Large-eddy simulation of flow past a circular cylinder for Reynolds numbers 400 to 3900

Hongyi Jiang¹, and Liang Cheng^{1,2†}

¹School of Engineering, The University of Western Australia, 35 Stirling Highway, Perth, WA 6009, Australia

²State Key Laboratory of Coastal and Offshore Engineering, Dalian University of Technology, Dalian, 116024, China

Abstract

The benchmarking case of flow past a circular cylinder at the Reynolds number (Re) of 3900 is computed with two open-source codes, OpenFOAM and Nektar++, which are based on the conventional finite volume method and the high-order spectral/ hp element method, respectively. By using the Nektar++ model, mesh convergence for the case $Re = 3900$ is demonstrated (perhaps for the first time) through a systematic mesh dependence study, which includes separate examinations of the spanwise domain length (L_z/D), spanwise resolution, and the resolution in the plane perpendicular to the spanwise direction. The computational efficiencies for the Nektar++ and OpenFOAM approaches are then compared. This benchmarking study adds value to the broad Nektar++ and OpenFOAM communities and to the numerical modelling of bluff-body flows in general. Based on the Nektar++ approach, the computations are then generalised to a range of $Re = 400 - 3900$. It is found that $L_z/D = 3$ is adequate for $Re = 2500 - 3900$, while an increased $L_z/D = 6$ is recommended for $Re = 400 - 2000$. Based on the present high-fidelity numerical data, the physical mechanisms for the variations in the wake recirculation length and the hydrodynamic forces and pressure on the cylinder with Re are explored. In particular, the physics behind the inverse correlation between the root-mean-square lift coefficient (C_L') and the wake recirculation length, which includes a significant decrease in C_L' over $Re = 270 - 1500$, is highlighted.

1. Introduction

Steady incoming flow past a smooth and slender circular cylinder (referred to as flow past a circular cylinder hereafter) has been a classical problem in fluid mechanics for over one hundred years, owing to its fundamental significance as well as practical applications in the fields of civil, hydraulic, mechanical, nuclear, offshore and wind engineering (Zdravkovich, 1997). The case of flow past a circular cylinder is governed by a single dimensionless parameter, i.e. the Reynolds number Re (=

[†]Correspondence author: liang.cheng@uwa.edu.au

UD/ν), defined based on the velocity of the incoming flow (U), the diameter of the cylinder (D), and the kinematic viscosity of the fluid (ν). Despite its geometric simplicity, a number of flow regimes are observed with increasing Re , including the onset of two-dimensional (2D) vortex shedding at $Re \sim 47$, onset of three-dimensionality at $Re \sim 190$, three-dimensional (3D) wake transition over $Re \sim 190 - 270$, and successive transition to turbulence in the wake, the separating shear layer and the boundary layer at $Re \sim 270$, 1200 and 2×10^5 , respectively (e.g. Williamson, 1996a; Zdravkovich, 1997).

Owing to a rapid increase in the computing power over the past two decades, there has been a surge in the numerical modelling of flow past a circular cylinder at subcritical Re of $\sim 10^3 - 10^5$ using either large-eddy simulation (LES) or (sometimes under-resolved) direct numerical simulation (DNS), with different purposes including

- (i) Resolving basic and fundamental flow behaviours, e.g. flow structures, wake characteristics, turbulence statistics, hydrodynamic forces, etc.,
- (ii) Guiding practical applications, e.g. in the contexts of flow control (Choi et al., 2008; Yan et al., 2018), vortex-induced vibration (Williamson and Govardhan, 2004; Gsell et al., 2018), flow around cylinder bundles (Afgan et al., 2011), etc., and
- (iii) Testing the accuracy and robustness of new or different numerical methods and schemes, e.g. Kravchenko and Moin (2000), Franke and Frank (2002), etc.

A prerequisite for achieving these purposes is to perform a high-quality numerical simulation of the problem, which includes proper choices of the numerical method, discretisation schemes, computational domain size, mesh resolution, statistical time period, and a number of other parameters.

Among different Re values, the most well-studied case is $Re = 3900$, where flow characteristics and numerical experience have been reported by more than 20 studies. Table 1 lists several numerical studies which predicted flow characteristics relatively close to the experimental data of e.g. Parnaudeau et al. (2008). Among different flow characteristics, Parnaudeau et al. (2008) suggested that the agreement of the wake recirculation length (L_r) with the experimental result serves as the best indicator in determining the accuracy of the numerical simulation. The wake recirculation length is defined as the horizontal distance from the rear point of the cylinder to the wake stagnation point, at which the time-averaged streamwise velocity on the wake centreline changes sign (see the inset in Fig. 6(a)). Table 1 lists the L_r/D values reported by different studies, along with their relative differences to the experimental result of $L_r/D = 1.51$ reported by Parnaudeau et al. (2008). Dong et al. (2006) also reported experimental result of $L_r/D = 1.47$ for $Re = 4000$, which agrees very well with that of Parnaudeau et al. (2008), considering a gradual decrease in L_r with increasing Re (Norberg, 1998).

Table 1. Numerical studies of flow past a circular cylinder at $Re = 3900$. When multiple cases were investigated in a study, the case with recommend numerical model and schemes, highest resolution and/or largest statistical time range is listed in

this table. The abbreviations FDM, FVM and FEM represent finite difference method, finite volume method and finite element method, respectively.

Reference	Method	LES or DNS	L_z/D	N_z	L_r/D (and relative difference to 1.51)
Beaudan and Moin (1994)	FDM	LES	π	48	1.50 (−0.7%)
Breuer (1998) (case D3)	FVM	LES	π	64	1.372 (−9.1%)
Kravchenko and Moin (2000)	<i>B</i> -spline	LES	π	48	1.35 (−10.6%)
Franke and Frank (2002)	FVM	LES	π	33	1.64 (+8.6%)
Parnaudeau et al. (2008)	FDM	LES	π	48	1.56 (+3.3%)
Afgan et al. (2011)	FVM	LES	4	256	1.49 (−1.3%)
Wornom et al. (2011)	FEM and FVM	LES	π	100	1.45 (−4.0%)
Lysenko et al. (2012)	FVM	LES	π	64	1.67 (+10.6%)
Lehmkuhl et al. (2013)		DNS	π	128	1.36 (−9.9%)
Gallardo et al., (2014)	FVM	DNS	6	240	1.535 (+1.7%)
Cheng et al. (2017)	FDM	LES	3	64	1.34 (−11.3%)

However, due to the significant computational cost for $Re = 3900$, most of the previous studies generally limited their scope/contribution to the appropriate choice of one or two parameters, as summarised below.

- (i) The subgrid scale model. Beaudan and Moin (1994) and Breuer (1998) found that the dynamic Smagorinsky model, which automatically updates the Smagorinsky constant over both time and the computational domain (Germano et al., 1991), outperforms the conventional Smagorinsky model. Lysenko et al. (2012) found that the dynamic k -equation eddy-viscosity model also outperforms the conventional Smagorinsky model. It is also noteworthy that the choice of the subgrid scale model becomes less important when the mesh resolution is sufficiently high (Parnaudeau et al., 2008).
- (ii) Length of the statistical time period. Franke and Frank (2002) suggested that a statistical period of larger than 200 non-dimensional time units (defined as $t^* = tU/D$) is required, while Parnaudeau et al. (2008) suggested a statistical period of 1200 time units for full convergence. In addition, Lehmkuhl et al. (2013) observed a low-frequency swapping of two different wake patterns (where L_r/D differed by 21%) with an averaged period of 156 time units, which supports the use of a long statistical period.
- (iii) The spanwise domain length (L_z/D). As shown in Table 1, there has been a general consensus in the choice of $L_z/D = \pi$ among different studies. Parnaudeau et al. (2008) and Lehmkuhl et al. (2013) investigated the influence of L_z/D by doubling L_z/D from π to 2π , and observed 10% and 0.2% variations in L_r , respectively. However, Ma et al. (2000) showed that an increase in L_z/D from π to 2π resulted in a 30% decrease in L_r from 1.59 to 1.12 (much smaller than those shown in Table 1) and a qualitative change in the pattern of the time-averaged streamwise velocity profile at

$x/D = 1.06$ from a U-shape to a V-shape. Similar conclusions were drawn in Dong et al. (2006). The results of Ma et al. (2000) and Dong et al. (2006) were at odds with the experimental result of Parnaudeau et al. (2008) and the numerical results listed in Table 1. Kravchenko and Moin (2000) and Lysenko et al. (2012) attributed the V-shaped pattern to insufficient mesh resolutions.

