ASSESSMENT OF UNSTRUCTURED LES WITH BOTH STRUCTURED LES AND EXPERIMENTAL DATABASE: FLOW PAST A SQUARE CYLINDER AT RE=2.2×10⁴

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The high Reynolds number flow past a square cylinder is simulated by large-eddy simulation (LES). The unstructured LES is comprehensively examined from the practical view point with both structured LES and experimental databases. The open-source code of OpenFOAM is employed for the unstructured LES, while the finite differencing method is used for the structured LES. The aerodynamic responses on the cylinder and the surrounding flow are analyzed. The influences are emphasized from the relatively low numerical schemes for the convective term. Three common schemes are tested in the present study, i.e., LUST, limited linear and linearUpwind. Results show that there is no big difference generally between the unstructured LES and structured LES when the similar "structured" grids are used. But one of exceptions for the unstructured LES is the over-prediction of fluctuating pressure on the side faces, which has been explained. Another exception is the earlier decay of turbulence inertial sub-range in the wake for LUST and linearUpwind. Also the TVD scheme shows clearly unphysical turbulence inertial sub-range distribution. Furthermore, their remedies with the feature of easy handling are suggested in this paper.

1. Introduction

Square cylinders are the common configuration arrangement in the environmental situations. The wind effect becomes increasingly important with the rising height of buildings. The investigations of flow past a square cylinder have attracted an amount of studies in the theoretical, experimental and numerical methods. For the civil engineering in practice, the flows at high Reynolds number (Re) are of more interest. They involve the complex development, i.e., the laminar boundary layer, separation from the frontal corners, formation of shear layers and the formation and downstream travelling of Karman vortices. Due to its wide applications, there are a huge number of accessible experimental data, which can be the validation of the numerical methods.

To date the numerical prediction of such flows in the urban areas has relied predominantly on the Reynolds-averaged Navier-Stokes equations (RANS) in the engineering practices. In RANS, the Reynolds stress tensor is modeled by time- or ensemble- averaged solutions to the Navier-Stokes equations. But as summarized by Rodi (1997) and Kim (1999), the RANS models are not completely satisfactory in dealing with bluff-body aerodynamics, especially for the turbulence fluctuations. Thus the large-eddy simulation (LES) is more attractive in the recent years. But the applications of LES to such flow prediction are majorly based on structured grid and have obtained sufficient accuracy (Tamura, 2008; Rodi et al., 1997). Unfortunately, the structured grid is very difficult, if not possible, to make adequate meshing for the complex practical geometries. Furthermore, structured grids usually lead to a considerable portion of mesh being wasted in the area which is not really needed. Thus, the unstructured grids are becoming popular because of their mesh flexibility and adaptability.

Although some numerical schemes or solution algorithm are proposed in the past for the unstructured LES, the low-order numerical schemes are still widely used in the engineering as a matter of fact because of their easier programming or ready access. However, from the

authors' knowledge, the work of Camarri et al. (2002) and Boileau et al. (2013) are the only LES of the square-cylinder cases performed on an unstructured grid. The former focused on the tests on the coarse unstructured grids, while the latter concerned with the heat transfer and near-wall modeling. Thus it seems urgent to examine the LES performance of fine unstructured mesh based on the relatively low numerical schemes, which is used by most operational codes including the major commercial codes. The open-source toolbox named OpenFOAM is increasingly attractive and being used all around the world. It implements an unstructured finite volume method (FVM) with support for arbitrary unstructured meshes. It means the mesh cells can be of arbitrary shape. Like most operational codes, the relatively low numerical schemes are applied. But unfortunately, there is no official and feasible guide for LES simulation by using OpenFOAM. It is owing to the lack of examinations of numerical and modeling influences on LES simulations based on OpenFOAM. Moreover, it remains a debate whether the relatively low order accuracy for convective term is suitable for wind prediction around bluff bodies from the viewpoint of engineering. It is also unknown how big difference compared with the high-order accuracy based on structured grid. Therefore, it is necessary and significant to perform the comprehensive examinations of unstructured LES based on the relatively low numerical schemes and eventually provide the simulation guide. In this study, numerical tests are presented of the aerodynamic characteristics on a stationary square-section cylinder at Re= 2.2×10^4 , with the front face normal to the flow.

