A NEW METHOD FOR DIRECT NUMERICAL SIMULATION THAT DISCRETELY CONSERVES MASS, MOMENTUM, AND KINETIC ENERGY

Frank Ham, Fue-Sang Lien, and Al Strong
Department of Mechanical Engineering, University of Waterloo
Waterloo, Ontario, N2L 3G1, Canada
corresponding author: fslien@sunwise.uwaterloo.ca

ABSTRACT

A second-order accurate finite difference discretization of the incompressible Navier-Stokes is presented that discretely conserves mass, momentum, and kinetic energy (in the inviscid limit) in space and time. The method is thus completely free of numerical dissipation and potentially well suited for the direct numerical simulation (DNS) or large-eddy simulation (LES) of turbulent flow. The method uses a staggered arrangement of velocity and pressure on a structured Cartesian grid, and retains its discrete conservation properties for both uniform and non-uniform grid spacing. The predicted conservation properties are confirmed by inviscid simulations on both uniform and non-uniform grids. The suitability of the method for DNS is demonstrated by repeating the turbulent channel flow simulations of Choi and Moin (1994), where the effect of computational time step on the computed turbulence was investigated. Using the present fully-conservative scheme, turbulent flow solutions were achieved for all computational time steps investigated ($\Delta t^+ = \Delta t u_\tau^2/\nu = 0.4$, 0.8, 1.6, and 3.2). Little variation in statistical turbulence quantities was observed up to $\Delta t^+ = 1.6$. The present results differ significantly from those reported by Choi and Moin, who observed significant discrepancies in the turbulence statistics above $\Delta t^+ = 0.4$, and the complete re-laminarization of the flow at and above $\Delta t^+ = 1.6$.

INTRODUCTION

The DNS and LES of turbulent flow require accurate numerical methods to resolve the wide range of spatial and temporal scales inherent to turbulence. Experience has shown that it is not only the order of accuracy of the discrete approximations that determines the overall accuracy of a given method. Of equal or perhaps even greater importance are the discrete conservation properties of the method. Numerical schemes with good discrete conservation properties in terms of mass, momentum, and kinetic energy have been shown to produce superior results when compared to their non-conservative counterparts (Mittal and Moin 1997).

In a recent investigation, Morinishi *et al.* (1998) analyzed several finite-difference schemes for their conservation properties, and derived discretely conservative fourth-order schemes for uniform meshes. The schemes were extended to non-uniform meshes by Vasilyev (2000), although the simultaneous discrete conservation of mass, momentum, and kinetic energy was not possible. Only schemes that discretely conserved mass and momentum but not kinetic energy, or discretely conserved mass and kinetic energy, but not momentum could be developed. This is true even for second-order accurate schemes on non-uniform meshes. Vasilyev identified the source of the non-conservation as the commutation error between the discrete differencing and averaging operators on the non-uniform mesh.

The concept of discrete conservation can be applied to time as well as space. Morinishi *et al.* did not, however, consider discrete conservation in time as an analytical requirement for a proper set of discretization equations. In the analyses of both Morinishi *et al.* and Vasilyev, time-advancement was accomplished by a third-order Runge-Kutta time-stepping method. The authors justified the non-conservation by observing that the associated errors appeared to be dissipative, and decreased with the cube of the computational time step. The recent work of Perot (2000) on two-dimensional unstructured staggered schemes extends the discrete conservation analysis to include time.

The objective of the present work is to develop a second-order accurate finite difference

scheme for structured Cartesian meshes that discretely conserves mass, momentum, and kinetic energy in both space and time, and then test its suitability for DNS.

NUMERICAL METHOD

The numerical method of the present contribution is based on a second-order accurate discretization of the incompressible Navier-Stokes equations for structured Cartesian meshes with non-uniform spacing and a staggered arrangement of velocity and pressure. In the following subsections, the staggered variable arrangement is described in both space and time, several discrete averaging operators are introduced, and the conservative discretization equations are presented and analyzed. We also briefly describe an efficient solution technique for the resulting fully-implicit, non-linear system.

