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On Large Eddy Simulation with Centered and Upwind Compact Difference Schemes

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중심 및 상류 컴팩트 차분기법을 적용한 난류유동의 LES

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Key words : *Compact differencing, Large Eddy Simulation, Discretization Error*

Abstract

The suitability of high-order accurate, central and upwind-biased compact difference schemes is evaluated for the large-eddy simulations of flows in complex geometry. Two flow geometries are considered: channel and circular cylinder. The effects of numerical dissipation and aliasing error on the evaluation of subgrid scale stress are investigated by extending the analysis by Ghosal [1] to centered and upwind compact schemes. It is shown that the failure of upwind schemes mainly comes from the aliasing error.

1. Introduction

Large-eddy simulation (LES) of turbulent flows is normally performed on grids that are just fine enough to resolve the important large flow structures. Numerical discretization errors, which are composed of finite-differencing and aliasing errors, from these grids have considerable effects on the simulation results. Recent analysis and *posteriori* numerical experiments [1, 2] show that discretization errors outweigh modeling errors and that aliasing errors are the leading source of errors for high order schemes.

On the other hand, the need for using high order upwind schemes for LES arises when the problems with strong discontinuity are to be tackled such as the flow with shock/turbulence and shock/boundary layer interaction. Besides, upwind schemes are believed to have the ability to control aliasing errors due to embedded numerical dissipation. However, it become clear in recent years that dissipative schemes are not good candidates for use in LES of turbulent flows. Except in cases where the flow is extremely well resolved, it has been found that upwind schemes tend to damp out a significant portion of the small scales that can be resolved on the grid. A well-known case is the LES of flow past a circular cylinder performed by Beaudan & Moin [3] at Reynolds number of 3900, where 5th and 7th order schemes were used. However, some questions arise regarding this issue: Is the conclusion due to Beaudan & Moin [3] universal for other schemes such as recently developed high resolution upwind schemes? Does numerical dissipation really reduce aliasing error? If so, can we find an 'optimal' upwind scheme which balances aliasing error and finite-differencing error such that the total error should be minimized? To answer these questions is the main objective of this study. In addition, the investigation of the suitability of centered compact difference schemes for LES of flows in complex flows is another objective.

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2. Computational Method

Governing equations are compressible formulation of filtered conservation equations that consists of mass, momentum, energy equations and the state equation. Subgrid-scale (SGS) stress and heat flux are modeled by Smagorinsky model, whose constants are determined by the dynamic procedure proposed by Moin *et al.* [4]. For any scalar quantity ϕ, such as metric, flux component or flow variable, the derivative is obtained by standard 4th order compact difference scheme [5]. The only exception is the convection terms whose derivatives are given by a general compact scheme with one free parameter α, which is proposed by Zhong [6] :

$$\begin{aligned}&(15+15\alpha)\phi'_{i-1}+60\phi'_i+(15-15\alpha)\phi'_{i+1}\\&=\{(-45-30\alpha)\phi_{i-1}+60\alpha\phi_i+(45-30\alpha)\phi_{i+1}\}\end{aligned} \tag{1}$$

Eq. (1) reduces to 4th order compact scheme (denoted as COM4 hereinafter) with $\alpha=0$. For other values of α, Eq. (1) is 3rd order accurate upwind-biased scheme. As Zhong [6] recommended 0.25 as the proper choice of α, we will refer to Eq. (1) with $\alpha=0.25$ as CUDZ. $\alpha=1.5$ corresponds to a compact upwind scheme proposed by Tolstykh [7], which will be referred to as CUD3 following his notation. One can mimic most of high order upwind schemes with Eq. (1) by controlling the parameter α. For COM4 ($\alpha=0$), a skew-symmetric form as well as divergence form of convection term is adopted, whereas only divergence form is adopted for other cases. The spectral analysis of Kravchenko & Moin [8] (denoted as KM1) reveals the relation between the nonlinear term formulation and aliasing error, and recommends the following skew-symmetric form to minimize aliasing error

$$\frac{\partial\rho u_i u_j}{\partial x_j}=\frac{1}{2}\left(\frac{\partial\rho u_i u_j}{\partial x_j}+u_j\frac{\partial\rho u_i}{\partial x_j}+\rho u_i\frac{\partial u_j}{\partial x_j}\right) \tag{2}$$

3. Results

3.1 Fully developed channel flow at Re = 23000

The first problem is a fully developed channel flow at Re = 23000 based on the centerline velocity and the channel half-width δ. This case is selected to compare the present results with those from KM1, who conducted LES of the same flow with various finite-differencing scheme from 2nd order central difference (CD2) to de-aliased spectral methods. For all cases considered, 48×64×48 grid points are used in the streamwise, wall-normal, and spanwise directions, respectively, in a computational domain of $2\pi\delta\times2\delta\times\pi\delta/2$.