The paper is organized as follows. Firstly the numerical methods are introduced in terms of both structured LES with high order numerical scheme and unstructured LES with lower order numerical schemes. Secondly the experimental data are selected for the purpose of numerical validation. Following it, the comparisons between structured and unstructured LES are presented under the similar hexedral grids in terms of aerodynamic forces, pressure distribution and flow around the cylinder. At the last part, the remedies are suggested for the weakness of unstructured LES.

2. Computational methods

The Navier-Stokes and continuity equations for incompressible flow are shown below. From left to right, the terms in N-S equation are called the transient, convective, pressure and viscous term throughout this paper.

$$\frac{\partial u_i}{\partial t} + \frac{\partial u_i u_j}{\partial t} = -\frac{\partial p}{\partial x_i} + v \frac{\partial^2 u_i}{\partial x_j x_j} \qquad \frac{\partial u_i}{\partial x_i} = 0$$

2.1 Structured LES

The code used for structured LES is based on the finite difference method in the curvilinear grid system, which has been successfully applied to the flow past bluff bodies at high Res (Ono and Tamura, 2002; Tamura and Ono, 2003). A fractional step method is employed to advance the solutions of velocities and pressure in time. The time marching of the momentum equation is hybrid, viz., the Crank-Nicolson scheme is applied to the viscous terms and an explicit third-order Runge-Kutta method is used for the convective term. Spatial discretization is treated as the second-order central difference generally. However the convective term is approximated using the 4th order scheme. To avoid the numerical instability near the front corners of a square cylinder, a small amount of numerical dissipation is added through the convective term. The sub-grid scale domain is modeled by using dynamic Smagorinsky model (Germano, 1991; Lilly, 1992).

2.2 Unstructured LES

For the unstructured LES, OpenFOAM 2.3.0 is utilized, which is based on finite volume method. The variables of flow are stored at the cell centers. The fully implicit time marching (PIMPLE) is applied to solve the governing equations in the physical Cartesian coordinates. The transient, pressure and viscous terms are discretized by second-order implicit backward, second-order central differencing, and second-order central differencing schemes respectively. For the high Re flow simulation, the purely second-order linear interpolation scheme always results in the numerical instability. Thus the conventional remedy is to employ the upwind-biased schemes, viz., the accuracy is actually 1st~2nd order. From the authors' knowledge, the situation also applies to most operational codes, including the major commercial codes. Accounting for the popularity of applications, stability and viscosity amount, the following convective schemes are chosen for high-Re square cylinder simulation: linear-upwind stabilized transport (LUST), limitedLinear and linear upwind. LUST is a blending of linear and linearUpwind, corresponding to the factors of 0.75 and 0.25. The limitedLinear is one of TVD schemes, which is also well known as Sweby limiter. The linearUpwind is a so-called second-order upwind-biased scheme. The velocity and pressure equations were solved by using the preconditioned bi-conjugate gradient (PBiCG) method for the former and the generalized geometric-algebraic multi-grid (GAMG) method for the latter. The time step is determined to ensure that the maximum Courant number is around 2, accounting for the balance between the temporal resolution required for LES and the computational resources from the engineering viewpoint. Like the structured LES, the dynamic Smagorinsky model is applied, with the locally weighted averaging for the Smaogrinsky coefficients.

Fig. 1 shows the grid system used for the structured LES. But when focusing on the effect of numerical schemes (Section 4), we employed actually the similar grid system for the unstructured LES, which is not shown herein because of the space limit. The computational domain size

is $28D \times 24D \times 4D$, where *D* is the width of the square cylinder. The nearest cell height to the cylinder wall is determined by $0.1D/\text{Re}^{0.5}$. The spanwise resolution is 0.05D. The total cell number is $300 \times 300 \times 80=7.2$ million. The inlet boundary condition is uniform and smooth inflow. The circular cylinder is a no-slip wall. The spanwise end boundary conditions are periodic. The structured LES uses the convective condition for the outlet, while the unstructured LES uses the condition of zero pressure and zero-gradient velocity. This difference is thought as no significant influence due to far enough distance between the cylinder and the outlet.



Fig. 1 Grid system. (a) Whole mesh; (b) & (c) close-up near the cylinder.