Staggered Variable Arrangement

The staggered arrangement of velocity and pressure has the advantage of ensuring strong coupling between velocity and pressure without requiring special interpolation techniques. Staggering also appears necessary to produce discrete methods with good conservation properties, and as such forms the basis of the present scheme.

On the staggered grid, pressure p is stored at the control volume (CV) centers and denoted by the integer subscripts $[i, j, k]$. The Cartesian velocity components u, v, and w are stored at the center of the east, north, and top CV faces respectively. Their staggered location relative to the CV center is denoted by an appropriate half-index shift, as shown in Fig. 1a.

Vasilyev points out that, on non-uniform meshes, the locations of the velocity and pressure points are somewhat ambiguous: they can be determined as the geometric volume and face centers in either physical or computational space. In the present work we choose physical space, and define the mesh in terms of the face locations. For example, the west face of the CV at $[i, j, k]$ is at $x_{i-1/2}$, and the east face at $x_{i+1/2}$. The x-location of the cell center can then be calculated as the simple average of the adjacent face coordinates. The y and z directions are handled similarly.

Because the present work also considers conservation in time, we append the additional index n to all discrete variables to denote their time level. Fig. 1b illustrates how the velocity and pressure locations are also staggered in time. We adopt the convention that the new velocity values in any time step are at time level t_{n+1} and the previous values at t_n. Pressure is then located at the mid-point between these time levels, $t_{n+1/2}$.

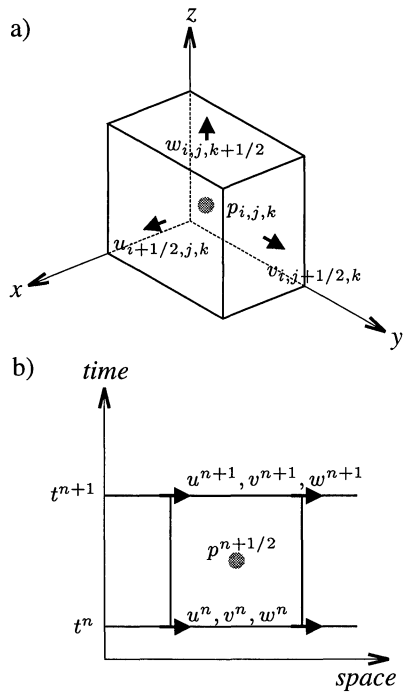

Figure 1: Staggered variable arrangement in a) space and b) space/time.

Discrete Operators

There are a variety of discretization techniques available for developing discrete approximations to a set of governing partial differential equations such as the Navier-Stokes equations. The finite volume method would seem a logical choice in this case because it is inherently conservative. A conservative finite volume discretization of momentum will not, however, guarantee conservation of kinetic energy. Because the discrete system is already fully defined through the mass and momentum discretizations, discrete conservation of kinetic energy depends implicitly on the discrete operators selected and the order they are applied. In the present work we use the finite difference method to develop the discretization equations, mainly because of the mathematical tools for discrete conservation analysis that have been developed to date.

Morinishi *et al.* (1998) introduced several discrete operators to investigate the conservation properties of various finite difference

schemes. Extending the notation of Morinishi to include time, the following discrete differencing operator is defined for structured Cartesian grids with non-uniform spacing:

$$\left.\frac{\delta_1\phi}{\delta_1 x}\right|_{i,j,k,n} \equiv \frac{\phi^n_{i+1/2,j,k} - \phi^n_{i-1/2,j,k}}{x_{i+1/2} - x_{i-1/2}} \quad (1)$$

In the above definition, ϕ represents a discrete variable and $[i, j, k, n]$ its associated mesh indices in the x, y, z, and t directions respectively. Although the stencil size used throughout the present analysis is always 1 (indicated by the "1" subscript), it is retained for consistency with the more general Morinishi definitions. Discrete operators in the y, z (alternatively x_2, x_3) and t directions are similarly defined.

