact MacCormack-type schemes are developed by Hixon and Turkel (2000).

This work is devoted to the application of the fourth-order compact MacCormack scheme for numerical solution of the conservative form of the two-dimensional non-hydrostatic and fully compressible Navier–Stokes equations governing an inviscid and adiabatic atmosphere. To our knowledge, the application of the fourth-order compact MacCormack for numerical simulation of two-dimensional and non-hydrostatic equations of a dry atmosphere has not been studied yet. However, there are research works devoted to the application of the compact finite difference methods to numerical solution of the two-dimensional shallow water equations (e.g., Spotz et al., 1998; Ghader et al., 2009; Ghader and Nordström, 2015).

Moreover, in the present work the second-order MacCormack scheme is also used to numerical solution of the two-dimensional non-hydrostatic and fully compressible equations of an inviscid and adiabatic atmosphere. Using this method enables us to measure some aspects of the computational results (such as efficiency and accuracy) compared to the fourth-order compact MacCormack scheme. Various aspects of the computations such as discretization of the equations for the interior and boundary points, the details of implementation of boundary conditions for different boundary types (e.g., rigid and open boundaries), time step, grid resolution and dissipation are presented (Wilhelmsen and Chen, 1982; Mendez-Nunez and Carroll, 1994; Straka et al., 1993; Giraldo and Restelli, 2007; Müller et al., 2013; Yelash et al., 2014).

In this work we have used the conventional second-order MacCormack scheme (MC2), the standard fourth-order compact MacCormack scheme (MC4) developed by Hixon and Turkel (2000) and a fourth-order compact MacCormack scheme with a four-stage Runge–Kutta time marching method (MCRK4) in our numerical simulations. In fact the main objective of the present work is to compare the performance of the MC4 and MCRK4 methods against the MC2 method for numerical solution of two-dimensional non-hydrostatic and fully compressible Navier–Stokes equations governing an inviscid and adiabatic atmosphere for some well-known test cases. In addition, the spatial differencing of the source term in vertical momentum equation using compact MacCormack method is addressed.

This paper is organized as follows. Section 2 presents details of the governing equations. The numerical method is given in Section 3. The numerical results are given in Section 4. Section 5 is devoted to the accuracy assessment. Finally, conclusions are given in Section 6.

2. Governing equations

An inviscid and isentropic flow of a perfect gas in an Eulerian framework can be expressed by the following equations in a two dimensional Cartesian coordinate as (e.g., Durran, 2010):

\[
\begin{align*}
\frac{d\mathbf{U}}{dt} + \frac{1}{\rho} \nabla p &= -g \mathbf{k}, \\
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{U}) &= 0, \\
\frac{d\theta}{dt} &= 0.
\end{align*}
\]

(1)

where Coriolis force is neglected and total derivative is defined as:

\[
\frac{d()}{dt} = \frac{\partial()}{\partial t} + \mathbf{U} \cdot \nabla().
\]

(2)

\(\mathbf{U} = (u, w)\) is the two-dimensional velocity vector, \(u\) is the velocity component in the x-direction, \(w\) is the velocity component in the z-direction, \(\rho\) is density, \(p\) is pressure, \(g\) is the gravitational acceleration, \(\mathbf{k}\) is unit vector in the vertical direction, and \(\theta\) is the potential temperature. Since, there are four equations involving 5 unknowns, the system is not closed. To close the system the equation of state for a perfect gas \(p = \rho RT\) may be used. Where, \(T\) is the temperature and \(R\) is the gas constant. From the definition of the potential temperature, \(\theta\), we have

\[
\theta = T \left( \frac{p_0}{p} \right) \frac{g}{\rho}.
\]

(3)

\(^1\) It should be mentioned that this matrix inversion can be simply done by using efficient algorithms, for example, Thomas algorithm for solving tridiagonal matrix system.
and we may solve it for $p$ and arrive at the following diagnostic equation:

$$p = p_0 \left( \frac{\rho R}{\rho_0} \right)^\frac{\gamma}{\gamma - 1}.$$  

(4)

In the above equations, $p_0 = 100,000 \text{ kg m}^{-1} \text{ s}^{-2}$ is the basic state pressure, $R = 287.0 \text{ J kg}^{-1} \text{ K}^{-1}$ ($R = c_p - c_v$) is the gas constant for dry air, $c_p = 1004.0 \text{ J kg}^{-1} \text{ K}^{-1}$ is the specific heat at constant pressure, and $c_v = 717.0 \text{ J kg}^{-1} \text{ K}^{-1}$ is the specific heat at constant volume, respectively.

The conservative form of the system of Eq. (1) in a Cartesian coordinate can be written as (e.g., Mendez-Nunez and Carroll, 1994; Straka et al., 1993):

$$\begin{align*}
\frac{\partial \rho}{\partial t} + \frac{\partial (\rho u)}{\partial x} + \frac{\partial (\rho w)}{\partial z} &= 0, \\
\frac{\partial \rho u}{\partial t} + \frac{\partial (\rho u^2 + p)}{\partial x} + \frac{\partial (\rho uw)}{\partial z} &= 0, \\
\frac{\partial \rho w}{\partial t} + \frac{\partial (\rho uw)}{\partial x} + \frac{\partial (\rho w^2 + p)}{\partial z} &= -\rho g, \\
\frac{\partial \rho \theta}{\partial t} + \frac{\partial (\rho u \theta)}{\partial x} + \frac{\partial (\rho w \theta)}{\partial z} &= 0.
\end{align*}$$