3. Experimental database

Two reasons necessitate us to select the experimental database to validate present numerical results. For one, there is a large-degree deviation even in the available experiments, which possibly affected by the experimental conditions, especially the aspect ratio of cylinder (AR), free-stream turbulence intensity (I_u) and blockage ratio (BR). For the other, the comprehensive experimental data is more preferable to perform the comparison with numerical results, e.g., pressure distribution, power spectrum of forces, flow statistics. Thus, we applied the rough rules of AR>9, I_u <1% and BR~5% to select the experimental data (Bearman and Obasaju, 1982; Lee, 1975; Luo et al., 1994; Norberg, 1993; Nishimura and Taniike, 2000; Nishimura, 2001; van Oudheusden et al., 2008; Okajima, 1983; Lyn and Rodi, 1994; Lyn et al., 1995). These data will be presented together with the numerical results in the following sections.

4. Results of structured LES and unstructured LES

In this section, the numerical aspects of unstructured LES are tested and assessed, i.e., the numerical schemes for the convective term and the time advancement method. Meanwhile, the results of structured LES and experimental data mentioned in Section 3 will be given as a validation.

Table 1 shows the comparison of aerodynamic characteristics, including the time-averaged drag, fluctuating drag and lift, and Strouhal number (St). Additionally, the collection of experimental data is also included which has been selected carefully under the satisfactory criteria of wind tunnel testing in Section 3. In terms of the structured LES, all of

aerodynamic responses considered are in good agreement with these experiments. Thus, the structured LES data can be the validation data with sufficient confidence. As for the unstructured LES, the time-averaged values and St are consistent with experiments and structured LES. But the fluctuating drags exhibit the dispersion to a certain degree. Moreover, the fluctuating lifts are larger than experiments and the structured LES regardless of the numerical schemes.

Table 1 Aerodynamic characteristics comparison					
	C_D -mean	C _D -rms	C _L -rms	St	
Structured	2.21	0.205	1.26	0.134	
LUST	2.21(0%)	0.165(-20%)	1.51(+20%)	0.133	
limitedLinear	2.14(-3%)	0.210(+2%)	1.47 (+17%)	0.126	
linearUpwind	2.16(-2%)	0.156(-24%)	1.54 (+22%)	0.126	
Experiments	2.05~2.34	0.187~0.235	1.22~1.33	0.122~0.140	

Table 1 Aerodynamic characteristics comparison

Fig. 2 shows the distributions of time-averaged and fluctuating pressure along the circumferential direction. Unless noted otherwise, the shorthand notations of "limited" and "upwind" in the legend correspond to "limitedLinear" and "linearUpwind" respectively. From Fig. 2 (a), the distributions of time-averaged pressure generally agree well with the experiments in terms of all cases based on structured and unstructured LES. In particular, on the leeward face all of numerical cases are consistent with each other. But the time-averaged pressures on the side faces are slightly smaller than the structured LES. Moreover, when OpenFOAM is used, the different numerical schemes do not influence the time-averaged pressure distribution. According to Fig. 2 (b), the distributions on the front and rear faces are similar with each other among all of the numerical cases. They are consistent with Bearman and Obasaju (1982) and Lee (1975), although the fluctuating pressure on the rear face is smaller than Nishimura (2001). On the other hand, the distributions display differently on the side faces. All of the unstructured cases are larger than the structured case. Also the unstructured cases are similar to each other regardless of the specific schemes. Thus it seems that the numerical schemes for the convective term tested in the present study have no big influence on the time-averaged pressure distribution when the unstructured LES is used. But they all tend to increase the fluctuating pressure on the side faces.

The preceding discussions focus on the responses on the cylinder surfaces, which are of interest for wind resistance designers. Following it, we will investigate the flow field around the cylinder, which is expected to explain the features of aerodynamic pressure and forces acting on the square cylinder. Fig. 3 shows the velocity profiles along the wake centerline. It can be seen that the unstructured LES can predict the time-averaged and fluctuating velocity in the wake. Additionally, the selection of numerical schemes is not big effect under the current grid resolution for prediction of the low-order moments. However, if we take more care about the interaction between the wake flow and the cylinder, we need higher requirements about the wake prediction. For this sake, the one-dimensional energy spectra are obtained along the wake centerline, as shown Fig. 4. According to it, we can find that the results of the LUST and linearUpwind are very similar, indicating that the amount of artificial dissipation addition seems not big difference under the current grid system. It is well know that the artificial dissipation will induce the earlier decay of turbulence inertial sub-range, which is reflected by the results of LUST and linearUpwind. However, the TVD schemes seem to exhibit different influences on the inertial sub-range, which is shown by the limitedLinear. That is, they tend to reduce the energy when the frequency is around $10f_{vsv}$ but increase the energy at the higher frequency. It is possibly due to the work of the negative dissipation somewhere and sometime. Because of the unnatural behavior within the inertial sub-range, the TVD schemes seem not advisable for turbulence simulation.