As summarised above, the choices of the subgrid scale model, the statistical time period and the spanwise domain length have been relatively well understood. However, there still lacks a systematic investigation on the adequacy of the mesh resolution in both the spanwise direction and the plane perpendicular to the spanwise direction (denoted the x - y plane), which is possibly due to prohibiting computational costs in demonstrating mesh convergence. Table 1 shows large scatters in the choice of the number of spanwise planes N_z (between 10.5 and 64 per unit span length). Breuer (1998) showed that an increase in N_z from 32 to 64 for $L_z/D = \pi$ resulted in an increase in L_r by 14.6% and a decrease in the mean drag coefficient ($\overline{C_D}$) by 5.1%.

This suggests that $N_z = 32$ is inadequate but may not guarantee mesh convergence at $N_z = 64$. On the other hand, Kravchenko and Moin (2000), Afgan et al. (2011), and Gallardo et al. (2014) reported noticeable variations in L_r and/or $\overline{C_D}$ with different mesh resolutions in the x - y plane. However, to the best knowledge of the authors, the mesh convergence has not been well demonstrated through e.g. showing close agreement of the flow characteristics (e.g. $\lesssim 3\%$ variation in L_r and $\lesssim 1\%$ variation in $\overline{C_D}$) predicted by two meshes of different resolutions (e.g. with mesh refinement resulting in an increase in the number of cells by at least 1.5 times).

It is worth noting that without a mesh dependence check, a close agreement between the numerical and experimental results does not necessarily indicate appropriate numerical setup. For example, the excellent agreement in L_r/D between the LES of Beaudan and Moin (1994) and the experiment of Parnaudeau et al. (2008) (Table 1) may not suggest adequacy of $N_z = 48$ for $L_z/D = \pi$. Close agreements may be due to coincident cancellation of opposite numerical effects. For example, Lehmkuhl et al. (2013) reported a less than 1% variation in L_r between a coarse mesh and a mesh refined in both the spanwise direction (with an increase in N_z from 32 to 128 for $L_z/D = \pi$) and the x - y plane, which seemed to suggest that the use of $N_z = 32$ is adequate. However, an increase in the spanwise resolution generally results in an increase in L_r , while an increase in the x - y plane resolution generally results in a reduction in L_r (shown later on in section 3.1), such that the mesh dependence may be smeared out.

To complement the earlier studies, the present study reports a systematic mesh dependence check and seeks appropriate mesh resolutions (for both the spanwise direction and the x - y plane) for numerical modelling of flow past a circular cylinder at $Re = 3900$. The numerical simulations were conducted using two open-source codes, OpenFOAM version 5.0 (www.openfoam.org) and Nektar++ version 4.4.1 (Cantwell et al., 2015), which are based on the finite volume method (FVM) and spectral/ hp

element method, respectively. The performances of the two codes are compared.

In addition, the numerical experience gained from $Re = 3900$ is generalised to a range of $Re = 400 - 3900$. While an adequate mesh resolution for $Re = 3900$ can be readily applied to $Re < 3900$, the use of $L_z/D \sim \pi$ may be inadequate. The required L_z generally increases with decreasing Re . Jiang et al. (2017) showed that for Re in the 3D wake transition regimes, specifically from the onset of three-dimensionality at $Re \sim 190$ (e.g. Williamson, 1996a) to ~ 270 , $L_z/D > 10$ is required to accommodate at least three spanwise periods of the relatively large-scale mode A wake structures (with a spanwise period of $\sim 3 - 4D$) and the associated vortex dislocations. With the disappearance of mode A at $Re \sim 270$ and the existence of the finer-scale mode B structures (with a spanwise period of $< 1D$) at higher Re , Jiang and Cheng (2017) showed that a reduced L_z/D of 6 is applicable to $Re = 400 - 1000$. Similarly, Gioria et al. (2011) recommended an L_z/D of 6 for $Re = 400$, while Posdziech and Grundmann (2001) recommended an L_z/D equal to two spanwise periods of mode A ($= 6.74$) for $Re = 280$. However, between the use of $L_z/D \sim 6$ for $Re = 400 - 1000$ and $L_z/D \sim \pi$ for $Re = 3900$, there remains a knowledge gap as to the L_z requirement for $Re = 1000 - 3900$. This knowledge gap is addressed in the present study.

The physical mechanisms for the variations in L_r and the hydrodynamic forces over $Re = 400 - 3900$ are then explored. In the literature, Norberg (2003) and Roshko (1993) attributed the variation in L_r to the variations in the circulation and the shear stress in the wake, respectively, where the circulation and the shear stress are affected by the transition to turbulence in the wake and the separating shear layer. Roshko (1955) suggested that the base pressure coefficient (C_{pb}) is affected by the low pressure region in the near wake due to vortex formation, establishing the correlation between C_{pb} and L_r . However, quantitative data supporting these qualitatively suggestions are scarce, which is likely due to the difficulty in measuring the circulation, the shear stress and the low pressure region in physical experiments. With the availability of the present high-fidelity numerical data, all wake characteristics can be examined quantitatively, which allows for a better interpretation of the physical mechanisms for the variations in L_r and C_{pb} with Re . In addition, the variations in $\overline{C_D}$ and the root-mean-square lift coefficient (C_L') with Re , including a phenomenon called “lift crisis” where C_L' experiences a significant decrease over $Re = 270 - 1500$ (Norberg, 2003), are also physically explained.

2. Numerical model

2.1. The OpenFOAM model

OpenFOAM was adopted in this study in performing the conventional type of LES, which was based on the use of a subgrid scale model. The governing equations for the LES were the filtered continuity and incompressible Navier–Stokes equations:

$$\frac{\partial \bar{u}_i}{\partial x_i} = 0, \quad (1)$$

$$\frac{\partial \bar{u}_i}{\partial t} + \bar{u}_j \frac{\partial \bar{u}_i}{\partial x_j} = -\frac{\partial \bar{p}}{\partial x_i} + \nu \frac{\partial^2 \bar{u}_i}{\partial x_j \partial x_j} - \frac{\partial \tau_{ij}}{\partial x_j}, \quad (2)$$

where $(x_1, x_2, x_3) = (x, y, z)$ are Cartesian coordinates, u_i is the velocity component in the direction x_i , t is time, p is kinematic pressure (i.e. pressure divided by fluid density), ν is kinematic viscosity, and τ_{ij} is the subgrid scale stress tensor. The overbar in equations (1) and (2) denotes a filtered quantity. The deviatoric part of τ_{ij} is:

$$\tau_{ij} - \frac{1}{3} \tau_{kk} \delta_{ij} = -2\nu_t \bar{S}_{ij}, \quad (3)$$

where $\bar{S}_{ij}$ is the rate-of-strain tensor written as:

$$\bar{S}_{ij} = \frac{1}{2} \left(\frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right), \quad (4)$$

and ν_t is the turbulent eddy viscosity, which was calculated in the present study through the wall-adapting local eddy-viscosity (WALE) model (Nicoud and Ducros, 1999):

$$\nu_t = (C_w V^{1/3})^2 \frac{(S_{ij}^d S_{ij}^d)^{3/2}}{(\bar{S}_{ij} \bar{S}_{ij})^{5/2} + (S_{ij}^d S_{ij}^d)^{5/4}}, \quad (5)$$

where $C_w = 0.325$ is the model constant, V is the volume of a cell, and S_{ij}^d is the traceless symmetric part of the square of the velocity gradient tensor, which is calculated as:

$$S_{ij}^d = \frac{1}{2} (\bar{g}_{ij}^2 + \bar{g}_{ji}^2) - \frac{1}{3} \delta_{ij} \bar{g}_{kk}^2, \quad (6)$$

where

$$\bar{g}_{ij} = \frac{\partial \bar{u}_i}{\partial x_j}, \quad (7)$$

$$\bar{g}_{ij}^2 = \bar{g}_{ik} \bar{g}_{kj}. \quad (8)$$

In the framework of OpenFOAM, the governing equations were solved by the conventional FVM and the PISO (Pressure Implicit with Splitting of Operators) algorithm (Issa, 1986). The convection, diffusion and time derivative terms were discretized, respectively, using a fourth-order cubic scheme, a second-order linear scheme, and a blended scheme consisting of the second-order Crank–Nicolson scheme and a first-order Euler implicit scheme. The same set of numerical schemes was used in Jiang and Cheng (2017) and Jiang (2020) for the DNS of flow past a circular cylinder over $Re = 50 - 1000$.