(5)

The vector form of system of Eq. (5) is (e.g., Mendez-Nunez and Carroll, 1994; Ahmad and Lindeman, 2007):

$$\begin{align*}
\frac{\partial \mathbf{V}}{\partial t} + \frac{\partial \mathbf{E}}{\partial x} + \frac{\partial \mathbf{F}}{\partial z} &= \mathbf{H},
\end{align*}$$

(6)

where,

$$\mathbf{V} = \begin{pmatrix} \rho \\ \rho u \\ \rho w \\ \rho \theta \end{pmatrix}, \quad \mathbf{E} = \begin{pmatrix} \rho u \\ \rho u^2 + p \\ \rho uw \\ \rho uw \end{pmatrix}, \quad \mathbf{F} = \begin{pmatrix} \rho w \\ \rho uw \\ \rho w^2 + p \\ \rho w \theta \end{pmatrix}, \quad \mathbf{H} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ -\rho g \end{pmatrix}.$$  

For numerical solution, it is required to add an artificial damping term to the right hand side of Eq. (6) to control nonlinear instability. In the present study, this term is defined as (e.g., Straka et al., 1993; Ahmad and Lindeman, 2007):

$$\mathbf{D} = \begin{pmatrix} 0 \\ \nabla \cdot \mathbf{u} \\ \nabla \cdot \mathbf{w} \\ \nabla \cdot \mathbf{\theta} \end{pmatrix}.$$  

(7)

In Eq. (7), $\mathbf{D}$ is the diffusion term and $\nabla$ is the diffusion coefficient. This coefficient is obtained by the numerical experiment and depends on the spatial resolution of numerical solution. In the numerical solution, a damping term is added to the right hand side of Eq. (6) as below:

$$\frac{\partial \mathbf{V}}{\partial t} + \frac{\partial \mathbf{E}}{\partial x} + \frac{\partial \mathbf{F}}{\partial z} = \mathbf{H} + \mathbf{D}.$$  

(8)

3. Numerical method

3.1. Spatial discretization

Formulation of the fourth order compact MacCormack scheme is described briefly. The general form of the family of compact spatial derivatives of a function $f$, may be written in a form as (Hixon and Turkel, 2000):

$$[B] \{D\} = \frac{1}{\Delta x} [C] \{f\}.$$  

(9)

where $D$ is the numerical approximation to the spatial derivative of the function $f$, $[C]$ is the matrix of explicit coefficients, and $[B]$ is the matrix of implicit coefficients and must be inverted to obtain $D$.

In a compact MacCormack-type scheme, the derivative operator is split into forward and backward implicit operators as follows:

$$[D] = \frac{[D^F] + [D^B]}{2}.$$  

(10)

In Eq. (10), $D^F$ and $D^B$ use one-sided forward and backward differences to estimate the first derivative, respectively.
To achieve the fourth order method, forward and backward operations are obtained as:

\[
\begin{align*}
 aD^B_{i+1} + (1 - a)D^F_i &= \left( \frac{1}{\Delta x} \right) (f_i - f_{i-1}), \\
 aD^F_{i+1} + (1 - a)D^B_i &= \left( \frac{1}{\Delta x} \right) (f_{i+1} - f_i),
\end{align*}
\]

where the coefficient \( a = \frac{1}{2} - \frac{1}{2\Delta x^2} \), \( \Delta x \) is grid points distance, \( D \) is spatial derivative and superscripts \( F \) and \( B \) denote forward and backward operators to estimate the first derivative and subscript \( i \) denotes the grid point. The sum of these two operators is of fourth order accuracy.

The details of truncation error of MC2, MC4 and MCRK4 methods for comparison are given in \( A \).

3.2. Temporal discretization

3.2.1. MacCormack-type

The standard fourth-order compact MacCormack scheme (MC4) is a two stage predictor-corrector time advancing method. Application of this method to system of Eq. (8) leads to:

Predictor

\[
V^p_{i,k} = V^l_{i,k} - \Delta t \frac{\partial E}{\partial x} \bigg|_{i,k}^{F} - \Delta t \frac{\partial F}{\partial z} \bigg|_{i,k}^{B} + \Delta t (\alpha_{k,k-1} \frac{\partial^2 \Delta}{\partial x} \bigg|_{i,k}^{d} (1 - \alpha_{k,k-1}) \frac{\partial^2 \Delta}{\partial x} \bigg|_{i,k}^{d} + \Delta t (D^F_{i,k}),
\]

Corrector

\[
V^c_{i,k} = \frac{1}{2} \left[ V^l_{i,k} + V^l_{i,k} - \Delta t \frac{\partial E}{\partial x} \bigg|_{i,k}^{F} - \Delta t \frac{\partial F}{\partial z} \bigg|_{i,k}^{F} + \Delta t (\alpha_{k,k+1} \frac{\partial^2 \Delta}{\partial x} \bigg|_{i,k}^{d} (1 - \alpha_{k,k+1}) \frac{\partial^2 \Delta}{\partial x} \bigg|_{i,k}^{d} + \Delta t (D^c_{i,k}) \right],
\]

in which \( i \) and \( k \) denote the grid point in the \( x \) and \( z \) directions and the superscript \( n \) denotes the time level. \( V \) is a temporary predicted value of \( V \) at time level \( n + 1 \). The coefficients \( \alpha_{k-1} \) and \( \alpha_{k+1} \) are used to determine the density of a layer between two consecutive height levels (see Appendix B). In this work, fourth-order compact finite difference method is applied to spatial differencing of the governing equations.