Five simulations are conducted with different discretization schemes with and without SGS model. The results are summarized in Table 1. The calculations with divergence form of the nonlinear terms are numerically unstable, which is consistent with the results of KM1. The results with skew-symmetric form are stable with and without SGS model, whereas those with divergence form show laminarization of flow with compact upwind schemes. Although the calculation with CUDZ, which has much smaller numerical dissipation than that with CUD3, seems to retain turbulence for a considerably long time, their statistics such as the mean velocity and RMS values tend to slowly move toward laminar solution instead of being converged.

Figs. 1(a) and 1(b) show the mean velocity and RMS velocity fluctuations for various schemes listed in Table 1 together with those from spectral LES (KM1) and experiments by Wei & Willmarth [9]. The results from CUDZ are shown for the purpose of comparison, although they are under laminarization. The results from present LES with COM4 in skew-symmetric from shows an excellent agreement with those from spectral LES and experiment. The results without SGS model underestimates the mean velocity and overestimates RMS values, which is consistent with KM1 and other LES results. The results from CUDZ are much worse than COM4 showing typical over-damped results. This aspect is more clearly demonstrated by one-dimensional energy spectra as shown in Fig. 2. The spectra from the LES with COM4 agree well with those from spectral method up to maximum resolvable wavenumbers by the numerical scheme, whereas simulation without SGS model over-predicts the spectra nearly at all wavenumbers, showing a clear effect of SGS model. However, the results from COM4 simulation without SGS model are still in reasonable agreement as compared to those from CUDZ. CUDZ seems to damp out energies at all wavenumbers.

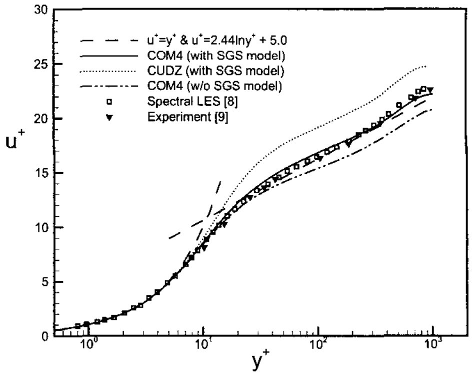
3.2 Flow past a circular cylinder at Re = 3900

The second problem considered is flow past a circular cylinder at Re = 3900 based on free-stream velocity and the cylinder diameter. It is one of the challenging problems for LES that has been tackled by various numerical schemes [3, 10].

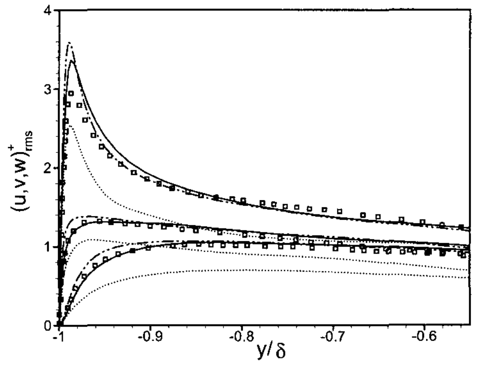
Table 1. Numerical simulations of turbulent channel flow with various discretization schemes.

Discretization	Nonlinear terms	SGS model	Results
COM4	Divergence	o	↑
COM4	Skew-symmetric	o	•
COM4	Skew-symmetric	×	•
CUDZ	Divergence	o	•↓
CUD3	Divergence	o	↓

• Stable; ↑ numerically unstable; ↓ flow laminarizes; •↓ flow laminarizes very slowly



(a) mean streamwise velocity



(b) RMS velocity fluctuations

Fig. 1 Mean quantities for a fully developed channel flow.