2.2. Computational domain and mesh for the OpenFOAM model

The reference mesh used for the OpenFOAM model is introduced below, while a systematic mesh dependence check will be performed in section 3. Fig. 1 shows the computational domain and mesh in the x - y plane. The computational domain had a radius $r = 30D$, with the centre of the cylinder located at $(x, y) = (0, 0)$. Fig. 2 details the cell sizes in the radial and circumferential directions (denoted Δr and $\Delta\theta$, respectively). Unlike many previous studies which used a uniform expansion of Δr and a uniform distribution of $\Delta\theta$ over the entire domain, the present mesh was locally refined in the near-wake region. In the radial direction, the size of the first layer of cells next to the cylinder was $\Delta r = 1 \times 10^{-4}D$, and a relatively high resolution was used for $r \leq 7D$ to resolve the near wake. In the circumferential direction, a relatively high resolution of $\Delta\theta = 0.6^\circ$ was used for the downstream half of the domain. The total numbers of cells in the radial and circumferential directions were 377 and 464, respectively. For the entire domain, the cell expansion ratio was kept below 1.08. The 3D mesh was constructed by replicating the mesh in the x - y plane along the spanwise direction. The spanwise domain length and cell size were $L_z = 3D$ and $\Delta z = 0.05D$, respectively. The total number of cells was thus $377 \times 464 \times 60 = 10,495,680$.

The boundary conditions were specified as follows. For the inlet boundary at $r = 30D$ and $x < 0$, a uniform velocity $(u_x, u_y, u_z) = (U, 0, 0)$ was specified, while the pressure was governed by the Neumann condition. For the outlet boundary at $r = 30D$ and $x > 0$, the Neumann condition was used for the velocity, while the pressure was specified as a reference value of zero. On the cylinder surface, a no-slip condition was used. At the two lateral boundaries perpendicular to the spanwise direction, the periodic boundary condition was applied, since it allows for travelling waves in the spanwise direction and imposes less numerical constraints than the symmetry boundary condition (Jiang et al., 2017). Specifically, the periodic boundary condition enforces:

$$u_i(x, y, z = 0, t) = u_i(x, y, z = L_z, t), \quad (9)$$

$$(\partial u_i / \partial z)(x, y, z = 0, t) = (\partial u_i / \partial z)(x, y, z = L_z, t), \quad (10)$$

$$p(x, y, z = 0, t) = p(x, y, z = L_z, t), \quad (11)$$

$$(\partial p / \partial z)(x, y, z = 0, t) = (\partial p / \partial z)(x, y, z = L_z, t), \quad (12)$$

while the symmetry boundary condition enforces:

$$\partial u_x / \partial z = \partial u_y / \partial z = \partial p / \partial z = u_z = 0, \quad \text{at } z = 0 \text{ and } L_z \quad (13)$$

which gives rise to:

$$\omega_x = \left(\frac{\partial u_z}{\partial y} - \frac{\partial u_y}{\partial z} \right) \frac{D}{U} = 0, \quad \text{at } z = 0 \text{ and } L_z \quad (14)$$

$$\omega_y = \left(\frac{\partial u_x}{\partial z} - \frac{\partial u_z}{\partial x} \right) \frac{D}{U} = 0, \quad \text{at } z = 0 \text{ and } L_z \quad (15)$$

where ω_x and ω_y are the streamwise and transverse vorticity, respectively. In short, the symmetry boundary condition suppresses the spanwise velocity and three-dimensional vortices at the boundary. This may also artificially weaken the spanwise velocity and three-dimensional vortices near the boundary (Jiang et al., 2017).

Fig. 1. (a) Computational mesh in the x-y plane for the OpenFOAM model, and (b) a close-up view of the mesh.

Fig. 2. Cell sizes in the (a) radial direction, and (b) circumferential direction. To facilitate comparison of the OpenFOAM and Nektar++ meshes, the cell sizes for the Nektar++ mesh have been divided by 5.

2.3. The Nektar++ model

For the Nektar++ model, the governing equations were the unfiltered continuity and incompressible Navier–Stokes equations:

$$\frac{\partial u_i}{\partial x_i} = 0, \quad (16)$$

$$\frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \nu \frac{\partial^2 u_i}{\partial x_j \partial x_j}. \quad (17)$$

The governing equations were solved by Nektar++ using the unsteady Navier–Stokes solver, along with a second-order implicit–explicit (IMEX) time-integration scheme, a velocity correction scheme (Karniadakis et al., 1991), and a continuous Galerkin projection. The Nektar++ implementation consisted of a high-order spectral/*hp* element method (Karniadakis and Sherwin, 2005) for the x - y plane coupled with a Fourier expansion (Karniadakis, 1990) in the geometrically homogeneous spanwise direction, which may offer a greater efficiency on modern computer systems than conventional FEM, FDM and FVM approaches (Cantwell et al., 2015; Moxey et al., 2020).

A difference between the conventional LES listed in Table 1 and the Nektar++ formulation is that Nektar++ does not employ a subgrid scale model. Instead, Nektar++ performs the implicit LES (iLES) by using a spectral vanishing viscosity (SVV) technique (Kirby and Sherwin, 2006) to stabilise the solution, which is achieved by increasing the viscosity on the expansion modes with the highest frequencies. By default, the SVV cut-off ratio is 0.75, i.e. the lowest 75% of the frequencies are not damped, while the SVV diffusion coefficient is 0.1 (Nektar++ User Guide). Pasquetti (2005) showed that for flow past a circular cylinder in a confined channel at $Re = 3900$, the wake characteristics (e.g. the L_r value) were affected by different choices of the SVV cut-off ratio and diffusion coefficient. The influence of the SVV coefficients is re-examined in the present study.

2.4. Computational domain and mesh for the Nektar++ model

The computational domain size and boundary conditions for the Nektar++ model were identical to those used for the OpenFOAM model, except for the use of a high-order Neumann condition for the pressure (Karniadakis et al., 1991) at the inlet and cylinder surface. The macro-element mesh for Nektar++ retained the general topology of the mesh for OpenFOAM, while the macro-element sizes were generally five times larger than those for OpenFOAM in both the radial and circumferential directions (Fig. 2), owing to the use of the high-order spectral/*hp* element method for the x - y plane. The expansion ratio of the macro-elements was kept below 1.3. The total numbers of macro-elements in the radial and circumferential directions were 72 and 92, respectively. Each macro-element was then subdivided using 4th-order Lagrange polynomials (denoted $N_p = 4$) on the Gauss-Lobatto-Legendre points for the quadrilateral expansion. For the 3D mesh, 64 Fourier planes were used over the spanwise length of $L_z = 3D$.

2.5. Initial condition and time integration

For the reference cases detailed in sections 2.1 – 2.4, the initial condition for the simulation was a fully developed flow field calculated with a coarser mesh in the x - y

plane, while the case with the coarser mesh was initialised with the fully developed flow field for a reduced Re of 1000. For the variation cases to be investigated, the initial condition was the fully developed flow field obtained from the reference case. The above setup ensures a better numerical stability for the initial stage of the flow than the use of an impulsive start (where the initial conditions for both velocity and pressure are set to zero).

In the present study, each case was simulated for at least 1000 non-dimensional time units. The first 400 time units were used to generate the fully developed flow. After that, at least another 600 time units (i.e. at least 125 vortex shedding periods) were used for the statistics of the hydrodynamic forces and wake characteristics so as to account for the long-time irregularity of the flow described by Franke and Frank (2002), Parnaudeau et al. (2008) and Lehmkuhl et al. (2013). For each case, the time-step size (Δt^*) was chosen based on a Courant–Friedrichs–Lewy (CFL) limit of no more than 0.5. Depending on the mesh resolution in the x - y plane, the time-step size varied within the range of 0.0008 – 0.002. The statistical period, CFL limit and time-step size for each of the present cases are given later on in Table 3.