In Eqs. (12) and (13), superscript \( F \) and \( B \) denote spatial forward and backward differential operators. As the one-sided forward and backward operators appear in Eqs. (12) and (13), to eliminate the bias due to this one sided differencing operators it is needed to sequentially alternate the forward and backward operators between the two spatial derivatives and also between the predictor and corrector steps at each successive time step. The sequence of operators in Eq. (12) is forward-backward and in Eq. (13) is backward-forward. We refer to this combination as \( FB/\text{FB} \). Combinations are \( FB/\text{BF}, BF/\text{BF}, \text{FF/BB} \) and \( \text{BB/FF} \) at each successive time forward. In addition, it is necessary to discretize the equation at boundaries of the computational domain. For example, if it is necessary to implement the zero gradient boundary condition at the right boundary of a rectangular domain in \( x \)-direction, the predictor and corrector equations will be (e.g., Mendez-Nunez and Carroll, 1994):

Predictor

\[
V^p_{N_x,k} = V^l_{N_x,k} - \Delta t \frac{\partial F}{\partial z} \bigg|_{N_x,k}^{B} + \Delta t (\alpha_{k,k+1} \frac{\partial^2 \Delta}{\partial x} \bigg|_{N_x,k}^{d} (1 - \alpha_{k,k+1}) \frac{\partial^2 \Delta}{\partial x} \bigg|_{N_x,k}^{d} ),
\]

Corrector

\[
V^c_{N_x,k} = \frac{1}{2} \left[ V^l_{N_x,k} + V^l_{N_x,k} - \Delta t \frac{\partial E}{\partial x} \bigg|_{N_x,k}^{B} - \Delta t \frac{\partial F}{\partial z} \bigg|_{N_x,k}^{F} + \Delta t (\alpha_{k,k+1} \frac{\partial^2 \Delta}{\partial x} \bigg|_{N_x,k}^{d} (1 - \alpha_{k,k+1}) \frac{\partial^2 \Delta}{\partial x} \bigg|_{N_x,k}^{d} + \Delta t (D^c_{i,k}) \right],
\]

where \( N_x \) is the number of grid points and \( i \) is the grid index in the \( x \)-direction. Eq. (14) is written considering the right boundary condition of \( \frac{\partial \Delta}{\partial x} \bigg|_{N_x,k} = 0 \), is implemented at \( i = N_x \) in \( x \)-direction.

To implement the zero gradient boundary condition at the upper boundary of the rectangular domain in \( z \)-direction the following predictor and corrector steps should be used at the boundary:

Predictor

\[
V^p_{i,N_z} = V^l_{i,N_z} - \Delta t \frac{\partial E}{\partial x} \bigg|_{i,N_z}^{F} - \Delta t \frac{\partial F}{\partial z} \bigg|_{i,N_z}^{B} + \Delta t (\alpha_{N_z,N_z-1} \frac{\partial^2 \Delta}{\partial x} \bigg|_{i,N_z}^{d} (1 - \alpha_{N_z,N_z-1}) \frac{\partial^2 \Delta}{\partial x} \bigg|_{i,N_z}^{d} ),
\]

Corrector

\[
V^c_{i,N_z} = \frac{1}{2} \left[ V^l_{i,N_z} + V^l_{i,N_z} - \Delta t \frac{\partial E}{\partial x} \bigg|_{i,N_z}^{F} - \Delta t \frac{\partial F}{\partial z} \bigg|_{i,N_z}^{F} + \Delta t (\alpha_{N_z,N_z+1} \frac{\partial^2 \Delta}{\partial x} \bigg|_{i,N_z}^{d} (1 - \alpha_{N_z,N_z+1}) \frac{\partial^2 \Delta}{\partial x} \bigg|_{i,N_z}^{d} ) \right],
\]

where \( N_z \) is the number of grid point and \( k \) is the grid index in the \( z \)-direction.
Furthermore, the hydrostatic equilibrium must be satisfied at the upper boundary of the computational domain in \(z\)-direction. In other words:

\[
\frac{\partial p}{\partial z} \bigg|_{i,N_z}^F = -\rho g. \tag{18}
\]

Therefore, to apply the zero gradient condition at the upper boundary while the hydrostatic condition is satisfied it is necessary to divide \(\mathbf{F}\) as follows:

\[
\mathbf{F}^* = \mathbf{F}^1 + \mathbf{F}^2, \tag{19}
\]

where,

\[
\mathbf{F}^1 = \begin{pmatrix}
w^* \rho^* \\
w^* \rho^* u^* \\
w^* \rho^* w^* \\
w^* \rho^* \theta^*
\end{pmatrix}, \quad \mathbf{F}^2 = \begin{pmatrix} 0 \\ 0 \\ 0 \\ p^* \end{pmatrix}.
\]

Thus, Eq. (17) can be rewritten as

\[
\mathbf{V}^{n+1}_{i,N_z} = \frac{1}{2} \left[ \mathbf{V}^0_{i,N_z} + \mathbf{V}^*_{i,N_z} - \Delta t \frac{\partial \mathbf{E}^*}{\partial x} \bigg|_{i,N_z}^B \right] . \tag{20}
\]

where conditions

\[
\frac{\partial \mathbf{F}^1}{\partial z} \bigg|_{i,N_z}^F = 0
\]

and

\[
\frac{\partial \mathbf{F}^2}{\partial z} \bigg|_{i,N_z}^F = \Delta t (\alpha_{N_z,N_z+1} \mathbf{H}^*_{i,N_z} + (1 - \alpha_{N_z,N_z+1}) \mathbf{H}^*_{i,N_z+1})
\]

are satisfied.