Fig. 2 The distributions of time-averaged and fluctuating pressure.



Fig. 3 Velocity profiles along the wake centreline. (a) Time-averaged streamwise velocity; (b) Fluctuation of vertical velocity.





Fig. 4 One-dimensional energy spectra along the wake centreline. (a) x/D=3.0; (b) x/D=5.0; (c) x/D=7.0.

(**d**)

With respect to the unstructured LES, another aspect of interest is the prediction accuracy near the shear layers since the fluctuating pressures on the side faces are smaller than the structured LES. Fig. 5 displays the streamlines of time-averaged velocity. It is clear shown that there is no secondary vortex for the structured LES beneath the shear layers and downstream the frontal corners. But there exit the secondary vortices for the unstructured LES. They alter the flow topologies within the shear layer regions, especially near the side faces. They are also the reason for the larger time-averaged vertical velocity beneath the shear layers, as shown Fig. 6 (a). The cause of their formation is thought due to the earlier instability of shear layers when the unstructured LES is used. It could be verified by the profiles of fluctuation of vertical velocity component which is more sensitive to the roll-up of shear layers above the side faces as shown Fig. 6 (b). That is, the fluctuation of unstructured LES is much larger than the structured LES. Fig. 7 shows the instantaneous span-wise vorticity distribution for the structured LES and the unstructured LES, corresponding to the instant when $C_L \approx 0$. It is clearly seen that the upper shear layer witnesses the roll-up near the side faces, which definitely leads to several closed contours of pressure.

In order to discover the reason for the earlier instability of the shear layers, we performed the ensemble-averaging technique to the instantaneous flows at the instant when the lifts reach the peaks. It should be noted that we set a C_L threshold of 1.5 to conduct the ensemble-averaging to exclude the effect of the "irregular" flow patterns which results in very small lift. Fig. 8 shows the span-wise vorticity distributions after ensemble-averaging. One can find the unstructured LESs have the following characteristics: (1) the reattachment of the upper shear layer on the trailing edge is greater than the structured LES in the range; (2) it decreases the curvature of the upper shear layer, resulting in more downstream location of the primary negative-vorticity vortex. The larger range of reattachment on the trailing edge is thought to induce the earlier instability of the shear layers at the more upstream regions.





Fig. 5 The streamlines of time-averaged velocity for all of numerical cases. (a) Structured LES; (b) unstructured LES, LUST; (c) unstructured LES, limitedLinear; (d) unstructured LES, linearUpwind.



Fig. 6 The profiles of vertical velocity component when *x/D*=0. (a) The time-averaged velocity; (b) the fluctuating velocity.



Fig. 7 The instantaneous span-wise vorticity distributions. (a) The structured LES; (b) the unstructured LES, linearUpwind.



Fig. 8 The ensemble-averaged span-wise vorticity distributions. (a) The structured LES; (b) the unstructured LES, LUST; (c) the unstructured LES, linearUpwind.

5. Remedies for the weakness of unstructured LES

In this section, the mesh-refinement in the wake region is expected to result in the enhancement of the inertial sub-range. For the structured grid, it is well known that it is difficult to control the mesh-density distribution over the computational domain. Thus, the purely unstructured grid is used which is composed of prism cells, together with three near-wall mesh layers. The grid is shown in Fig. 9. The size of computational domain, the nearest cell from the cylinder surface and the spanwise resolution are retained the same as that introduced in Section 4. Moreover, the total cell number (7.0 million) is also close to that. The biggest difference is the mesh-refinement in the wake. Because the unnatural prediction of the inertial sub-range by the TVD schemes reported in Fig. 4, we only tested the numerical scheme stabilized by addition of artificial dissipation, i.e., LUST and linearUpwind. Table 2 shows the comparison of aerodynamic characteristics with the structured LES, where the shorthand notation of "WR" means the wake-refinement unstructured LES. One can find that even under the purely unstructured grid, the time-averaged drag can be accurately predicted. In contrast with the reduced fluctuating drag under the grid used in Section 3, the wake-refinement under the purely unstructured grid gives rise to the fluctuation of drag, compared with the structured LES. But there is an encouraging tendency in the fluctuating lift. The degree of overestimation of fluctuating lift is decreased through the wake refinement for both numerical schemes.



Fig. 9 Grid system. (a) Whole mesh; (b) & (c) close-up near the cylinder.