3. Numerical modelling at $Re = 3900$

3.1. The OpenFOAM results

Table 2 lists the OpenFOAM cases simulated at $Re = 3900$. In Table 2, the Strouhal number (St) and the drag and lift coefficients (C_D and C_L) are defined as:

$$St = \frac{f_L D}{U}, \quad (18)$$

$$C_D = \frac{F_D}{\frac{1}{2} U^2 D L_z}, \quad (19)$$

$$C_L = \frac{F_L}{\frac{1}{2} U^2 D L_z}, \quad (20)$$

where f_L is the peak frequency derived from the fast Fourier transform (FFT) of the time history of C_L , and F_D and F_L are the drag and lift forces on the cylinder (divided by the fluid density already), respectively. The time-averaged drag and lift coefficients are denoted $\overline{C_D}$ and $\overline{C_L}$, respectively. The root-mean-square lift coefficient is calculated as:

$$C_L' = \sqrt{\frac{1}{N} \sum_{i=1}^N (C_{L,i} - \overline{C_L})^2}, \quad (21)$$

where N is the number of values in the time history. On the other hand, the base pressure coefficient (C_{pb}) and the wake recirculation length (L_r) are determined from the time-averaged flow field, where C_{pb} is calculated as:

$$C_{pb} = \frac{p_b - p_\infty}{\frac{1}{2}U^2} \quad (22)$$

where p_b is the time-averaged kinematic pressure at the rear point of the cylinder, and p_∞ is the reference kinematic pressure at the inlet boundary.

Table 2. Mesh dependence study of the OpenFOAM cases at $Re = 3900$. For cases 2 to 5, the relative differences in L_r/D with respect to the reference case are shown in the brackets.

Case description	L_z/D	$\Delta z/D$	St	$\overline{C_D}$	C'_L	$-C_{pb}$	L_r/D
1. Reference case (OpenFOAM)	3	0.05	0.212	0.994	0.161	0.893	1.444
2. Increase in spanwise length	6	0.05	0.211	0.992	0.152	0.889	1.447 (+0.2%)
3. Increase in spanwise resolution	3	0.025	0.210	0.959	0.111	0.842	1.634 (+13.2%)
4. Increase in x - y plane resolution	3	0.05	0.211	1.032	0.217	0.954	1.260 (−12.7%)
5. Without subgrid scale model	3	0.05	0.212	0.986	0.136	0.906	1.406 (−2.6%)
Experimental result			0.209		0.083	0.88	1.51

Table 3. Computational cost of the OpenFOAM and Nektar++ cases at $Re = 3900$.

Case description	Δt^*	CFL	Statistical time units	Cores	Cost for 1000 time units	
					Hours	Core hours
1. Reference case (OpenFOAM)	1.5×10^{-3}	≤ 0.50	600	10×24	533	127,920
2. Increase in spanwise length	1.5×10^{-3}	≤ 0.50	600	20×24	667	320,160
3. Increase in spanwise resolution	1.5×10^{-3}	≤ 0.50	600	20×24	686	329,280
4. Increase in x - y plane resolution	1.21×10^{-3}	≤ 0.50	600	15×24	1043	375,480
5. Without subgrid scale model	1.5×10^{-3}	≤ 0.50	600	10×24	494	118,560
6. Reference case (Nektar++)	1.25×10^{-3}	≤ 0.41	1350	2×24	552	26,496
7. Increase in spanwise length	1.25×10^{-3}	≤ 0.41	600	2×24	1067	51,216
8. Increase in spanwise resolution	1.25×10^{-3}	≤ 0.41	600	2×24	1057	50,736
9. Increase in h -type resolution	8×10^{-4}	≤ 0.38	600	2×24	1412	67,776
10. Increase in p -type resolution	8×10^{-4}	≤ 0.41	1050	2×24	1081	51,888
11. Decrease in p -type resolution	2×10^{-3}	≤ 0.38	1100	2×24	247	11,856

In Table 2, case 1 is the reference case introduced in section 2. Cases 2 to 5 are variations to case 1, where each case focused on one numerical aspect only. Specifically, case 2 doubled the spanwise domain length from $L_z/D = 3$ to 6. The excellent agreement in the numerical results between cases 1 and 2 suggests that the use of $L_z/D = 3$ is adequate. Table 3 lists the computational cost for each case. The present computations were performed on a Cray XC40 system supercomputer. For each case, parallel computation was conducted on multiple computer nodes (each containing 24 cores). The number of computer nodes was selected based on the scalability analysis reported in Appendix A. The computational cost is calculated as a multiplication of the number of cores used and the wall-clock time required for the

computation. As shown in Table 3, the computational cost for case 2 was 2.5 times that of case 1, which is due to the use of doubled nodes for doubled number of cells, coupled with the convergence and scalability issues.

Cases 3 and 4 examined the adequacy of the mesh resolution of case 1. Specifically, case 3 refined the spanwise resolution by reducing $\Delta z/D$ from 0.05 to 0.025, while case 4 refined the x - y plane resolution by reducing both Δr and $\Delta \theta$ by 1.24 times (see Fig. 2). The total number of cells for case 4 was 1.54 ($= 1.24 \times 1.24$) times that of case 1, while the time-step size was reduced by 1.24 times (see Table 3) so as to satisfy the same CFL limit. The ratio 1.24 was chosen based on the following considerations:

- (i) By considering the variations in the total number of cells and the time-step size due to mesh refinement, the increases in the nominal computational costs for cases 3 and 4 are similar (2 and 1.24^3 times that of case 1, respectively). *A posteriori* data in Table 3 also show that the actual computational costs for cases 3 and 4 were similar.
- (ii) The computational cost for a mesh finer than that of case 4 is prohibitive.

As shown in Table 2, moderate differences in the numerical results exist between case 1 and cases 3 and 4 (e.g. $\sim 13\%$ variations in L_r and $\sim 4\%$ variations in $\overline{C_D}$), which suggests that the mesh resolution of case 1 is still somewhat inadequate.

Theoretically, the adequacy of the spanwise resolution used in case 3 and the x - y plane resolution used in case 4 can be checked by computing additional cases with further mesh refinements and showing good agreement in the numerical results with cases 3 and 4 (e.g. $\lesssim 3\%$ variation in L_r and $\lesssim 1\%$ variation in $\overline{C_D}$ after further mesh refinement). However, Table 3 shows that the computational costs for cases 3 and 4 were 2.57 and 2.94 times that of case 1, respectively, which suggests that further mesh refinements may demand further increases in the computational cost by ~ 3 times and reach the level of one million core hours for one case, which is currently unaffordable. Therefore, without further mesh refinements to cases 3 and 4, the present study cannot determine the adequate spanwise and x - y plane resolutions required for the OpenFOAM case.

It is interesting to see in Table 2 that cases 3 and 4 show similar levels but opposite effects in the variations to case 1, which coincidentally brings up case 1 as a good match of the experimental results of St (Norberg, 2003), Cl' (Norberg, 2003), C_{pb} (Norberg, 1994) and L_r (Parnaudeau et al., 2008), whereas mesh refinements in cases 3 and 4 seem to worsen the prediction. These cases suggest that it is insufficient to merely confirm the agreement between the numerical and experimental results, since multiple influencing factors may be at play and they may partially cancel one another. Instead, a systematic mesh dependence study is necessary in seeking appropriate numerical setup and avoiding misleading conclusions.

Lastly, case 5 shows that the effect of the subgrid scale model on the flow characteristics is minor. The most important factors in governing the numerical accuracy are the mesh resolutions in the spanwise direction and the x - y plane.

3.2. The Nektar++ results

Table 4 summarises the Nektar++ cases simulated at $Re = 3900$. Case 6 is the reference case introduced in section 2, while cases 7 to 11 are five variations to case 6. Specifically, case 7 doubled the spanwise domain length from $L_z/D = 3$ to 6 and shows that $L_z/D = 3$ is adequate. Case 8 examined the spanwise resolution by doubling the Fourier planes from 64 to 128. Cases 9 and 10 examined the x - y plane resolution via h -type and p -type refinements, respectively. The h -type refinement in case 9 focused on local refinement of the macro-elements around the separating shear layers and the near wake (see Fig. 2, where mesh refinement was concentrated at $r \lesssim 4D$ and $90^\circ \lesssim \theta \lesssim 270^\circ$). On the other hand, the p -type refinement in case 10 was realised by increasing the N_p value, which offered a consistent increase in the resolution over the entire x - y plane. As shown in Table 4, the numerical results predicted by the variation cases 8 to 10 agree well with those of the reference case 6, which suggests that the mesh resolution used in case 6 is adequate.