3.2.2. Runge–Kutta MacCormack-type

Using a four stage Runge–Kutta method for time marching will lead to the MCRK4 formulation, where, Eq. (6) can be rewritten as:

\[
\frac{\partial \mathbf{V}}{\partial t} + \mathbf{G}(\mathbf{V}) = 0 \tag{21}
\]

where

\[
\mathbf{G}(\mathbf{V}) = \frac{\partial \mathbf{E}}{\partial x} + \frac{\partial \mathbf{F}}{\partial z} - \mathbf{H} . \tag{22}
\]

A four-stage Runge–Kutta MacCormack-type can be written in the following form (Hixon and Turkel, 2000):

\[
\mathbf{h}^{(1)} = -\Delta t D^F [\mathbf{G}(\mathbf{V}^n)], \tag{23}
\]

\[
\mathbf{h}^{(2)} = -\Delta t D^B [\mathbf{G}(\mathbf{V}^n + \alpha_2 \mathbf{h}^{(1)})], \tag{24}
\]

\[
\mathbf{h}^{(3)} = -\Delta t D^F [\mathbf{G}(\mathbf{V}^n + \alpha_3 \mathbf{h}^{(2)})], \tag{25}
\]

\[
\mathbf{h}^{(4)} = -\Delta t D^B [\mathbf{G}(\mathbf{V}^n + \alpha_4 \mathbf{h}^{(3)})], \tag{26}
\]

\[
\mathbf{V}^{n+1} = \mathbf{V}^n + \beta_1 \mathbf{h}^{(1)} + \beta_2 \mathbf{h}^{(2)} + \beta_3 \mathbf{h}^{(3)} + \beta_4 \mathbf{h}^{(4)}. \tag{27}
\]

where, \(D^F\) and \(D^B\) refers to forward and backward spatial differencing operators of fourth-order compact finite difference method, respectively. Normally, the sequence of forward and backward differences is interchanged at every step to avoid numerical bias. The coefficients of this time marching method are given in Table 1. The boundary conditions for MCRK4 are the same as the MC4.
4. Numerical results

Two test problems are adopted to investigate the numerical performance of the MC2, MC4 and MCRK4 schemes. The test cases that are widely used to examine the performance of a numerical method implemented for the solution of governing compressible and non-hydrostatic equations of the atmosphere, are the evolution of a warm bubble in a neutral atmosphere, in domains with rigid and open boundary conditions, (for example, Lilly, 1962; Carpenter et al., 1990; Robert, 1993; Mendez-Nunez and Carroll, 1994; Wicker and Skamarock, 1998; Ahmad and Lindeman, 2007; Müller et al., 2013) and evolution of a cold bubble in a neutral atmosphere (density current benchmark proposed by Straka et al., 1993).

4.1. Straka density current test case

The first test case used to examine the performance of our scheme is the evolution of a cold bubble in a neutral atmosphere proposed by Straka et al. (1993).

For this test case the computational domain is bounded within $[-26.5\text{ km}: 26.5\text{ km}] \times [0: 6.4\text{ km}]$. The lateral and the upper and bottom boundaries are assumed as solid walls. The domain is initialized for a neutral atmosphere at $\theta = 300 \text{ K}$ in hydrostatic balance. The initial $u$ and $w$ velocity components are set to zero.

In this test case, initial conditions of the temperature field perturbation are defined as follows (Straka et al., 1993):

$$\Delta T = \left\{ \begin{array}{ll} 0.0 & \beta > 1.0 \\ -15.0 \left( \frac{\cos(\pi \beta) + 1.0}{2} \right) & \beta \leq 1.0 \end{array} \right. $$

(28)

where

$$\beta = \sqrt{ \left( \frac{x - x_c}{x_r} \right)^2 + \left( \frac{z - z_c}{z_r} \right)^2 }$$

(29)

and $x_c = 0.0 \text{ km}$, $z_c = 3.0 \text{ km}$, $x_r = 4.0 \text{ km}$ and $z_r = 2.0 \text{ km}$. In addition a fixed diffusion coefficient, $\nu = 75 \text{ m}^2 \text{s}^{-1}$, is used to be able to compare our results with those reported by Straka et al. (1993). However, we have conducted some numerical experiments and it is observed that we can use smaller values of $\nu$ for different resolutions while the numerical stability is preserved. For example, it is found that for the MC2 method a value of $\nu = 30 \text{ m}^2 \text{s}^{-1}$ can be used for $\Delta x(=\Delta z) = 100 \text{ m}$ resolution. In a similar way, for the MC4 and MCRK4 methods a value of $\nu = 8 \text{ m}^2 \text{s}^{-1}$ is working at resolution $\Delta x(=\Delta z) = 100 \text{ m}$.

The grid resolutions used in the Straka test case are $\Delta x(=\Delta z) = 25 \text{ m}$, $50 \text{ m}$, $100 \text{ m}$, $200 \text{ m}$ and $400 \text{ m}$ in which the number of grid points are $N_x \times N_z = [1025 \times 257]$, [513 \times 129], [257 \times 169] and [65 \times 17] in the horizontal and vertical directions, respectively. According to the numerical stability condition, time steps corresponding to these resolutions are [0.015625], [0.03125], [0.0625], [0.0125] and [0.25] second, respectively.

