Reduced conservation error of kinetic energy using a Runge-Kutta algorithm with reduced numerical dissipation

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Abstract. This paper describes an approach that reduces the error in the conservation law of velocity fluctuation intensities and turbulent kinetic energy resulting from a numerical analysis of incompressible flow. The optimized fourth-order Runge-Kutta method used to analyze acoustic problems in previous studies was used here to reduce the numerical dissipation. In order to strictly validate the conservation law of velocity fluctuation intensities and turbulent kinetic energy, the authors used a periodic box filled with an inviscid flow, where velocity fluctuation intensities and turbulent kinetic energy could be analytically held. By using the optimized Runge-Kutta method, the numerical dissipation, which is the error in conservation laws, is of the order of 1/100. The reduction in the numerical dissipation shown in this study increased with an increasing time increment. To investigate the effect of numerical dissipation, higher-order statistics of turbulent kinetic energy were calculated. This study also derived a simple mathematical form to estimate the conservation error of higher-order statistics for turbulent kinetic energy.

1. Introduction
Incompressible turbulence is an essential issue in the field of fluids engineering. However, the governing equations of incompressible turbulence cannot be solved analytically. To solve the governing equations using numerical analysis, the governing equations must be discretized using an appropriate discrete formula, with error terms that are (ideally) small. Large-eddy simulation (LES) is commonly used in the field of turbulence engineering and should be performed with a high degree of accuracy. The governing equations represent conservation laws in the form of mathematical expressions. From the governing equations, a kinetic energy conservation law can be derived. Maintaining the law of conservation of kinetic energy has been considered significant for the accurate analysis of incompressible turbulence.

The continuity and Navier-Stokes (NS) equations, the governing equations for incompressible flow, describe the conservation of mass and momentum, respectively [1]. From these conservation laws, the conservation laws of kinetic energy, specifically the intensities of velocity fluctuation and turbulent kinetic energy, are also derived. By satisfying these conservation laws of intensities of velocity fluctuation and turbulent kinetic energy in a numerical simulation, the accuracy of the numerical
simulation to analyze incompressible flow is maintained (e.g., [2]). In LES, a higher-order discretization scheme should be used. A previous study proposed a high-order accuracy discretization scheme that can maintain this conservation law explicitly [3]. This discretization scheme has been used in many studies. Suzuki et al. [4-6] apply the commonly used scheme to numerically analyze grid-generated turbulence. Another study [7] describes a numerical analysis whose accuracy using the difference method is further improved by using a high-order accuracy discretization scheme to discretize the viscous terms. From this high-order accuracy discretization scheme, a discrete formula for discretizing the governing equations in the cylindrical coordinate system has been developed [8].

The high-order discretization schemes produced by previous studies that explicitly conserve kinetic energy do not include discrete error terms, but still allow errors due to numerical integration. In earlier studies (e.g., [3]), inviscid flow has been used to validate the conservation characteristics of kinetic energy. In an inviscid flow, kinetic energy is completely maintained, but due to numerical integration error, the kinetic energy conservation characteristic has an error term. This error term is due to the error of the time integration method. Previous works studied the accuracy of incompressible turbulence using the numerical dissipation [9-12].

Numerical dissipation caused by time integration has previously been addressed. For example, a time integration method optimized to reduce numerical dissipation was developed to analyze an acoustic field [13]. If kinetic energy is conserved explicitly, the kinetic energy conservation error will be reduced by using a time integration method with reduced numerical dissipation.

The purpose of this study is to demonstrate the reduction in kinetic energy conservation error produced by applying a previously developed time integration method with reduced numerical dissipation. Specifically, the time integration scheme developed by Berland et al. [13] is employed. In order to strictly validate the conservation error of kinetic energy, inviscid flow is used as in previous studies. In addition, the effect of kinetic energy conservation error on higher-order statistics is addressed.

2. Methods

2.1. Present numerical simulation

The governing equations for the numerical analysis in this study are the continuity equation and the NS equation. These equations describe mass and momentum conservation, respectively. The equations are discretized using a discretization scheme developed in a previous study [3]. In the numerical analysis in this study, the fourth-order central differential scheme is employed. Here, a skew-symmetric form is used as the form of the convection terms. As shown in the previous study [3], by using the skew-symmetric form, the conservation laws of the velocity fluctuation intensities and turbulent kinetic energy are explicitly held in the simulation without making a numerical assumption regarding the continuity equation. Moreover, it is appropriate to use the fourth-order accuracy central differential scheme rather than the second-order scheme in applying the scheme to LES. The code for the present numerical analysis is based on that in previous works [4-7].