Using this differencing operator, a finite difference equation is said to discretely conserve ϕ in space and time if it can be shown to have the following form (Morinishi 1998, Perot 2000):

$$\frac{\delta_1\phi}{\delta_1 t} + \frac{\delta_1 F_j(\phi)}{\delta_1 x_j} = 0 \quad (2)$$

$F_j(\phi)$ is a discrete approximation for the flux of ϕ (its exact form is not important here), and subscripts represent Cartesian tensor notation with summation implied when repeated (not to be confused with the mesh indices). In addition to the discrete differencing operator defined by Eq. (1), the following averaging operators will be required to develop and analyze the conservative discretization:

$$\left.\overline{\phi}^{1x}\right|_{i,j,k,n} \equiv \frac{\phi^n_{i+1/2,j,k} + \phi^n_{i-1/2,j,k}}{2} \quad (3)$$

$$\left.\widetilde{\phi\psi}^{1x}\right|_{i,j,k,n} \equiv \frac{1}{2}\left(\phi^n_{i+1/2,j,k}\psi^n_{i-1/2,j,k} + \phi^n_{i-1/2,j,k}\psi^n_{i+1/2,j,k}\right) \quad (4)$$

In the above definitions, ϕ and ψ represent discrete variables that may be cell-centered or staggered, and $[i, j, k, n]$ are the associated indices in the x, y, z, and t directions respectively. Discrete operators in the y, z and t directions are similarly defined.

Unfortunately, kinetic energy conservation is not possible on non-uniform meshes when only these operators are used to discretize the incompressible Navier-Stokes equations. As pointed out by Vasilyev (2000), the violation in conservation is related to the commutation error between the discrete differencing and averaging operators. To produce conservative schemes on non-uniform meshes, it is necessary to introduce the following weighted averaging operators:

$$\left.\overline{\phi}^{1\widehat{x}}\right|_{i,j,k,n} \equiv a\phi^n_{i+1/2,j,k} + b\phi^n_{i-1/2,j,k} \quad (5)$$

$$\left.\overline{\phi}^{1\breve{x}}\right|_{i,j,k,n} \equiv b\phi^n_{i+1/2,j,k} + a\phi^n_{i-1/2,j,k} \quad (6)$$

where the weights a and b are defined:

$$a = \frac{x_i - x_{i-1/2}}{x_{i+1/2} - x_{i-1/2}} \quad (7)$$

$$b = \frac{x_{i+1/2} - x_i}{x_{i+1/2} - x_{i-1/2}} \quad (8)$$

Note that, on uniform meshes, both of these averaging operators reduce to the uniform averaging operator of Eq. (3). Also note that, when evaluated at the cell-center locations, both of these averaging operators are the same as the uniform averaging operator of Eq. (3), even on non-uniform meshes. This is a result of our definition of cell centers as the geometric center between face locations in physical space. When evaluated at the staggered locations, however, these two operators have quite different interpretations. Eq. (5) is simply the standard linear interpolation. In Eq. (6) the weights are reversed, and it can be thought of as a volume-weighted average.

Discretization Equations

Using the discrete operators defined previously, the discretized incompressible Navier-Stokes equations are now presented. The continuity equation is evaluated at the mesh location $[i, j, k, n+1]$ using the following discretization:

$$\frac{\delta_1 u_i}{\delta_1 x_i} = 0 \quad (9)$$

The x, y, and z components of the momentum equation are evaluated at the staggered mesh locations $[i + 1/2, j, k, n + 1/2]$, $[i, j+1/2, k, n+1/2]$, and $[i, j, k+1/2, n+1/2]$ respectively using the following discretization:

$$\frac{\delta_1 u_i}{\delta_1 t} + \frac{\delta_1 \overline{\overline{u_j}^{1t}}^{1\breve{x}_i} \overline{\overline{u_i}^{1t}}^{1x_j}}{\delta_1 x_j} + \frac{\delta_1 p}{\delta_1 x_i} - \frac{\delta_1 \tau_{ij}}{\delta_1 x_j} = 0 \quad (10)$$