Table 4. Mesh and parameter dependence study of the Nektar++ cases at $Re = 3900$. The relative differences in L_r/D for cases 7 to 11 are calculated with respect to case 6, while the relative differences in L_r/D for cases 12 to 16 are calculated with respect to case 11.

Case description	N_p	L_z/D	Fourier planes	St	$\overline{C_D}$	C_L'	$-C_{pb}$	L_r/D
6. Reference case (Nektar++)	4	3	64	0.209	0.980	0.145	0.869	1.504
7. Increase in spanwise length	4	6	128	0.209	0.972	0.129	0.860	1.529 (+1.7%)
8. Increase in spanwise resolution	4	3	128	0.209	0.972	0.136	0.862	1.533 (+1.9%)
9. Increase in h -type resolution	4	3	64	0.209	0.968	0.122	0.858	1.547 (+2.9%)
10. Increase in p -type resolution	5	3	64	0.209	0.983	0.154	0.877	1.496 (−0.5%)
11. Decrease in p -type resolution	3	3	64	0.210	0.957	0.107	0.837	1.614 (+7.3%)
Experimental result				0.209		0.083	0.88	1.51
Case 11 (ref. for cases 12 to 16)	3	3	64	0.210	0.957	0.107	0.837	1.614
12. Increase in spanwise length	3	6	128	0.211	0.951	0.095	0.830	1.641 (+1.7%)
13. Increase in spanwise resolution	3	3	128	0.211	0.952	0.100	0.832	1.631 (+1.1%)
14. SVV cut-off ratio 0.5	3	3	64	0.211	0.955	0.100	0.833	1.637 (+1.4%)
15. SVV diffusion coefficient 0.05	3	3	64	0.211	0.954	0.106	0.834	1.635 (+1.3%)
16. SVV diffusion coefficient 0.2	3	3	64	0.211	0.970	0.133	0.858	1.543 (−4.4%)

However, with a reduction in the p -type resolution from $N_p = 4$ to 3 (case 11 in Table 4), a moderate variation in L_r is observed. Nevertheless, in terms of the computational efficiency, case 11 was more than twice faster than case 6 (Table 3). Therefore, case 11 was used as a reference for some further parameter dependence studies. Specifically, cases 12 and 13 re-examined the influence of the spanwise domain length and resolution, respectively. The variations in the numerical results with respect to case 11 display similarities to the $N_p = 4$ counterparts (i.e. cases 6 to 8).

Cases 14 to 16 investigated the influence of the SVV coefficients. Specifically, cases 14 and 15 show respectively that a reduction in the SVV cut-off ratio from 0.75 to 0.5 and an increase in the SVV diffusion coefficient from 0.05 to 0.1 (both resulted in increased numerical dissipation) have minimal influence on the numerical results, which support the use of the default SVV coefficients in this study. For completeness, case 16 shows that a further increase in the SVV diffusion coefficient from 0.1 to 0.2 leads to moderate variations in the numerical results.

In addition to the comparison of L_r and other quantities in Table 4, Fig. 3 compares the time-averaged velocity and velocity fluctuation profiles sampled at $x/D = 1.06, 1.54$ and 2.02 , where $\bar{u}_i$ and $u'_i (= u_i - \bar{u}_i)$ denote time-averaged and fluctuation components of the velocity, respectively. The close agreement between case 6 and cases 8 and 10 suggests that the use of $N_p = 4$ and 64 Fourier planes for the reference case 6 is adequate. The numerical accuracy of cases 6, 8 and 10 is further confirmed by a close agreement with the experimental results of Parnaudeau et al. (2008). On the other hand, moderate differences are observed between cases 6 and 11, which suggests that $N_p = 3$ is slightly inadequate. As expected, an inadequate x - y plane resolution tends to under-predict the velocity fluctuations (Fig. 3c-e).

Fig. 3. Time-averaged velocity and velocity fluctuation profiles sampled at $x/D = 1.06$, 1.54 and 2.02 for $Re = 3900$: (a) streamwise velocity, (b) transverse velocity, (c) variance of the streamwise velocity fluctuation, (d) variance of the transverse velocity fluctuation, and (e) covariance of the velocity fluctuation. For ease of presentation, the velocity profiles at $x/D = 1.54$ and 2.02 have been shifted by certain values. The experimental results used for comparison are from “PIV case 1” of Parnaudeau et al. (2008).

Based on the reference case 6, Fig. 4 shows the frequency spectra of the transverse velocity u_y sampled at $(x/D, y/D) = (1, 0.8)$, $(3, 0)$ and $(7, 0)$ over a period of 260 time units. The frequency spectra were obtained from the FFT of the time history of u_y , where f and A are the frequency and amplitude of u_y derived from the FFT, respectively. The frequency spectra were averaged over the 64 spanwise planes. Fig. 4(a) shows the frequency spectrum at $(x/D, y/D) = (1, 0.8)$. This point is the same as that used in the experimental study of Prasad and Williamson (1997) and is just above the upper separating shear layer. Therefore, both the Kármán vortex shedding

frequency (f_K) and the shear-layer frequency (f_{SL}) are observed. Based on a 4th-order polynomial curve fitting of the spectrum over the range $f/f_K = 4 - 9$, f_{SL} was determined as the peak of the fitted curve at $6.2f_K$. In addition, the mesh convergence of the ratio f_{SL}/f_K was checked by performing the same analysis using case 10 (with $N_p = 5$), where f_{SL} was determined at $6.3f_K$. The present ratio agrees well with the experimental result of $f_{SL} = 6.0f_K$ for $Re = 3900$ obtained from the empirical formula $f_{SL}/f_K = 0.0235 \times Re^{0.67}$ proposed by Prasad and Williamson (1997). On the other hand, Fig. 4(b) shows the frequency spectra in the wake region at $(x/D, y/D) = (3, 0)$ and $(7, 0)$, where only f_K and its harmonics are observed. The frequency spectra follow the $-5/3$ slope (i.e. the inertial subrange) over an order of magnitude of f/f_K . This feature agrees well with the experimental results of Parnaudeau et al. (2008).

Fig. 4. Frequency spectra of the transverse velocity sampled at (a) $(x/D, y/D) = (1, 0.8)$, and (b) $(x/D, y/D) = (3, 0)$ and $(7, 0)$, based on the reference case 6.

The mesh resolution for the reference case 6 is also compared against the Kolmogorov length scales for $Re = 3900$. The Kolmogorov length scale (η) for an instantaneous flow field is calculated as:

$$\eta = \left(\frac{\nu^3}{\varepsilon} \right)^{1/4}, \quad (23)$$

where ε is the kinetic energy dissipation rate calculated as:

$$\varepsilon = \nu \frac{\partial u'_i}{\partial x_j} \left(\frac{\partial u'_i}{\partial x_j} + \frac{\partial u'_j}{\partial x_i} \right) \quad (24)$$

Fig. 5(a) shows the time- and span-averaged η/D values sampled along the wake centreline. The time average was performed over a period of 260 time units, and the sample interval was 0.5 time unit. The adequacy of the sample interval was confirmed by almost identical results shown in Fig. 5(a) obtained with sample intervals of 0.5

and 1 time unit. Fig. 5(b) compares the mesh resolutions in the streamwise and transverse directions ($\Delta x/N_p$ and $\Delta y/N_p$, respectively) against the η values shown in Fig. 5(a). It is also noted that by using the high-order spectral/ hp element method, the actual mesh resolution is better than a simple division of the macro-element size by N_p , such that the ratios shown in Fig. 5(b) are on the conservative side.

Fig. 5. (a) Time- and span-averaged Kolmogorov length scales sampled along the wake centreline, and (b) ratio between the cell size and the Kolmogorov length scale.