In the numerical analysis in this study, the conservation laws of velocity fluctuation intensities and turbulent kinetic energy need to be strictly validated. In order to validate these conservation laws, the authors used a flow field in which these conservation laws are held analytically. Specifically, a three-dimensional inviscid flow was used. In this flow, the velocity fluctuation intensities and the turbulent kinetic energy are analytically constant with time. In order to strictly validate these conservation laws, a periodic box is used as a computational region. Figure 1 shows a schematic figure of the present numerical simulation. By using the periodic box, the use of boundary conditions does not affect the temporal profile of the velocity fluctuation intensities and turbulent kinetic energy. The size of the periodic box is set to $L^3 = 2\pi^3$. The computational region of the periodic box is discretized using a grid with equally spaced points. The number of grid points of the periodic box is set to $N^3 = 16^3$.

The initial velocity field is obtained by rotating a normal random vector. By using this method, the initial velocity field analytically satisfies the continuity equation, which is one of the governing
equations. The series of uniform random numbers was generated using the Mersenne twister scheme [14]. The normal random number vectors were calculated from a series of uniform random numbers produced by the Box-Muller method [15]. The spatial mean value of the initial velocity field is zero. The initial velocity field is normalized so that the initial kinetic energy is unity. Normalization by the initial kinetic energy is performed in the post-processing stage. A value of CFL is set to be sufficiently smaller than unity in the present numerical simulation by controlling the amplitude of the random number vector. The governing equations were analyzed using the fractional step method. The Poisson equation for pressure was solved directly using a fast Fourier transform. Here, the Poisson equation is needed to be solved at each fractional time step. Therefore, the error in the continuity equation is of the order of machine zero because of using the present direct Poisson solver at the fractional steps. The error in the continuity equation can affect the obtained flow field significantly. The kinetic energy conservation error is given as a function of the time increment. Therefore, the time increment is taken to be a principal parameter in the present study. We consider that the generality of the results obtained in this study is sufficiently high. The flow field of this research is taken to be isotropic. The local turbulence in the sufficient high Reynolds number turbulence is isotropic, like the flow field in this study. The kinetic energy conservation error observed in this study can be found when a real turbulent flow field is simulated.

![Figure 1. Schematic figure of present numerical simulation: Inviscid fluid is filled in a periodic box in the present numerical simulation; The initial flow field is given by normal random number vector field.](image)

2.2. Applying a Runge-Kutta method with reduced numerical dissipation

Application of the explicit time integration method slightly dissipates velocity fluctuation intensity and turbulent kinetic energy in the stages of the time integration. The numerical dissipation due to a time integration scheme depends on the form of the time integration scheme. For example, the numerical dissipation of the fourth-order Runge-Kutta method is much smaller than that of the first-order Euler method. By optimizing the value of the constants included in the integral form of the fourth-order Runge-Kutta method, the numerical dissipation of the method can be reduced. This study uses a fourth-order Runge-Kutta method suitable for acoustic problems that require numerical analysis with lower numerical dissipation [13]. The fourth-order Runge-Kutta method used in this study has been used in many previous studies. The discretization formula for calculating incompressible flow, which is the focus of this study, satisfies the conservation laws of velocity fluctuation intensities and turbulent kinetic energy explicitly. However, the time integration method will cause slight errors. By using the optimized fourth-order Runge-Kutta method with reduced numerical dissipation, the error in the conservation laws of velocity fluctuation intensities and turbulent kinetic energy may be further reduced.

In order to validate the numerical analysis using inviscid flow, an analysis using various time integration methods is first carried out. The discretized form proposed in previous research explicitly conserves kinetic energy [3]. Kinetic energy conservation error is caused by the numerical dissipation due to the use of a time integration method. The order of numerical dissipation of a time integration
method is given by the accuracy order of the method. For example, the numerical dissipation of the second-order Adams-Bashforth method is of the second-order of the time increment. This study uses this characteristic to validate the numerical analysis. Specifically, the first-order Euler method, the second-order Adams-Bashforth method, the third-order Runge-Kutta method [16], and the fourth-order Runge-Kutta method based on five stages [17] are used for validation. The magnitudes of the numerical dissipation of the first-order Euler method, the second-order Adams-Bashforth method, the third-order Runge-Kutta method, and the fourth-order Runge-Kutta method based on five steps are the first order, the second order, the third order, and the fourth order of the time increment, respectively. Table 1 shows coefficients of the Runge-Kutta schemes based on five and six stages, where $A_j$ and $B_j$ are the coefficients of a Runge-Kutta schemes for $j$ stage. Note that the numerical dissipation of the fourth-order Runge-Kutta method based on five stages is significantly larger than that of the fourth-order Runge-Kutta method with the reduced numerical dissipation shown above.