The viscous shear stress is calculated using the following:

$$\tau_{ij} = \bar{\nu}\left(\frac{\delta_1 \overline{u_i}^{1t}}{\delta_1 x_j} + \frac{\delta_1 \overline{u_j}^{1t}}{\delta_1 x_i}\right) \tag{11}$$

$$\bar{\nu} = \begin{cases} \nu & \text{for } i = j \\ \overline{\nu}^{1x_i 1x_j} & \text{for } i \neq j \end{cases} \tag{12}$$

Clearly both the mass and momentum equations are in the discrete form of Eq. (2), and thus the scheme will discretely conserve mass and momentum in space and time.

As pointed out by Morinishi, local kinetic energy cannot be defined unambiguously on the staggered grid because the velocity components are stored at different locations. The kinetic energy norm conserved by the present system requires the discrete kinetic energy equation to be developed about the mesh location $[i, j, k, n+1/2]$. The vector dot product of the velocity with the momentum equation (10) produces the kinetic energy equation which, including the appropriate discrete 2nd-order interpolations, takes the form

$$\overline{\overline{u_i}^{1t}\left(\frac{\delta_1 u_i}{\delta_1 t} + \frac{\delta_1 \overline{\overline{u_j}^{1t}}^{1\breve{x}_i}\overline{\overline{u_i}^{1t}}^{1x_j}}{\delta_1 x_j} + \frac{\delta_1 p}{\delta_1 x_i}\right)}^{1x_i} = 0 \tag{13}$$

Note that the viscous terms have been omitted. Expanding Eq. (13), each of the three resulting terms can be rearranged as follows:

$$(Time) = \overline{\overline{u_i}^{1t}\frac{\delta_1 u_i}{\delta_1 t}}^{1x_i} \tag{14}$$

$$= \frac{\delta_1 \overline{u_i u_i/2}^{1x_i}}{\delta_1 t} \tag{15}$$

$$(Conv.) = \overline{\overline{u_i}^{1t}\frac{\delta_1 \overline{\overline{u_j}^{1t}}^{1\breve{x}_i}\overline{\overline{u_i}^{1t}}^{1x_j}}{\delta_1 x_j}}^{1x_i} \tag{16}$$

$$= \frac{1}{2}\frac{\delta_1 \overline{\overline{\overline{u_j}^{1t}}^{1\breve{x}_i}\widetilde{\overline{u_i}^{1t}\overline{u_i}^{1t}}^{1x_j}}^{1\widehat{x}_i}}{\delta_1 x_j} + \overline{\frac{1}{2}\overline{u_i}^{1t}\overline{u_i}^{1t}\frac{\delta_1 \overline{u_j}^{1\breve{x}_i}}{\delta_1 x_j}}^{1x_i} \tag{17}$$

$$(Pres.) = \overline{\overline{u_i}^{1t}\frac{\delta_1 p}{\delta_1 x_i}}^{1x_i} \tag{18}$$

$$= \frac{\delta_1 \overline{u_i}^{1t}\overline{p}^{1\widehat{x}_i}}{\delta_1 x_i} - p\overline{\frac{\delta_1 u_i}{\delta_1 x_i}}^{1t} \tag{19}$$

Because the discrete continuity equation is identically zero, the kinetic energy equation also takes the discrete form of equation (2), and thus the scheme discretely conserves kinetic energy in space and time. The conserved norm can be taken from the time term:

$$K = \overline{u_i u_i/2}^{1x_i} \tag{20}$$

and evaluated at the mesh location $[i, j, k, n]$ or $[i, j, k, n+1]$.