An O-mesh with 144×201×48 point in the azimuthal, radial and spanwise direction is used in a spanwise domain length of πD. Some of the important flow parameters from the computation are summarized in Table 2 together with those from previous LES and available experiments. The present results are obtained from COM4 (in skew-symmetric form) with SGS model. All the parameters are in fairly good agreement with the experimental data and previous simulations. Fig. 3 compares the instantaneous fields showing separating shear layer and development of Karman vortex street. CUDZ and COM4 show nearly the same structure near wake region where the flow is well resolved. Unlike the results from COM4, however, that from CUDZ has nearly no small-scale structure in the region of $x/D > 3$.

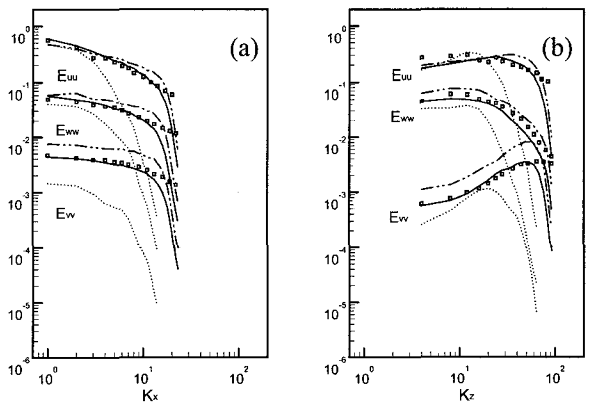
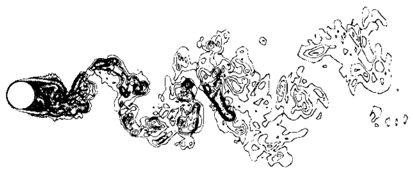


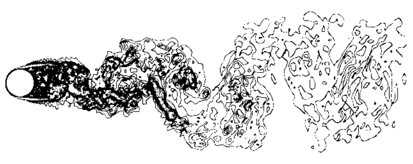
Fig. 2 One-dimensional energy spectra at $y^+\approx15$ for a fully developed channel flow: (a) streamwise wavenumber; (b) spanwise wavenumber. See caption of Fig. 1 for details.

Table 2. Flow parameters from cylinder flow computation

	C_D	$-C_{P_b}$	St	$U_{\min}$
Exp.[11-13]	0.99±0.05	0.88±0.05	0.215±0.005	-0.24±0.1
Upwind [3]	1.00	0.95	0.203	-0.32
B-spline[10]	1.04	0.94	0.210	-0.37
Present	1.02	0.89	0.209	-0.33



COM4 (with SGS model)



COM4 (without SGS model)

CUDZ (with SGS model)

Fig. 3 Separating shear layer and development of Karman vortex street in the flow over a circular cylinder.

Fig. 4 shows streamwise velocities in the wake. In this region, the effect of dissipation and SGS model seems to be small so that two results from COM4 show negligible difference and good agreements with experimental data, although those from CUDZ shows some discrepancy possibly due to the delayed shear layer transition. The effect of numerical dissipation is clearly shown from the one-dimensional frequency spectra at x/D = 7.0 as shown in Fig. 5

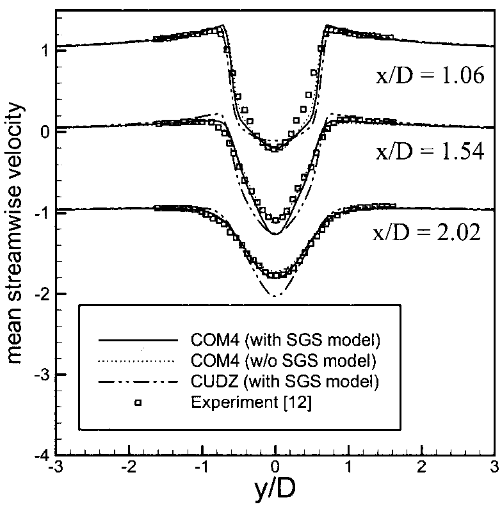


Fig. 4 Mean streamwise velocity at three locations in the wake.