Table 1. Coefficients of the Runge-Kutta schemes.

| Coefficients | Fourth-order Runge-Kutta due to five stages (RK4-5) | Fourth-order Runge-Kutta due to six stages (RK4-6) |
|--------------|-----------------------------------------------------|-----------------------------------------------------|
| $A_1$        | 0                                                   | 0                                                   |
| $A_2$        | $- \frac{567301805773}{1357537059087}$             | $-0.73710139279$                                     |
| $A_3$        | $- \frac{2404267990393}{2016746695238}$            | $-1.63470794341$                                    |
| $A_4$        | $- \frac{3550918686646}{2091501179385}$           | $-0.74473900378$                                    |
| $A_5$        | $- \frac{1275806237668}{842570457699}$            | $-1.46989735815$                                    |
| $A_6$        | N/A                                                 | $-2.81397138804$                                    |
| $B_1$        | $\frac{1432997174477}{9575080441755}$              | $0.032918605146$                                    |
| $B_2$        | $\frac{5161836677717}{13612068292357}$            | $0.823256997200$                                    |
| $B_3$        | $\frac{1720146321549}{2090206949498}$             | $0.381530948900$                                    |
| $B_4$        | $\frac{3134564353537}{4481467310338}$             | $0.200092213184$                                    |
| $B_5$        | $\frac{2277821191437}{14882151754819}$            | $1.718581042715$                                    |
| $B_6$        | N/A                                                 | 0.27                                                |

3. Results and discussion

3.1. Reduced conservation error

The focus of this study is on the non-dissipative nature of an inviscid flow. In an inviscid flow, kinetic energy is never dissipated analytically. Therefore, the dissipation that occurs in an inviscid flow can only be due to errors in the numerical analysis. This characteristic enables the present study to validate strictly the kinetic energy conservation error in numerical analysis. Kinetic energy deviates from the
initial value as time proceeds due to the conservation error in the numerical analysis. This deviation grows with time. The time evolution of the deviation can be approximated using a linear function with sufficient accuracy specifically as follows:

\[ K = K_0 + \left( \frac{dK}{dt} \right) t \ldots \text{or} \ K / K_{|t=0} = 1 + \varepsilon t + \ldots, \text{where} \ \varepsilon = \frac{dK}{dt}. \tag{1} \]

Here \( \varepsilon \) is equivalent to the conservation error of the kinetic energy: \( K_{|t=0} = 1 \). Also, \( K \) is the mean kinetic energy in the box. The following quadratic function is used in this study to accurately calculate the time rate of change of kinetic energy \( \frac{dK}{dt} \):

\[ K = K_0 + \left( \frac{dK}{dt} \right) t + \left( \frac{a}{2} \right) \left( \frac{dK}{dt} \right)^2 t^2. \]

Here, analytically, the rate of temporal change of kinetic energy is exactly zero. Figure 2 shows the absolute value of the conservation error calculated by the above scheme as a function of time increment \( \Delta t \). As shown in Figure 2, the absolute value of the conservation error decreases with a decreasing time step. The absolute value of the conservation error also depends on the time integration method being used. As indicated in Figure 2, the magnitude of the conservation error decreases as the accuracy order of the time integration scheme increases. The increasing conservation error is due to the use of double precision real numbers in this simulation.

![Figure 2](image_url)

**Figure 2.** Dependency of kinetic-energy conservation error on time increment \( \Delta t \), where the rate of change of the kinetic energy is calculated at the initial time: As shown here, the dependency on the time increment follows a power law whose accuracy order is equal to that of the specific time integration scheme; Here E1, AB2, RK3, and RK4(5) indicate results of the first-order Euler method, the second-order Adams-Bashforth method, the third-order Runge-Kutta method [16], and the fourth-order Runge-Kutta method based on five stages [17], respectively.