3.3. Comparison between the OpenFOAM and Nektar++ models

Based on the OpenFOAM model used in section 3.1, it is found that for the reference case 1 the spanwise resolution of $\Delta z/D = 0.05$ and the x - y plane resolution shown in Fig. 2 are both inadequate. If one assumes that the mesh refinements from case 1 to cases 3 and 4 would result in adequate mesh resolutions in the spanwise direction and the x - y plane, respectively, the computational cost for a mesh-independent simulation is estimated to be $2.57 \times 2.94 = 7.56$ times that of case 1, i.e. approximately one million core hours. The tremendous computational cost is possibly the reason why mesh convergence is difficult to be demonstrated through conventional FVM (and similarly FEM and FDM) used in this study and many of the previous studies (e.g. Table 1).

On the other hand, the Nektar++ model offers a more computationally efficient approach by using a high-order spectral/ hp element method for the x - y plane and a Fourier expansion in the spanwise direction. It is shown in section 3.2 that mesh convergence is achieved by the reference case 6, which uses 64 Fourier planes over $L_z = 3D$ and the x - y plane resolution shown in Fig. 2 with an $N_p = 4$. If one assumes that the x - y plane mesh in case 4 (by OpenFOAM) is also adequate, the OpenFOAM mesh is $5 \times 1.24 = 6.2$ times finer than the macro-element mesh for Nektar++ in both the radial and circumferential directions. However, owing to the use of the p -type refinement in Nektar++, the N_p value required for the mesh convergence is smaller

than 6.2.

A comparison of the computational costs for the OpenFOAM and Nektar++ models is meaningful when both numerical simulations reach the level of mesh convergence. Compared with the estimated cost of approximately one million core hours for a mesh-independent simulation using FVM-based OpenFOAM, the computational cost for the Nektar++ model (case 6 in Table 3) is only $\sim 3\%$ of the former. The general conclusions are expected to be applicable to the numerical modelling of other bluff-body flows.

4. Numerical results for $Re = 400 - 3900$

4.1. Hydrodynamic characteristics over $Re = 400 - 3900$

In addition to the case $Re = 3900$ investigated in section 3, this section investigates further the cases over a range of $Re = 400 - 3900$. Theoretically, with decreasing Re the mesh resolution in both the spanwise direction and the x - y plane can be progressively reduced, on the basis that the Kolmogorov length scale η/D scales with $Re^{-3/4}$ (Pope, 2000). Practically, to avoid complete re-examinations of the mesh convergence for multiple Re values, the mesh resolution for $Re = 3900$ (based on the reference case 6) is applied to $Re = 400 - 3900$ directly. However, the spanwise domain length of $L_z/D = 3$ used for $Re = 3900$ may be inadequate for $Re < 3900$. Therefore, both $L_z/D = 3$ and 6 were tested in this study for $Re = 1000 - 3900$ so as to determine the range of Re for the applicability of $L_z/D = 3$. The cases with $L_z/D = 3$ and 6 adopted the meshes identical to those used for the cases 6 and 7 for $Re = 3900$ (Table 4). For $Re = 400 - 1000$, $L_z/D = 6$ was used, since Jiang and Cheng (2017) demonstrated the adequacy of $L_z/D = 6$ based on a comparison of $L_z/D = 6$ and 12 for both $Re = 400$ and 1000.

Fig. 6 shows the present numerical results obtained with both $L_z/D = 3$ and 6. The results obtained with $L_z/D = 3$ and 6 show agreement at $Re \geq 2500$ but moderate differences at $Re \leq 2000$, which suggests that $L_z/D = 3$ can be used for $Re \geq 2500$ but is inadequate for $Re \leq 2000$. Compared with the experimental results reported in the literature (see Fig. 6), it is found that the present numerical results with $L_z/D = 6$ match the experimental results better than their counterparts with $L_z/D = 3$ for the range $Re \leq 2000$. In particular, the numerical results with $L_z/D = 6$ reveal an obvious change in the variation trends of the L_z-Re , $\overline{C_p}-Re$, $C_L'-Re$, $C_{pb}-Re$ and $St-Re$ relationships at $Re = 1000 - 1500$, where physically the separating shear layer transitions to turbulence (Prasad and Williamson, 1997). However, for the cases with $L_z/D = 3$, such a changeover is observed at $Re > 2000$, which suggests that an insufficient L_z may restrict and delay the transition to turbulence in the separating shear layer.

It is worth noting that the present numerical results with $L_z/D = 6$ agree well with the experimental results over the entire range of Re investigated. The good agreement demonstrates the accuracy and robustness of the present LES approach in simulating

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flow past a circular cylinder.

Fig. 6. The (a) L_z-Re , (b) $\overline{C_D}-Re$, (c) $C_L'-Re$, (d) $C_{pb}-Re$, and (e) $St-Re$ relationships for flow past a circular cylinder. The present numerical results are obtained with both $L_z/D = 3$ and 6. The cases with $L_z/D = 3$ and 6 adopt the meshes identical to those used for the cases 6 and 7 for $Re = 3900$. The $C_L'-Re$ and $St-Re$ relationships from Norberg (2003) are piecewise empirical formulae fitted from experimental data reported by several studies, such that discrete data points are omitted. The DNS results of Jiang and Cheng (2017) and Jiang et al. (2016) for $Re = 100 - 300$ are included for completeness.

Henderson (1997) suggested based on the numerical analysis at $Re = 1000$ that with increase in L_z/D from 2π to 4π and 8π the C_L' value may decrease, owing to the phase differences in vortex shedding at different spanwise locations and therefore partial cancellation of the span-averaged C_L' value (see equation (20) where C_L is span-averaged). Similarly, Norberg (2003) concluded that the sectional C_L' value is larger than the C_L' value integrated over a finite span length. Therefore, one may wonder if the decrease in the C_L' values with increase in L_z/D from 3 to 6 (Fig. 6c) is affected by the above-mentioned physical cause, or purely due to numerical setup (i.e. an inadequate L_z).

To address this issue, the case $Re = 1000$ and $L_z/D = 6$ was computed again with a modified mesh that divided the cylinder surface into six spanwise sections. In this way, the time history of C_L of each section can be obtained separately. This case was

computed using OpenFOAM, owing to the convenient definition of multiple sections over the spanwise mesh layers. The computational mesh was the reference mesh used in Jiang and Cheng (2017), which was coarser than those used in section 3 for $Re = 3900$. The six spanwise sections of the cylinder are listed in Table 5. The shortest spanwise sections (sections 2, 4 and 6) each contained only one spanwise mesh layer, and was used to determine the sectional forces. Table 5 summarises the $\overline{C_D}$ and C_L' values integrated within each section and over some combinations of the sections (for spanwise lengths $3D$ and $6D$). As the spanwise length for the integration of C_L' increases from $0.05D$ to $3D$ and $6D$, the C_L' values do reduce slightly, which is due to the physical cause of phase differences in the vortex shedding. In contrast, the $\overline{C_D}$ values are almost unchanged, since $\overline{C_D}$ is not cancelled by the phase differences. Nevertheless, the minor differences in the C_L' values integrated over spanwise lengths $0.05D$ to $6D$ are much smaller than those induced by the mesh and numerical parameters (e.g. Table 2 and Table 4). Therefore, the C_L' values integrated over $L_z/D = 3$ and 6 can be approximated as the sectional C_L' , for the purpose of comparing with the sectional C_L' measured in the experimental studies (e.g. Norberg, 2003).

Table 5. The case $Re = 1000$ and $L_z/D = 6$ where the cylinder surface is divided into six spanwise sections.

Section index	Range of z/D	Section length (D)	$\overline{C_D}$	C_L'
1	0 – 0.95	0.95	1.0179	0.1247
2	0.95 – 1	0.05	1.0171	0.1241
3	1 – 2.95	1.95	1.0180	0.1263
4	2.95 – 3	0.05	1.0195	0.1298
5	3 – 5.95	2.95	1.0186	0.1253
6	5.95 – 6	0.05	1.0198	0.1263
1 – 4	0 – 3	3	1.0180	0.1247
5 – 6	3 – 6	3	1.0186	0.1252
Average of 2, 4 and 6		0.05	1.0188	0.1267
Average of 1 – 4 and 5 – 6		3	1.0183	0.1249
1 – 6	0 – 6	6	1.0183	0.1239

On the other hand, to examine the influence of numerical restriction on C_L' , we computed an addition case of $Re = 1000$ with $L_z/D = 3$. The C_L' value predicted by this case was 0.1615, which was much larger than the sectional C_L' of ~ 0.1267 obtained with $L_z/D = 6$ (Table 5). Therefore, it is concluded that the major cause for the increase in C_L' with decrease in L_z/D from 6 to 3 (Fig. 6c) is the inadequacy of $L_z/D = 3$ in the numerical setup.