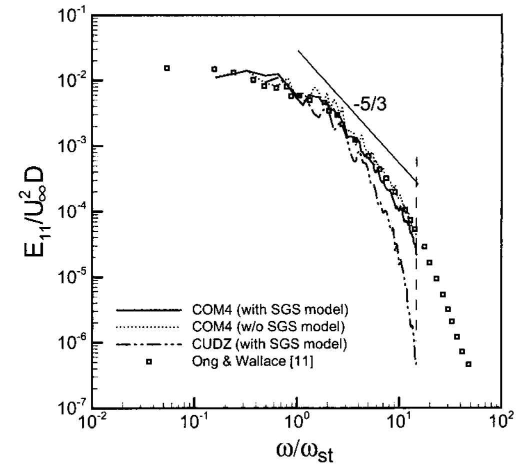


Fig. 5 One-dimensional frequency spectra at $x / D = 7.0$. ω_{st} is the vortex shedding frequency.

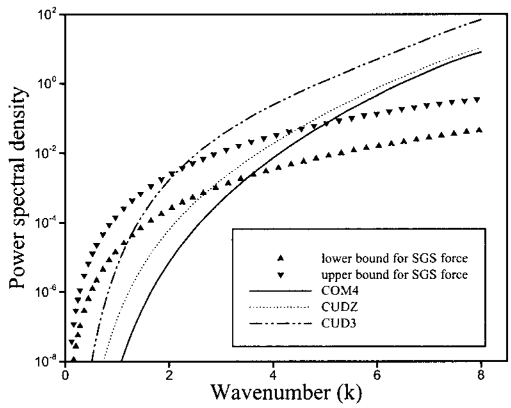


Fig. 6 Finite differencing errors for compact difference schemes.

The spectrum from COM4 with SGS model gives an excellent agreement with the experimental data of Ong & Wallace [11] up to grid-cut-off wavenumber. The spectrum from COM4 without SGS model shows also a good agreement. However, the spectrum from CUDZ shows a rapid fall-off at high frequencies.

4. Analysis on Discretization Errors

In this section, the effect of numerical errors on the accuracy of LES is evaluated analytically. Discretization errors are evaluated by their power spectrum for a given energy spectrum. If we assume isotropic turbulence, the spectrum of finite differencing error is given by

$$
\begin{aligned}
\varepsilon^{FD}(k) &= 4\pi k^2 \lim_{V\to\infty}\frac{8\pi^2}{V}\left\{E_i^{FD}(\mathbf{k})E_i^{FD}(\mathbf{k})^*\right\}_\Omega \\
&= \left[F_1(k)+F_2(k)\right]\left\{\sum_{i,m,n}\left|\Delta_{imn}(\mathbf{k},\tilde{\mathbf{k}})\right|^2\right\}_\Omega \\
&\quad +F_3(k)\left\{\sum_{i,m,n,p}\frac{k_n k_p}{k^2}\Delta_{imn}(\mathbf{k},\tilde{\mathbf{k}})\Delta^*_{ipn}(\mathbf{k},\tilde{\mathbf{k}})\right\}_\Omega \\
&\quad +2F_4(k)\left\{\sum_{i,m,n,p,q}\frac{k_n k_p k_n k_q}{k^4}\Delta_{imn}(\mathbf{k},\tilde{\mathbf{k}})\Delta^*_{ipq}(\mathbf{k},\tilde{\mathbf{k}})\right\}_\Omega \\
&\quad +2\nu E(k)\left\{\left|\tilde{k}^2-k^2\right|^2\right\}_\Omega
\end{aligned}
\qquad (3)
$$

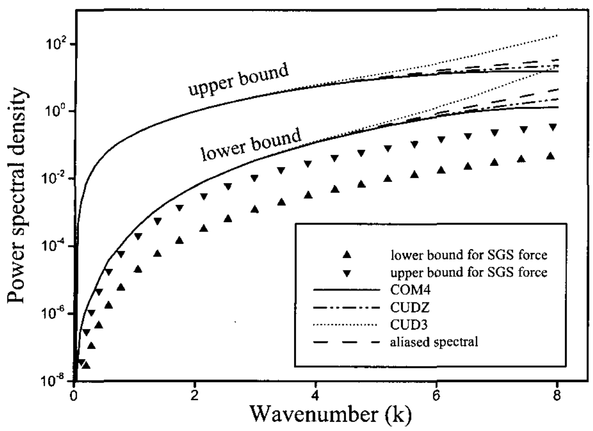


Fig. 7 Aliasing errors for compact difference schemes.