The accuracy of the time integration scheme used in this study is set in the range from first to fourth. The accuracy order of the time integration scheme precisely affects the conservation error, as the scheme used in this study is explicit. As shown in Figure 2, the \( \Delta t \) distribution of the absolute value of the conservation error is described by a power-law function with the power number equal to the accuracy order of the time integration scheme. This result is confirmed for the first-order accuracy Euler scheme through the fourth-order Runge-Kutta method. In the discretization scheme used in this study, kinetic energy is explicitly conserved. Thus, the kinetic energy conservation error is due to the numerical dissipation caused by the time integration scheme. The results displayed in Figure 2 are consistent with this result, which indicates that the discretization formula for the convection term used
in this study explicitly conserves the kinetic energy. These results also show that the discretization formula here is constructed correctly in the analysis. The errors due to the use of the fourth-order Runge-Kutta method appear not be approximated by a power-law $\Delta t^4$ with time steps in the range $\Delta t = 10^{-2}$ to $10^{-3}$ due to the fact that the machine zero in the analysis is on the order of $10^{-16}$. This result is clearly found in Figure 3.

![Figure 3. Dependency of kinetic-energy conservation error on time increment $\Delta t$ for two Runge-Kutta schemes: In applying the lower-dissipation Runge-Kutta schemes, RK4-6 [13], conservation error of kinetic energy is notably reduced over the time increment compared to that of the Runge-Kutta scheme with five stages (RK4-5); The order of the conservation error depending on the time increment is the same for the two Runge-Kutta schemes in the range of $\Delta t = 10^{-2}$ to $10^{-1}$.](image)

As shown in Figure 2, in the discretization scheme used in this study, the kinetic energy conservation error depends on the time integration scheme. Accordingly, this error can be reduced by reducing the numerical dissipation as a numerical error in the time integration scheme. Figure 3 shows the conservation error based on the use of the time integration scheme with reduced numerical dissipation. In this case, the time integration is given by the function $\Delta t = 10^{-3/2M}$, where $I = 0$ to $M$ with $M = 2000$. Figure 3 allows visual comparison of the conservation error for this scheme with the error for the time integration scheme without the reduction of the numerical dissipation. As shown, the conservation error of the kinetic energy is significantly reduced by using the time integration scheme with reduced numerical dissipation error. This result demonstrates that the time integration scheme with the reduction of the numerical dissipation is useful in reducing the kinetic energy conservation error.

It should be noted that the decrease in the conservation error due to the use of the time integration scheme with the reduction of the numerical dissipation increases with increases in the time increment. This result is due to the characteristics of the numerical dissipation of the time integration method used in the study. There may be cases where a large time step is required to reduce the large computational cost. In this case, the conservation error of the kinetic energy is significantly reduced by using the time integration scheme with reduced numerical dissipation.

3.2. Effects on higher-order turbulence statistics
The dimension of kinetic energy is the square of velocity. In actual turbulent flow analysis, higher-order statistics of velocity fluctuations are often calculated. For instance, in acoustic analysis, etc.,
higher-order statistics of kinetic energy are calculated. Accordingly, the conservation error of higher-order statistics of kinetic energy was examined in the present study. In order to increase the conservation error for purposes of clarity, the first-order conservation error associated with the first-order Euler method (as shown in Figure 2) was used. Figure 4 shows the temporal evolutions of kinetic energy and its higher-order statistics. Here \( < > \) denotes the spatial average; \( \tilde{k} \) is the fluctuation of kinetic energy. Two time step values are used to examine the effect of the time increment size on the conservation error of the higher-order statistics. As shown, the conservation error of the higher-order kinetic energy statistics increases with increasing time. The temporal rate of the increase of the error increases as the order of the kinetic energy statistics increases. These results are found for both time steps. The conservation error of the kinetic energy is reduced by using the time integration scheme with suppressed numerical dissipation, as shown in Figure 3, in this study. The results show that the use of the time integration method with reduced numerical dissipation increases in usefulness as the order of the kinetic energy statistics increases.

![Figure 4](image_url)

**Figure 4.** Temporal profiles of the conservation error of higher-order statistics of kinetic energy, where the first-order Euler scheme is used to integrate the equation and \( \tilde{k} \) is fluctuation of kinetic energy; Also \( < > \) denotes mean: For (a) and (b), the values of the time increment are set to \( \Delta t = 0.2 \) and \( 0.002 \), respectively.