Solution Procedure

The fully-implicit, non-linear system of equations resulting from this choice of discretization can be quite stiff, particularly on the highly stretched grids typical of LES and DNS of wall-bounded shear flows. In the present work, the system is solved iteratively at each time step using Newton linearization, and algebraic multigrid with smoothing based on the Symmetric Coupled Gauss-Siedel method of Vanka (1986). The system's stiffness is handled by coarsening preferentially in the direction of greatest coefficient strength, a multigrid technique referred to as semi-coarsening (Wesseling 1991). With the judicious selection of coarse grids, it was possible to reduce the maximum residual by 6 orders of magnitude with about 50 workunits per time step (where 1 workunit is equivalent to one smoothing sweep through the finest grid). Although relatively expensive per time step when compared to other DNS/LES solution methods, the present fully-implicit system is numerically stable for any choice of computational time step, and the discrete conservation properties ensure the method is free from numerical dissipation.

SIMULATIONS IN A PERIODIC BOX

To test the predicted conservation properties of the method, inviscid simulations were carried out in $1 \times 1 \times 1$ periodic boxes with both uniform and non-uniform grid spacing. The simulations were initialized with a random solenoidal velocity field, and integrated ahead in time with finite viscosity. At some point the viscosity was set to zero and the equations were integrated further ahead in time, monitoring the total momentum and kinetic energy. On both the uniform and non-uniform grids, both quantities were conserved to machine accuracy, confirming the predicted conservation properties of the method.

Energy Spectra

Fig. 2 plots the time history of the total kinetic energy for one simulation carried out on a 64^3 uniform grid. During the initial viscous part of the simulation ($0 < t < 3$), the total kinetic energy is seen to decay rapidly due to viscous dissipation.

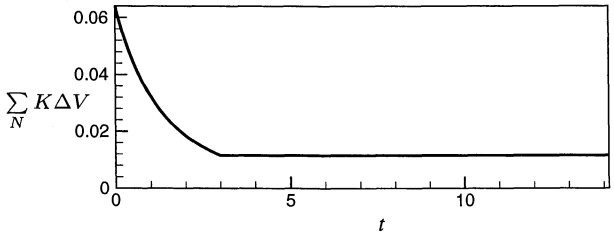

Figure 2: Time history of total kinetic energy for 64^3 periodic box simulation. Initial viscosity $\nu = 1/2000$ set to zero at $t = 3$.

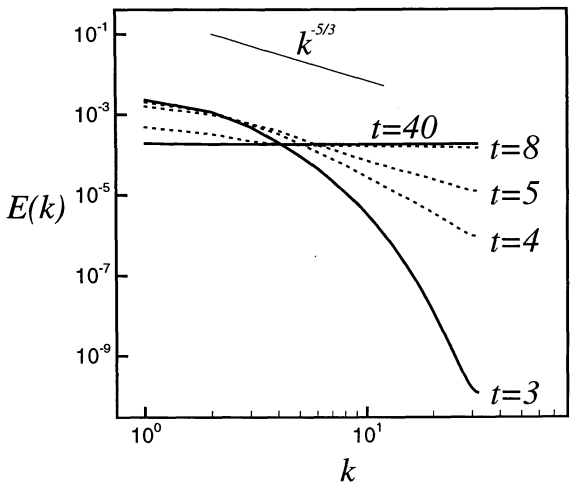

Figure 3: Computed spatial energy spectra from 64^3 periodic box during the inviscid part of simulation illustrating the eventual equi-distribution of energy amongst wave numbers. Times refer to Fig. 2.

At $t = 3$ the viscosity was set to zero. As Fig. 2 shows, the kinetic energy remained precisely constant thereafter. It is interesting to note how the energy redistributes itself in wave space in the absence of viscosity. Fig. 3 shows the spatial energy spectra calculated at times $t = 3$, 4, 5, 8, and 40. At $t = 3$, the spectra shows a strong drop off at higher wave numbers, and little or no energy pileup at the highest wave number. The immediate loss of viscous dissipation causes the energy at the highest wave numbers to increase rapidly. The net energy transfer is out of the lowest wave numbers, although at a much slower rate. Eventually, the distribution stabilizes at a point where the energy is equally distributed in wave space - a condition of maximum entropy for this isolated numerical system!