Fig. 1 shows the time evolution of perturbation potential temperature field ($\theta'$) generated by the MCRK4 scheme for a 25 m resolution. The reference solution (REFC) provided by Straka et al. (1993) is also shown in Fig. 1. A qualitative comparison indicates the validity of the results and shows that the results of the MCRK4 scheme are in good agreement with the Straka et al. (1993) benchmark (see Table 2).

In addition, the perturbation pressure ($p'$), $\theta'$, $u$-velocity and $w$-velocity generated by the MCRK4 scheme at time=900 s are shown in Fig. 2.

Maximum and minimum values of $\theta'$ at time=900 s for 25 m resolution are given in Table 2. Table presents results of MCRK4, MC4, MC2 schemes and the reference solution (REFC) by Straka et al. (1993).

Fig. 3 shows the $\theta'$ at time=900 s generated by the MCRK4 scheme for 50 m, 100 m, 200 m and 400 m resolutions. The reference solution (REFC) given by Straka et al. (1993) is also shown in this figure. It can be seen that, MCRK4 even at the very coarse resolution of 400 m, is able to detect the shape of Kelvin–Helmholtz rotors and in 200 m resolution the second rotor is improved compared to Straka et al. (1993).

### Table 1

| Coefficients for MCRK4 method (Hixon and Turkel, 2000). |
|----------------|----------------|----------------|----------------|----------------|
| $\alpha_1$   | $\alpha_2$   | $\alpha_3$   | $\alpha_4$   |
| $\frac{1}{2}$ | $\frac{1}{2}$ | 1             | $\frac{1}{8}$ |
| $\beta_1$    | $\beta_2$    | $\beta_3$    | $\beta_4$    |
| $\frac{1}{4}$ | $\frac{1}{4}$ | $\frac{1}{10}$ | $\frac{1}{10}$ |

### Table 2

<table>
<thead>
<tr>
<th>Variable</th>
<th>MCRK4</th>
<th>MC4</th>
<th>MC2</th>
<th>REFC</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\theta_{max}$ (C)</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>$\theta_{min}$ (C)</td>
<td>-9.58</td>
<td>-9.59</td>
<td>-9.68</td>
<td>-9.77</td>
</tr>
<tr>
<td>Front location (m)</td>
<td>15,421.0</td>
<td>15,451.0</td>
<td>15,487.0</td>
<td>15,537.44</td>
</tr>
</tbody>
</table>
Fig. 4 shows the $\theta^*$ at time $= 900$ s generated by the MCRK4, MC4, MC2 schemes for a 200 m resolution. The solution given by the MCRK4 for a 25 m resolution at time $= 900$ s is also shown in the figure. It is observed that, for a coarse grid the MCRK4 and MC4 are more accurate than the MC2 method and they are able to better resolve the shape of rotors.

The density current benchmark suggested by Straka et al. (1993) can be considered as an idealized micro-burst, strong downdraft movement at center of the cold bubble is formed, because the cold air descends due to negative buoyancy. When the cold air reaches the ground, it is rolled up and a front is formed. The density current benchmark solution (Straka et al., 1993) consists of three rotors, which develop at top boundary of the front due to the Kelvin–Helmholtz-type instability. The formation of the front and the development of these rotors can be seen in Fig. 5 (that are similar to results reported by Ahmad and Lindeman (2007)).

Fig. 5 shows that the location of front is at 15,421 m after 900 s integration. The location of the front for the MCRK4, MC4, MC2 and for the reference solution (REFC) by Straka et al. (1993) is given in Table 2.

In addition, to measure the computational cost of the methods, Table 3 presents CPU times for MC2, MC4 and MCRK4 methods at different resolutions for the Straka density current test case at time $= 900$ s. For a meaningful comparison, the CPU times have been normalized by the CPU time of MC2 method for 200m resolution. It can be seen that the MC2 schemes are less expensive than the MC4 schemes and MCRK4 schemes.

4.2. Convection in neutral atmosphere

In this section, the results of warm bubble test case in a neutral atmosphere are presented. The domain for this test case is bounded within $[0:40.0 \text{ km}] \times [0:15.0 \text{ km}]$. The mesh resolution is set to 50 m in both the $x$- and $z$-directions. The lateral and top boundaries of domain are open. The domain is initialized for a neutral and hydrostatic atmosphere at $\theta = 300$ K. The initial $u$ and $w$ are set to zero. In this test case, initial conditions of the temperature field perturbation is defined as follows (Mendez-Nunez and Carroll, 1994):

$$\Delta T = 6.6 \left[ \cos \left( \frac{\pi \beta}{2} \right) \right] \beta \leq 1.0$$

Table 3
The CPU times for different methods at time $= 900$ s. The unit of CPU time is taken to be that of the MC2 method for 200 m resolution.