4.2. Physical mechanisms for the variations in the hydrodynamic forces

The Re range of 100 – 5000 in Fig. 6 spans several flow regimes, including the 2D laminar regime ($Re \sim 47 - 190$), 3D wake transition regimes ($Re \sim 190 - 270$), wake transition to turbulence ($Re \sim 270 - 1200$) and shear-layer transition to turbulence ($Re \gtrsim 1200$) (Williamson, 1996a; Zdravkovich, 1997). Correspondingly, the hydrodynamic characteristics shown in Fig. 6 display changes in the variation trends at these critical Re values. Since the 2D laminar and 3D wake transition regimes have been investigated by a number of studies in the literature (e.g. Williamson (1996a,b) and the references therein), the present study focuses mainly on the variation trends over $Re = 270 - 3900$.

4.2.1. The L_r – Re relationship

For the L_r – Re relationship shown in Fig. 6(a), the transition to turbulence in the wake (in the form of increasingly disordered and turbulent 3D fine-scale mode B structures) results in an increase in L_r over $Re \sim 270 - 1500$. An increase in L_r indicates a more downstream roll up and shedding of the Kármán vortices. Norberg (2003) suggested that “the increase in secondary (essentially streamwise) circulation occurs probably at the expense of the primary (essentially spanwise) circulation associated with the roll-up of the von Kármán vortices”. To validate this suggestion, the spanwise circulation for $Re = 100 - 3900$ is quantified in this study by using the DNS results of Jiang et al. (2016) for $Re = 100 - 300$ and the present LES results for $Re = 400 - 3900$ (with $L_z/D = 6$). The total spanwise circulation prior to the formation of the Kármán vortices consists of three parts, namely (i) the circulation entering the wake and forming the laminar separating shear layers, (ii) the circulation of the small-scale shear-layer vortices, and (iii) the circulation of the smaller-scale turbulence. While parts (i) and (ii) may be responsible for the roll up of the Kármán vortices, part (iii) is largely irrelevant. However, it is difficult to separate parts (ii) and (iii), due to the intermittent emergence of the shear-layer vortices in time and space (Prasad and Williamson, 1997). Therefore, only part (i) is quantified in this study. Part (i) is calculated based on the time- and span-averaged flow field, and is defined as the spanwise circulation past $x = 0$ (i.e. entering the wake) per unit time:

$$\Gamma_{z,x=0} = \frac{1}{2} \left(\int_{0.5}^{\infty} \frac{u_x}{U} |\omega_z| d\left(\frac{y}{D}\right) + \int_{-\infty}^{-0.5} \frac{u_x}{U} |\omega_z| d\left(\frac{y}{D}\right) \right), \quad (25)$$

where

$$\omega_z = \left(\frac{\partial u_y}{\partial x} - \frac{\partial u_x}{\partial y} \right) \frac{D}{U}. \quad (26)$$

Fig. 7(b) shows the $\Gamma_{z,x=0}$ – Re relationship over $Re = 100 - 3900$. The $\Gamma_{z,x=0}$ – Re relationship correlates inversely with the L_r – Re relationship up to $Re \sim 1500$ (Fig. 7a,b), i.e. the spanwise circulation entering the wake does govern the streamwise location for the roll up of the separating shear layers into the Kármán vortices. However, the inverse correlation between $\Gamma_{z,x=0}$ and L_r ends at $Re \sim 1500$. This is because the contribution of part (ii), which takes effect at $Re \gtrsim 1500$, is not included

in $\Gamma_{z,x=0}$.

Another way to quantify the effect of the shear-layer instability at $Re \gtrsim 1500$ is to examine the variation in the shear stress $u'_x u'_y / U^2$ with Re (Roshko, 1993; Williamson, 1996a). Fig. 7(c) shows the relationship between the time- and span-averaged maximum shear stress in the near wake $(u'_x u'_y / U^2)_{\max}$ and Re . The emergence of the shear-layer instability is revealed by the changeover in the variation trend of $(u'_x u'_y / U^2)_{\max}$ at $Re = 1500$. The $(u'_x u'_y / U^2)_{\max}-Re$ and L_r-Re relationships display an inverse correlation over the entire range of Re investigated.

Fig. 7. The (a) L_r-Re , (b) $\Gamma_{z,x=0}-Re$, and (c) $(u'_x u'_y / U^2)_{\max}-Re$ relationships for flow past a circular cylinder. For ease of comparison, the L_r-Re relationship is reproduced from Fig. 6(a).

4.2.2. The $C_{pb}-Re$ relationship

The inverse correlation between the $(-C_{pb})-Re$ and L_r-Re relationships was investigated by Roshko (1955), who suggested that the base suction is affected by the low pressure region in the near wake due to vortex formation. For example, Fig. 8(a) shows the phase-averaged spanwise vorticity field for $Re = 1000$, where the phase corresponds to the peaks in the time history of the lift coefficient. At this phase, the upper shear layer is rolling up into a Kármán vortex, and correspondingly a significant low pressure region is observed in the phase-averaged pressure field shown in Fig. 8(b). Having confirmed the correspondence between the low pressure region and vortex formation, the time-averaged pressure field (e.g. Fig. 8c) is used to quantify the influence of Re on the low pressure region near the wake stagnation point. Fig. 9

quantifies the minimum pressure in the low pressure region (p_{min}) and its streamwise location for $Re = 100 - 3900$. Both the minimum pressure and its streamwise location vary with the variation in L_r (or the wake stagnation point at $x = L_r + 0.5D$). Since an increase in L_r results in a reduction in $|p_{min}|$ and an increase in the distance between the cylinder base and the low pressure region, the influence of the low pressure region on the $-C_{pb}$ value is reduced, resulting in the inverse correlation between $-C_{pb}$ and L_r .

Fig. 8. Span-averaged wake characteristics for flow past a circular cylinder at $Re = 1000$: (a) phase-averaged spanwise vorticity field, (b) phase-averaged pressure field, and (c) time-averaged pressure field.

Fig. 9. Characteristics of the time-averaged low pressure region near the wake stagnation point: (a) the minimum pressure in the low pressure region, and (b) the streamwise location for the minimum pressure.

4.2.3. The $\overline{C_D}$ – Re relationship

While $-C_{pb}$ and CL' correlate inversely with L_r , the inverse correlation between $\overline{C_D}$ and L_r is less obvious (Fig. 6). The reason is that the drag coefficient consists of the viscous and pressure components, and the viscous drag decreases almost monotonically with increasing Re (except for a $\sim 1\%$ increase in the viscous drag at $Re = 250 - 260$ due to a sharp decrease in the degree of flow three-dimensionality associated with the wake transition from mode A to mode B). By removing the viscous drag from the total drag, it is seen in Fig. 10 that the pressure drag displays a better inverse correlation with L_r over both $Re \lesssim 190$ and $Re \gtrsim 1500$.

Fig. 10. The total drag and pressure drag coefficients for flow past a circular cylinder.

Fig. 11 shows the variations in the pressure coefficient along the cylinder surface for $Re = 400 - 3900$. It is seen that the low pressure region in the near wake affects not only the base point (i.e. $\theta = 180^\circ$) but also a significant portion of the cylinder surface ($\theta \sim 60 - 300^\circ$). Therefore, the pressure drag also displays an inverse correlation with L_r (Fig. 10).

Fig. 11. Variations of the pressure coefficient along the cylinder surface for $Re = 400 - 3900$.