DNS OF PLANE CHANNEL FLOW

The first rigorous investigation of the effect of computational time step on the DNS of turbulent flow was performed relatively recently by Choi and Moin (1994). They used a fully implicit scheme to conclude that the optimal computational time step for the DNS of turbulent channel flow was, expressed in wall units, about $\Delta t^+ = \Delta t u_\tau^2/\nu = 0.4$. For time steps larger than 0.4, their numerical experiments showed the calculated turbulence statistics to vary significantly from their time-step-independent values. Further, they observed the turbulence to completely decay to a laminar state for time steps of 1.6 or greater. In conclusion, they suggested the following physical explanation for their observations: *"turbulence fluctuations can only be sustained if the computational time step is appreciably less than the Kolmogorov time scale"*. They estimated the Kolmogorov time scale in the sublayer to be about 2.4 in wall units.

Using the fully conservative method of the present work, the identical investigation was repeated. Following Choi and Moin, the channel domain and grid distribution was taken from the *minimum flow unit* of Jiminez and Moin (1991), with dimensions $2\pi\delta \times 2\delta \times 0.289\pi\delta$ in the streamwise, wall-normal, and spanwise directions respectively. The mesh size (in terms of cells) was $16 \times 128 \times 32$, with uniform spacing in both the streamwise and spanwise directions, and a hyperbolic tangent distribution in the wall normal direction, as described by Jimenez and Moin. All computations were performed at Reynolds number based on bulk velocity $Re_b = U_b\delta/\nu = 2800$, which corresponds to a Reynolds number based on wall-shear velocity of $Re_\tau = u_\tau\delta/\nu \approx 190$.

Fig. 4 compares the calculated rms velocity fluctuations for four of the time steps investigated: $\Delta t^+ = 0.4$, 0.8, 1.6, and 3.2. In terms of CFL number, these computational time steps correspond approximately to $CFL = max\left(|u_i|/\Delta x_i\right) = 1$, 2, 4, and 8. Little variation in statistical turbulence quantities was observed up to $\Delta t^+ = 1.6$. Even at $\Delta t^+ = 3.2$, the variation is only a few percent, substantial smaller than that observed by Choi and Moin. Fig. 5 compares the Reynolds shear stress for the same computational time steps.

Even for the largest computational time

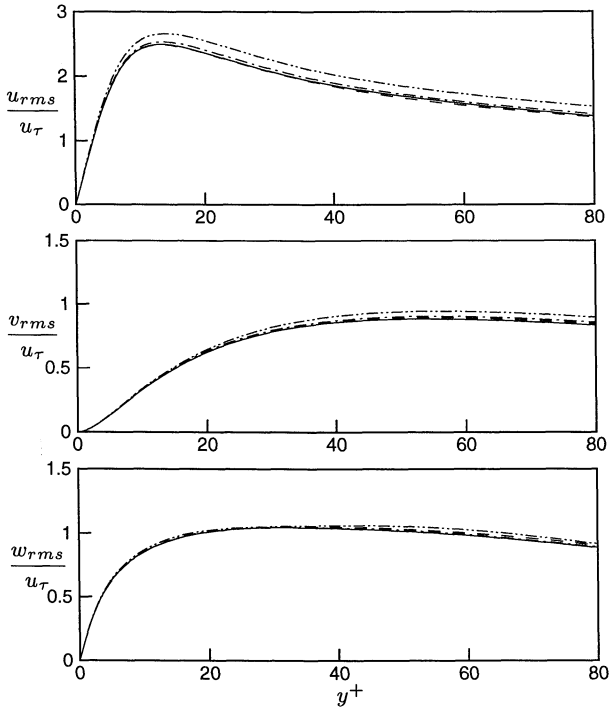

Figure 4: Variation of root-mean-square velocity fluctuations with the computational time step: ——— $\Delta t^+ = 0.4$; - - - - $\Delta t^+ = 0.8$; —·— $\Delta t^+ = 1.6$; —··— $\Delta t^+ = 3.2$.