<table>
<thead>
<tr>
<th>Resolution</th>
<th>200 m</th>
<th>100 m</th>
<th>50 m</th>
</tr>
</thead>
<tbody>
<tr>
<td>MC2</td>
<td>1</td>
<td>10</td>
<td>89</td>
</tr>
<tr>
<td>MC4</td>
<td>2</td>
<td>12</td>
<td>103</td>
</tr>
<tr>
<td>MCRK4</td>
<td>3</td>
<td>25</td>
<td>207</td>
</tr>
</tbody>
</table>
Fig. 2. Contour plots (solid contours are positive, dashed negative values) of the (a) $u$-velocity (m s$^{-1}$) $[-16, 32; 2]$, (b) $w$-velocity (m s$^{-1}$) $[-30, 30; 2]$, (c) $p'$ (mb) $[-700.0, 400.0; 50]$ and (d) $\vartheta'(C)$ $[-16.5, -0.5; 1]$ at time =900 s for the resolution 25 m generated by the MCRK4 scheme. Only the right half of the computational domain is shown in the figures.

where

$$\beta = \sqrt{\left(\frac{x - x_c}{x_t}\right)^2 + \left(\frac{z - z_c}{z_t}\right)^2}$$

(31)

in which $x_c = 20.0$ km, $z_c = 2.75$ km, $x_t = 2.5$ km and $z_t = 2.5$ km. The diffusion coefficient, $\nu$, is not added. According to Eq. (30), the maximum perturbation of potential temperature is located at center of the bubble, so the bubbles move upward quickly.

Fig. 6 shows the initial condition of the potential temperature perturbation field ($\vartheta'$) for a 50 m resolution at $t = 0$ s.

Fig. 7 shows the time evolution of the potential temperature perturbation field at 120 s intervals generated by the MCRK4 scheme. It can be seen, the potential temperature gradient has increased over time.

Fig. 8 shows the time evolution of the $u$-velocity at 120 s intervals generated by the MCRK4 scheme.

5. Accuracy analysis

In this section we use the one-dimensional advection equation with known analytical solution to assess the accuracy of the compact MacCormack schemes. Then, the method of manufactured solution (MMS) is employed to construct an analytical solution for the 2D compressible and non-hydrostatic atmospheric equations (with source terms) that enables us to compare the accuracy of the MC2 and MC4 methods in a meaningful way.
5.1. One-dimensional linear wave equation

Consider the one-dimensional advection equation with constant speed (e.g., Hixon and Turkel, 2000):

\[ U_t + U_x = 0, \]  

(32)
Fig. 6. Contour plot of initial potential temperature perturbation field (K) [0.0, 6.5; 0.5] at time = 0 s.

Fig. 7. Time evolution of the potential temperature perturbation field (K) [0.0, 6.5; 0.5] at 120 s intervals generated by the MCRK4 scheme. Solid and dashed lines are for positive and negative contours, respectively.
with initial condition

$$U(x, 0) = \frac{1}{2} \exp \left( - \ln(2) \left( \frac{x}{3} \right)^2 \right) ,$$  \hspace{1cm} (33)

where

$$-20 \leq x \leq 450$$

To implement the boundary condition at $x=20$, which is the inflow boundary, the derivative of $U$ is set to zero. At $x=450$, which is the outflow boundary, the derivative of $U$ is calculated explicitly from the interior using one-sided boundary stencils.

The following global $l_2$ norm is used to measure the error:

$$l_2 = \left\{ \frac{1}{N} \sum_{i=1}^{N} |Q(i) - Q_{ref}(i)| \right\}^{1/2} \hspace{1cm} (34)$$
Table 4
The convergence rate, $q$, for the second-order methods.

<table>
<thead>
<tr>
<th>$\Delta x$</th>
<th>Lax–Wendroff</th>
<th>Leap-frog</th>
<th>Beam–Warming</th>
<th>MC2</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.0</td>
<td>1.887</td>
<td>1.887</td>
<td>1.887</td>
<td>1.887</td>
</tr>
<tr>
<td>0.5</td>
<td>1.929</td>
<td>1.929</td>
<td>1.929</td>
<td>1.929</td>
</tr>
<tr>
<td>0.25</td>
<td>1.950</td>
<td>1.950</td>
<td>1.950</td>
<td>1.887</td>
</tr>
<tr>
<td>0.125</td>
<td>1.962</td>
<td>1.962</td>
<td>1.962</td>
<td>1.962</td>
</tr>
</tbody>
</table>

where $Q$ is numerical solution, $Q_{\text{ref}}$ is exact solution and $N$ is the number of grid point. When the norms are calculated for a given method in different resolutions, the convergence rate, $q$, can also be measured (for example, Salari and Knupp, 2000; Roy et al., 2002, 2004; Williamson et al., 1992). The following relation is used to calculate the convergence rate

$$ q = \frac{\log_{10} \left( \frac{L_2(Q)^{\Delta x_1}}{L_2(Q)^{\Delta x}} \right)}{\log_{10} \left( \frac{\Delta x_1}{\Delta x} \right)} $$

(35)

where $L_2(Q)^{\Delta x_1}$ denotes the $L_2$ norm of numerical solution corresponding with spatial grid space $\Delta x_1$. Values of $q$ are reported in Tables 4 and 5 for different methods. Here, for comparison the results for Lax–Wendroff (Lax and Wendroff, 1960; Durran, 2010), leap-frog and Beam–Warming (Beam and Warming, 1976, 1978; Cebecci et al., 2005) methods with second-order and fourth-order compact finite difference methods in space are also included in tables.