where $\{\}_\Omega$ denotes angular average in wavenumber space over the surface of the sphere $|\mathbf{k}| = k$ and V is the volume of the physical box. $\tilde{\mathbf{k}}$ is the modified wavenumber for differencing scheme. The last term denotes viscous term. F_1~F_4 are determined once the three-dimensional energy spectrum is given. For more details on the derivation of terms in Eq. (3), see Ghosal [1]. Similarly, aliasing error is given by

$$\begin{aligned}\varepsilon^{alias}(k) &= 8\pi k^2 \sum_{\mathbf{a}\in\Lambda_0} \Big\{ P_{imn}(\tilde{\mathbf{k}}) P^*_{ipq}(\mathbf{k}) \int_B \int_B \\ &\quad d\mathbf{k}' d\mathbf{k}'' \Phi^*_{mp}(\mathbf{k}') \Phi^*_{nq}(\mathbf{k}'') \delta(\mathbf{k}+\mathbf{a}-\mathbf{k}'-\mathbf{k}'') \Big\}_\Omega \\ &= \sum_{\mathbf{a}\in\Lambda_0} \Big\{ [F_1(K)+F_2(K)] \sum_{i,m,n} \left| P_{imn}(\tilde{\mathbf{k}}) \right|^2 \\ &\quad + 2F_3(K) \sum_{i,m,n,p} \frac{K_m K_p}{K^2} P_{imn}(\tilde{\mathbf{k}}) P^*_{ipn}(\tilde{\mathbf{k}}) \\ &\quad + F_4(K) \sum_{i,m,n,p,q} \frac{K_m K_p K_n K_q}{K^4} P_{imn}(\tilde{\mathbf{k}}) P^*_{ipn}(\tilde{\mathbf{k}}) \Big\}_\Omega \end{aligned} \quad (4)$$

where **K=k+a**. The subscript B in the integral denotes the integration over a cubic box. Λ_0 is the set of wavevectors of the form $(2pk_m, 2qk_m, 2rk_m)$ where p, q and r are integers, and k_m is the maximum resolvable wavenumber at a given grid. It should be noted that in the derivation of Eqs. (3) and (4), conservative convection term is assumed for simplicity.

The SGS force is given as

$$\sigma(k) = k^2 [F_1(k) + F_2(k) + F_3(k)] \quad (5)$$

The Von Karman spectrum [1] is used as the prescribed energy spectrum. Fig. 6 shows the power spectrum of finite- differencing error for various schemes ($k_m = 8$) together with the lower and upper bounds of SGS force. Upwind schemes have larger finite differencing error at all wavenumbers than their non-dissipative counterpart.. Fig. 7 shows the aliasing error. It is found, contrary to the common belief, that the aliasing error further increases with upwind schemes. From the Fig. 7, aliasing error is more serious than finite differencing error overwhelming SGS force at all wavenumbers regardless of discretization schemes. These results indicate that the aliasing error and finite differencing error increase simultaneously as the magnitude of the imaginary part of the modified wavenumber increases. Therefore, there exists no optimal upwind scheme. It is interesting to note that falsely dissipated energy at high wavenumbers is due to aliasing error. The aliasing error of this kind that produced by dissipative schemes may be called as the aliasing error in "reverse direction". In addition to increased aliasing and finite differencing error, the conservative form for convection terms is responsible for the failure of LES with upwind schemes. That is, the concept of 'flux vector' in upwind schemes enforces the conservative form of convection terms, whereas non-dissipative scheme can be used in a skew- symmetric form to reduce the aliasing error.

5. Conclusions

The suitability of high order accurate compact differencing was evaluated for large eddy simulation of complex turbulent flows from the simulation and the analysis. Non-dissipative compact schemes were shown to be good candidates for large eddy simulation provided that a proper dealiasing of nonlinear terms is performed. The unsuitability of upwind schemes for large eddy simulation is confirmed with compact upwind schemes. It was also found the failure of upwind schemes mainly comes from the aliasing error rather than finite differencing error.

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