4.2.4. The C_L' – Re relationship

The influence of the low pressure region on the C_L' value is investigated with the fluctuation component of the pressure field of $Re = 1000$ shown in Fig. 12. Fig. 12(a) is shown at the phase when C_L reaches a local maximum (denoted phase 0/4), while Fig. 12(b–d) are shown at 1/4, 2/4 and 3/4 vortex shedding period apart, respectively. The fluctuation component of the pressure field is calculated as the difference between the instantaneous and the time-averaged pressure fields. For example, Fig. 12(a) is the difference between Fig. 8(b) and Fig. 8(c). At phases 0/4 and 2/4 (i.e. local maximum and minimum of C_L , respectively), the alternate roll up of the Kármán vortices (e.g. Fig. 8a) results in the alternate development of low pressure regions at the two sides of the wake centreline (e.g. Fig. 8b). Since each low pressure region is asymmetric about the wake centreline, it induces pressure fluctuations at both sides of the wake centreline (Fig. 12a,c). As shown in Fig. 12(a,c), the pressure fluctuation in the near wake exerts its influence back to the cylinder surface. The opposite-signed fluctuations at the two sides of the wake centreline result in a net lift on the cylinder. At phases 0/4 and 2/4, the local peaks of the two low pressure regions are observed at $(x/D, y/D) \sim (1.54, \pm 0.39)$, and the pressure difference between the two peaks is 0.545. Based on a similar analysis for the case $Re = 300$, the two peaks are observed at $(x/D, y/D) \sim (0.97, \pm 0.39)$, and the pressure difference is 0.555. A comparison between $Re = 1000$ and 300 suggests that the C_L' value is mainly changed by the streamwise location of the low pressure regions, whereas the influence of the pressure difference is minor. In summary, the inverse correlation between C_L' and L_r stems from the generation of an increased net lift when the pressure fluctuation due to vortex formation takes place closer to the cylinder.

Fig. 12. Span- and phase-averaged fluctuation component of the pressure field for flow past a circular cylinder at $Re = 1000$. Panel (a) is shown at the phase when the lift coefficient reaches a local maximum, while panels (b) – (d) are shown at $1/4$, $2/4$ and $3/4$ vortex shedding period apart, respectively.

Over the range of $Re = 270 - 1500$, the C_L' value decreases significantly by 88% (Fig. 6c). Norberg (2003) termed this phenomenon as the “lift crisis”. In comparison, the $\overline{C_D}$ and $-C_{pb}$ values only decrease by 29% over this range of Re (Fig. 6b,d). The reason for the significant drop in C_L' is that the C_L' value is solely due to vortex formation and the associated development of the low pressure regions asymmetric about the wake centreline. With the increase in L_r and the downstream movement of the low pressure regions, the influence on C_L' may become extremely small. This physical mechanism has practical implications on the suppression of C_L' and the associated vortex-induced vibration, which can be achieved through directing the vortex formation away from the body, e.g. by using a splitter plate in the wake.

In contrast, the $\overline{C_D}$ and $-C_{pb}$ values are not solely due to vortex formation and the associated low pressure region. This is demonstrated by an additional case where the circular cylinder is attached with a splitter plate along the wake centreline to prevent vortex formation. The case was simulated at $Re = 190$, and it was tested that a splitter plate of at least $8D$ in length was required to suppress vortex shedding. The use of $Re = 190$ is because for the corresponding isolated cylinder case, this Re value is marginally prior to the wake transition to three-dimensionality, such that three-dimensionality and turbulence are ruled out in the comparison of the two cases.

Fig. 13 shows the pressure distributions around the cylinder for the cases with and without a splitter plate (i.e. without and with vortex shedding, respectively). A comparison of the two cases indicates that there remain large portions of the pressure drag and base suction unrelated to the vortex shedding. Therefore, the percentage decreases in the $\overline{C_D}$ and $-C_{pb}$ values due to the increase in L_r are much smaller than that for the CL' value.

Fig. 13. Variations of the pressure coefficient along the cylinder surface for $Re = 190$.

6. Conclusions

This study investigates numerically the canonical case of flow past a circular cylinder over $Re = 100 - 3900$. The case $Re = 3900$ was computed with two open-source codes, OpenFOAM and Nektar++, which are based on the conventional FVM and the high-order spectral/ hp element method, respectively. For the Nektar++ model, mesh convergence is demonstrated (perhaps for the first time) through a systematic mesh dependence study, which includes separate examinations of the spanwise domain length, spanwise resolution, and the x - y plane resolution. For the OpenFOAM model, the estimated computational cost for a mesh-independent simulation is approximately one million core hours. The tremendous computational cost is possibly the reason why mesh convergence is difficult to be demonstrated in the literature through conventional FVM, FEM and FDM approaches. In comparison, the Nektar++ approach is more computationally efficient. For a mesh-converged simulation, its computational cost is only a few percent of the estimated cost for the FVM-based OpenFOAM approach.

In order to generalise the computations to a range of $Re = 400 - 3900$, the requirement of the spanwise domain length is examined. The present numerical

results show that $L_z = 3D$ is adequate for $Re = 2500 - 3900$, while $L_z = 6D$ is recommended for $Re = 400 - 2000$. Over the entire range of Re investigated in this study, the present numerical results, including the wake recirculation length and the hydrodynamic forces and pressure on the cylinder, agree well with the experimental results reported in the literature.

With the availability of the present high-fidelity numerical data over $Re = 400 - 3900$, the physical mechanisms governing the L_r-Re , $C_{pb}-Re$, $\overline{C_D}-Re$ and $C_L'-Re$ relationships are explored. The variation of L_r with Re is investigated by quantifying the spanwise circulation entering the wake and the maximum shear stress in the near wake, where the former correlates inversely with L_r up to $Re \sim 1500$, while the latter correlates inversely with L_r over the entire range of Re investigated ($Re = 100 - 3900$). The variations of C_{pb} and the pressure drag with Re are investigated by quantifying the minimum pressure of the low pressure region in the near wake and its streamwise location, where both the minimum pressure and its streamwise location correlate with L_r over the entire range of Re investigated. The streamwise location of the transient low pressure regions also explains the variation of C_L' with Re . The reason for the phenomenon called “lift crisis” (Norberg, 2003), i.e. a significant decrease in C_L' over $Re = 270 - 1500$, is that the C_L' value is solely due to vortex formation and the associated development of the low pressure regions asymmetric about the wake centreline. In contrast, the $\overline{C_D}$ and C_{pb} values are not solely due to vortex formation and the associated low pressure region, such that the decreases in the $\overline{C_D}$ and C_{pb} values over the same range of Re are much smaller.

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Appendix A. Scalability of the parallel computations

Based on the reference cases 1 and 6 for $Re = 3900$, the scalability of the OpenFOAM and Nektar++ models was examined with parallel computations using different numbers of computer nodes. The test cases started from a checkpoint where the flow had become fully developed and ran for one hour of wall-clock time. In

addition to the computation of the flow, the drag and lift forces on the cylinder and the time-averaged and root-mean-square velocity and pressure fields (which are essential for the analysis) were also computed.

Fig. 14(a) summarises the speedup performances of the two cases on different numbers of computer nodes. With increasing computer nodes, both cases show increasing deviations from the ideal performance. This is mainly attributed to an increase in the workload on the Message Passing Interface (MPI) communication relative to the workload assigned to each processor (which reduces with increasing processors). For the Nektar++ case, the parallel computation involves decomposition of $72 \times 92 = 6624$ macro-elements, at least when the number of processors is larger than the number of Fourier modes (of 32, which is half of the Fourier planes). In comparison, for the OpenFOAM case the number of cells in the x - y plane is $377 \times 464 = 174,928$. Therefore, under the same number of computer nodes, the issue of MPI communication is likely less dominant in the OpenFOAM case than the Nektar++ case, such that the OpenFOAM case is less deviated from the ideal performance than the Nektar++ case. Fig. 14(b) shows the wall-clock time required for the computation of 1000 time units of flow evolution. In consideration of a feasible wall-clock time (e.g. within a month) and the speedup performance, the present OpenFOAM and Nektar++ cases were computed using 10 and 2 nodes, respectively (shown with filled symbols in Fig. 14).

Fig. 14. Scalability of the OpenFOAM and Nektar++ models for the case $Re = 3900$: (a) Speedup performances on different numbers of computer nodes, and (b) wall-clock time required for the computation of 1000 time units of flow evolution. The number of nodes selected for the present study is shown with filled symbols.

Data Availability Statement

Raw data were generated at the Pawsey Supercomputing Centre. Derived data supporting the findings of this study are available from the corresponding author upon

reasonable request.

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