Tables 4 and 5 present the convergence rates for different methods in different resolutions. The space resolutions used are, $\Delta x = 1$ m, $\Delta x = 0.5$ m, $\Delta x = 0.25$ m and $\Delta x = 0.125$ m. A fixed small time step $\Delta t = 0.5 \times 10^{-7}$ s is used for all resolutions. It can be seen that the convergence rates are in agreement with theoretical order of convergence. It is also observed that the MCRK4 and MC2 exhibit a similar spatial convergence rate.

5.2. Method of manufactured solution

In this part, the method of manufactured solution (MMS) (e.g., Roache, 1998, 2002) is used to generate analytical solutions which can be used to assess the accuracy of the MC2, MC4 and MCRK4 methods. In the MMS, a solution form is first constructed, then, governing equations are modified by the addition of analytical source terms. The MMS has been used in many research works (for example, Salari and Knupp, 2000; Roy et al., 2002, 2004; Waltz et al., 2014).

System of Eq. (5) by using MMS method can be rewritten as:

$$ \begin{align*}
\frac{\partial \rho}{\partial t} + \frac{\partial \rho u}{\partial x} + \frac{\partial \rho w}{\partial z} &= S_\rho, \\
\frac{\partial \rho u}{\partial t} + \frac{\partial (\rho u u + p)}{\partial x} + \frac{\partial \rho w u}{\partial z} &= S_u, \\
\frac{\partial \rho w}{\partial t} + \frac{\partial (\rho w u + p)}{\partial x} + \frac{\partial \rho w^2}{\partial z} &= S_w - \rho g, \\
\frac{\partial \rho \theta}{\partial t} + \frac{\partial \rho u \theta}{\partial x} + \frac{\partial \rho w \theta}{\partial z} &= S_\theta.
\end{align*} $$

(36)

in which $S_\rho$, $S_u$, $S_w$ and $S_\theta$ are the source terms that arise from the application of the MMS. The general form chosen for the MMS, for $\theta$, $u$, $w$, $p$ are given as follows

$$ \begin{align*}
\theta(x, z, t) &= \theta_1 + \theta_2 \cos(\pi \beta) e^{-\alpha t}, \\
u(x, z, t) &= u_1 + u_2 \sin(\pi \beta) e^{-\alpha t}, \\
w(x, z, t) &= w_1 + w_2 \cos(\pi \beta) e^{-\alpha t}, \\
p(x, z, t) &= p_1 + p_2 e^{-\alpha t},
\end{align*} $$

(37)

where $\theta_1$, $u_1$, $w_1$ and $p_1$ are constants. Constants $\theta_1$, $u_1$, $w_1$, $p_1$ and coefficients $\theta_2$, $u_2$, $w_2$, $p_2$ are chosen to satisfy the initial and boundary conditions. To perform the calculations the following constants are used: $\theta_1 = 300$, $p_1 = 0$, $u_1 = \sin(\pi \beta)$, $w_1 = \cos(\pi \beta)$ and $\alpha = 1$.

Table 5
The convergence rate, $q$, for the fourth-order methods.

<table>
<thead>
<tr>
<th>$\Delta x$</th>
<th>Lax–Wendroff</th>
<th>Leap-frog</th>
<th>Beam–Warming</th>
<th>MC4</th>
<th>MCRK4</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.0</td>
<td>4.408</td>
<td>4.408</td>
<td>4.436</td>
<td>4.408</td>
<td>4.408</td>
</tr>
<tr>
<td>0.5</td>
<td>4.259</td>
<td>4.259</td>
<td>4.273</td>
<td>4.259</td>
<td>4.259</td>
</tr>
<tr>
<td>0.25</td>
<td>4.182</td>
<td>4.182</td>
<td>4.191</td>
<td>4.182</td>
<td>4.182</td>
</tr>
</tbody>
</table>
where, $l_2$ indicates conclusion in atmospheric benchmark dimensional respectively. Cormack addition, results the also support that, and is grateful to his helpful comments during the development of the codes.

Acknowledgments

In this case to measure the global error, the following $l_2$ norm is used (e.g., Straka et al., 1993):

$$l_2(Q) = \left\{ \frac{1}{N_x N_z} \sum_{i=1}^{N_x} \sum_{k=1}^{N_z} \left| Q(x_i, z_k) - Q_{\text{ref}}(x_{ii}, z_{kk}) \right| \right\}^{1/2}$$

where $Q$ is numerical solution, $Q_{\text{ref}}$ is analytical solution of MMS method [Eq. (37)]. $N_x$ and $N_z$ are the number of grid points in $x$- and $z$-directions, $i$ and $k$ are the grid indexes in the $x$- and $z$-directions, $ii$ and $kk$ are the grid indexes for the MMS, respectively.

Fig. 9 presents the global error ($l_2$ norm) for potential temperature perturbation obtained for the MMS method for MC2 and MC4 methods (after 500 time steps with $\Delta t = 1 \times 10^{-5}$ s). It is seen that the MC4 schemes produces less error than MC2 scheme. In addition, figure shows higher convergence rate for the MC4 than the MC2 method. It is also worth to mention that, MC4 and MCRK4 methods exhibit similar spatial convergence rate (not shown here).

6. Conclusions

In this work we used the traditional second-order MacCormack scheme (MC2), the standard fourth-order compact MacCormack scheme (MC4) developed by Hixon and Turkel (2000) and a fourth-order compact MacCormack scheme with a four-stage Runge–Kutta time marching method (MCRK4) for numerical solution of 2D compressible and non-hydrostatic atmospheric equations.