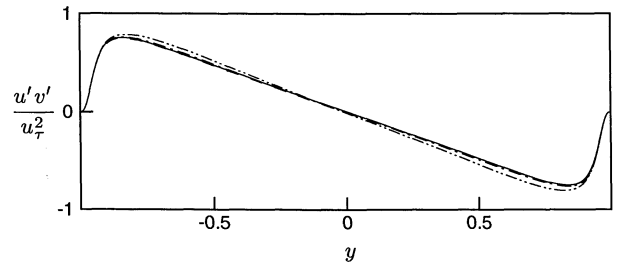

Figure 5: Variation of Reynolds shear stress with the computational time step: ——— $\Delta t^+ = 0.4$; - - - - $\Delta t^+ = 0.8$; —·— $\Delta t^+ = 1.6$; —··— $\Delta t^+ = 3.2$.

steps investigated of $\Delta t^+ = 5.0$, corresponding to $CFL \approx 12$, the flow remained turbulent with an approximately correct statistical behavior. The present results suggest that the observations of Choi and Moin may have been a result of dissipative numerical errors associated with their fractional step time advancement scheme, rather than the more physical explanation they proposed.

SUMMARY

A second-order accurate finite difference discretization of the incompressible Navier-Stokes has been presented that discretely conserves mass, momentum, and kinetic energy (in the inviscid limit) in both space and time. The method uses a staggered arrangement of velocity and pressure on a structured Cartesian grid, and retains its discrete conservation properties for both uniform and non-uniform grid spacing. The predicted conservation properties have been confirmed by inviscid simulations on both uniform and non-uniform grids. The suitability of the method for DNS has been demonstrated by repeating the turbulent channel flow simulations of Choi and Moin (1994), where the effect of computational time step on the computed turbulence was investigated. Using the present fully-conservative scheme, turbulent flow solutions were achieved for all computational time steps investigated ($\Delta t^+ = \Delta t u_\tau^2/\nu = 0.4$, 0.8, 1.6, and 3.2). Little variation in statistical turbulence quantities was observed up to $\Delta t^+ = 1.6$, corresponding to $CFL = 4$. The present results differ significantly from those reported by Choi and Moin, and suggest that the cause of their observed sensitivity to computational time step may have been dissipative numerical errors associated with their fractional step time-advancement scheme, rather than the more physical explanation they proposed.

References

Choi, H., and Moin, P., 1994, "Effects of the Computational Time Step on Numerical Solutions of Turbulent Flow", *J. Comput. Phys.* **113**, p. 1.

Jimenez, J., and Moin, P., 1991, "The minimal flow unit in near-wall turbulence", *J. Fluid Mech.* **225**, pp. 213-240.

Mittal, R., and Moin, P., 1997, "Suitability of upwind-biased finite difference schemes for large-eddy simulation of turbulent flows", *AIAA Journal* **35** (8), p. 1415.

Morinishi, Y., Lund, T. S., Vasilyev, O. V., and Moin, P., 1998, "Fully Conservative Higher Order Finite Difference Schemes for Incompressible Flow", *J. Comput. Phys.* **143**, p. 90.

Perot, B., 2000, "Conservation Properties of Unstructured Staggered Mesh Schemes", *J. Comput. Phys.* **159**, p. 58.

Vanka, S. P., 1986, "A Calculation Procedure for Three-Dimensional Steady Recirculating Flows Using Multigrid Methods", *Comp. Meth. Appl. Mech. Eng.* **55**, pp. 321-338.

Vasilyev, O., 2000, "High Order Finite Difference Schemes on Non-uniform Meshes with Good Conservation Properties", *J. Comput. Phys.* **157**, p. 746.

Wesseling, P., 1991, *An Introduction to Multigrid Methods*, John Wiley and Sons.