 Table 2 Aerodynamic characteristics of wake-refinement unstructured

 LES

	C_D -mean	C_D -rms	C_L -rms
Structured	2.21	0.205	1.26
LUST-WR	2.24(+1%)	0.290(+41%)	1.39(+10%)
linearUpwind-WR	2.30(+4%)	0.267(+30%	1.49 (+18%)

Fig. 10 shows the distributions of time-averaged and fluctuating pressure for the wake-refinement LES. It seems that the time-averaged pressure still retains the agreement with the structured LES even though the purely unstructured grid is used. From (b), the fluctuating pressure on the side faces shows a slight reduction compared with the results reported in Section 4. Unfortunately, they are still larger than the structured LES. On the other hand, the fluctuating pressure on the rear face is larger than the structured LES.

After checking the 1st and 2nd moment of the wake velocity, there are two identifiable tendencies under the effect of the wake-refinement. One is the fluctuation of streamwise velocity becomes larger; the other is the profile of time-averaged streamwise velocity along the centerline becomes gentler (see Fig. 11), and the formation length of vortex is slightly lengthened. It is possibly because of the higher proportion of weak vortex shedding characterized by the relatively parallel arrangement of upper and lower shear layers.

With regard to the earlier decay of higher frequency in the wake reported in Section 4 (see Fig. 4), one primary purpose of wake mesh-refinement is to enhance the prediction of higher frequency in the wake region. For this sake, the one-dimensional energy spectra are shown in Fig. 12, where the results of the coarse mesh in the wake are also included. It can be easily seen that the wake-refinement can extend the range of inertial sub-range even with the upwind-biased numerical scheme.

Moreover, the flow prediction within the shear-layer region is also

examined. Like that in Section 4, the time-averaged location of the shear layer can be predicted accurately compared with the structured LES. Regarding the earlier instability of shear layers, the profiles of vertical velocity component are shown in Fig. 13. One can find that compare with Fig. 6 (a), the side effect of the topology of time-averaged velocity has been reduced since the secondary vortex just behind the frontal corner has been compressed. Moreover, the reduction of fluctuation of vertical velocity indicates that the roll-up of shear layers near the side faces has been relieved. It is possibly because the formation length of vortex is lengthened by the wake-refinement.



Fig. 10 The distributions of time-averaged and fluctuating pressure for the wake-refinement LES.



Fig. 11 Profile of time-averaged streamwise velocity along the wake centreline.





spectra along the wake centreline for the wake-refinement LES with the linearUpwind scheme. (a) x/D=3.0; (b) x/D=5.0; (c)

0.2

Fig. 13 The profiles of vertical velocity component when x/D=0 for the wake-refinement LES. (a) The time-averaged velocity; (b) the fluctuating velocity.

6. Conclusions

Large eddy simulation is used to simulate the flow past a square cylinder at the high Reynolds number ($=2.2\times10^4$) under the fine mesh from the view point of engineering. The unstructured LES (based on OpenFOAM) is examined in detail in comparison with the structured LES and experimental database. The low-order numerical schemes are primarily considered under the similar grid system. In particular, we focus on the effect of artificial dissipation and the application of TVD scheme.

(1) The unstructured cases tested can predict the time-averaged drag force generally under the present grid resolution.

(2) The unstructured cases tested tend to increase the fluctuation of lift forces and the fluctuating pressure on the side faces.

(3) The addition of artificial dissipation tends to enhance the reattachment of shear layers on the trailing edges; it will promote the earlier roll-up of vortices in the shear layers near the side faces; secondary vortices occur just behind the frontal corners, which would alter slightly the time-averaged flow topology beneath the shear layer.

(5) The TVD schemes seem not preferable due to the unnatural distribution of turbulence inertial sub-range.

(6) The artificial dissipation induces the earlier decay of higher frequency components in the wake region.

The remedy with the feature of easy handling is suggested. The purely unstructured grid is used to refine the wake mesh under the similar total cell number. Several positive tendencies could be obtained: the fluctuating lift is reduced somewhat; the inertial sub-range in the wake is extended to higher frequencies; the earlier roll-up of shear layers has been relieved to a certain degree; the secondary vortices just behind the frontal corners have been compressed, resulting in more reasonable flow topology beneath the shear layers. But the fluctuating pressures on the rear face become further away from the structured LES, which is not clearly known and will be investigated further. The influence of mesh density around the cylinder will be considered in the future.

7. Bibliography

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