Two test cases including evolution of a warm bubble in a neutral atmosphere (in domains with open boundary conditions proposed by Mendez-Nunez and Carroll (1994)) and evolution of a cold bubble in a neutral atmosphere (density current benchmark proposed by Straka et al. (1993)) are used for numerical experiments.

The accuracy analysis is performed by using one-dimensional advection equation with constant speed and the MMS method. Results of the accuracy assessment indicates the superiority of the MCRK4 and MC4 schemes over the MC2 scheme in terms of global error and convergence rate. In addition, comparison of numerical results generated in this work with the results reported by others (for example, Mendez-Nunez and Carroll, 1994; Straka et al., 1993; Ahmad and Lindeman, 2007) indicates better performance of the MCRK4 and MC4 schemes over the MC2 method. However, it should be noted that this conclusion is limited to the test cases used in this research work. More investigation is needed to assess the performance of the MCRK4 and MC4 for real-world atmospheric applications.

It is also worth to mention that for real atmospheric applications the present work should be extended to three-dimensional geometry and the orography is needed to be handled by using a terrain-following vertical coordinate.

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Appendix A. Truncation error

The truncation errors of MC2, MC4 and MCRK4 for the one-dimensional advection equation is given in this appendix.

A.1. MC2

Consider the one-dimensional advection equation with constant speed (e.g., Hixon and Turkel, 2000):

\[ U_t + (F(U))_x = 0, \]  \hspace{1cm} (A.1)

where \( F(U) = cU \). Application of MC2 scheme to Eq. (A.1) leads to

Predictor

\[ U^* = U^n - \Delta t \delta^F(F(U^n)), \]  \hspace{1cm} (A.2)

Corrector

\[ U^{n+1} = \frac{1}{2} \{ U^n + U^* - \Delta t \delta^B(F(U^*)) \}, \]  \hspace{1cm} (A.3)

where \( \delta^F \) and \( \delta^B \) refer to forward and backward spatial difference operators. \( U^* \) is a temporary predicted value of \( U \) at time level \( n + 1 \). Substitution of (A.2) into (A.3) leads to:

\[ U^{n+1} = \frac{1}{2} \{ U^n + (U^n - \Delta t \delta^F(F(U^n))) - \Delta t \delta^B(F(U^*)) \}, \]  \hspace{1cm} (A.4)

Then by using Taylor series for \( U(t + \Delta t) \) and \( U(x + \Delta x) \) and substituting into (A.4) the truncation error of MC2 method is obtained. The truncation error for this method is given in Table A.6. It can be seen that the MC2 method is of second-order in time and space.

A.2. MC4 and MCRK4

To find the truncation error for the fourth-order MacCormack methods the Taylor series expansion of the forward and backward operators of equation (11) are needed and the rest of the procedure is similar to what used for the MC2 method. Truncation errors of MC4 and MCRK4 methods are also shown in Table A.6. It is observed that the MC4 method is fourth-order in space and second-order in time and MCRK4 is fourth-order in space and time.

Appendix B. Initialization procedure

The procedure for the initialization is similar to what proposed by Mendez-Nunez and Carroll (1994). Here, we explain how the coefficients \( \alpha_{k,k-1} \) and \( \alpha_{k,k+1} \) appearing in Eqs. (12) and (13) are calculated. Fig. B.10 shows three levels of computational mesh in z-direction, namely, \( k - 1, k, k + 1 \).

| \( p_{k+1} \) | \( \alpha_{k,k+1} \) |
| \( p_k \) | \( \alpha_{k,k} \) |
| \( p_{k-1} \) |

Fig. B.10. The sequential levels \( k - 1, k, k + 1 \) related to each pressure level.
The discrete form of the hydrostatic equation on these levels can be written as:

$$\frac{\partial p}{\partial z} = -g(\alpha_{k,k+1} \rho_k + (1 - \alpha_{k,k+1}) \rho_{k+1})$$

$$\frac{\partial p}{\partial z} = -g(\alpha_{k,k+1} \rho_k + (1 - \alpha_{k,k+1}) \rho_k).$$

(B.1)

In Eq. (B.1), it is seen that the sum of coefficients of the densities [i.e., $\alpha_{k,k+1}, (1-\alpha_{k,k+1})$] are equal to one.

This ensures that the discrete form of the hydrostatic equation is consistent with the continuous form of the hydrostatic equation.

For a given pressure gradient a relation can be found for the coefficient $\alpha_{k,k+1}$ as:

$$\alpha_{k,k+1} = \frac{-\frac{\partial p}{\partial z} g_{k+1} - \rho_k}{-\frac{\partial p}{\partial z} g_k - \frac{\partial p}{\partial z} g_{k+1} - 2\rho_k} - \frac{\partial p}{\partial z} g_k - \frac{\partial p}{\partial z} g_{k+1} - 2\rho_k$$

(B.2)

By substitution of the forward and backward operators of the MC4 into Eq. (B.2) the coefficient $\alpha_{k,k+1}$ is obtained for this method. However, for the second-order MacCormack method, as a special case, the forward and backward operators are

$$\frac{\partial p}{\partial z} = \frac{p_{i,k+1} - p_{i,k}}{\Delta z}, \quad \frac{\partial p}{\partial z} = \frac{p_{i,k+1} - p_{i,k}}{\Delta z}.$$

(B.3)

by substitution of (B.3) into (B.2) we have

$$\alpha_{k,k+1} = \frac{1}{2}$$

(B.4)

for the MC2.

References