As shown in Figure 4, the temporal evolutions of the conservation error of the high-order statistics are similar for the time increments set in this study. This result suggests that there may be a simple form to describe the conservation error of the higher-order statistics of kinetic energy. Consequently, an attempt was made to identify an appropriate simple form describing the conservation error of the higher-order statistics. To this end, with instantaneous kinetic energy \( \tilde{k} \), mean kinetic energy \( K \), and fluctuation of kinetic energy \( k \), \( \tilde{k} = K + k \), where \( K = < \tilde{k} > \), was used. The intensity of kinetic energy fluctuation is described as \( < k^2 > = < \tilde{k}^2 > - K^2 \). Since the flow field of this analysis is homogeneous and isotropic, the following equation is derived:

\[
<k^2> = < (3/2) u^2 > - < (1/2) u^2 >^2 = (3^2 / 2^2) (<u^4 > - <u^2 >^2) \]
\[
<k^2> = (F - 1) (3^2/2^2) <u^2 >^2 = (F - 1) K^2. \tag{2}
\]

Here \( <u^4 > = F <u^2 >^2 \), where \( F \) is the flatness factor. The above equation can hold even at the initial time. This study focuses on the relative value of the intensity of kinetic energy fluctuation to that at the initial value \( <k^2>/ <k^2>_t=0 \) at a.

This results in the following equation:

\[
<k^2>/ <k^2>_t=0 = ((F - 1) / (F - 1)) (K^2 / K^2_t=0) = (K/K_t=0)^2. \tag{3}
\]

As shown in this equation, the relative magnitude of the conservation error of the kinetic energy fluctuation is equal to the square of the relative magnitude of the conservation error of the kinetic energy.
energy. Using this equation, equations for the third- and fourth-order statistics of kinetic energy fluctuation can also be derived:

\[
<\kappa^3>/<\kappa^2>_{t=0} = (K/K_{t=0})^3 \quad \text{and} \quad <\kappa^4>/<\kappa^2>_{t=0} = (K/K_{t=0})^4.
\]

As indicated in these equations, the conservation error of the higher-order statistics of kinetic energy is simply shown using the conservation error of the kinetic energy itself. The mean kinetic energy with conservation error is shown in Equation (1). Using this equation, the following equations can be derived, as the conservation error is small:

\[
<\kappa^2>/<\kappa^2>_{t=0} = (K/K_{t=0})^2 = 1 + 2\varepsilon t + \cdots,
\]

\[
<k^2>/<\kappa^2>_{t=0} = (K/K_{t=0})^3 = 1 + 3\varepsilon t + \cdots, \quad \text{and}
\]

\[
<k^2>/<\kappa^2>_{t=0} = (K/K_{t=0})^4 = 1 + 4\varepsilon t + \cdots.
\]

As shown in these equations, the rate of the time increase of the conservation error of the higher-order statistics of kinetic energy is equal to the order of the statistics.

4. Conclusions

In order to discretize the governing equations of incompressible turbulent flow, an appropriate higher-order central discretization scheme is proposed. Since this discretization scheme explicitly conserves kinetic energy, the error of the time integration method used affects kinetic energy conservation characteristics as numerical dissipation due to the scheme. This study demonstrates the reduction in the kinetic energy conservation error achieved by applying a previously developed time integration method with reduced numerical dissipation [13]. In the numerical analysis described here, an inviscid flow was analyzed in order to strictly investigate the kinetic energy conservation error. Here, the inviscid flow conserves kinetic energy analytically. In addition, the conservation error of higher-order statistics of kinetic energy was also examined.

The effects of differences in time integration schemes on the conservation error of kinetic energy were shown. It was demonstrated that the kinetic energy conservation error is decreased according to the order of the time integration scheme. Based on the observed dependence of the kinetic energy conservation error on the time increment, the explicit conservation characteristics of the kinetic energy were validated. Given this result, the conservation error due to the use of a time integration scheme with reduced numerical dissipation was then investigated. By using such a time integration scheme, the kinetic energy conservation error was significantly reduced with changes in the time increment. Moreover, the decrease of the conservation error due to the use of the scheme was found to be significant in the region where the time increment was larger. The conservation error of higher-order statistics of kinetic energy was then examined. It was shown that the conservation error of the higher-order statistics increases with increases in the order of the statistics. Notably, the conservation error of higher-order statistics can be expressed in a simple form using the kinetic energy conservation error itself.

It was also shown that even if the time increment is large, the conservation error can be sufficiently reduced by using the proposed time integration method with reduced numerical dissipation. In addition, the effect of applying the technique increases with the increasing order of the turbulent statistics. In the numerical analysis of acoustic fields, higher-order statistics of the velocity field are often required. The method proposed in this study made the conservation error smaller than the single precision machine zero at the large time increment. Therefore, we consider that the present error reduction is sufficient for acoustic simulation. By using the approach proposed in this study, the accuracy of numerical analysis on turbulent and acoustic fields can be substantially improved.

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