A high-order CFD method using successive differentiation

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A B S T R A C T
There has been a growing interest in higher-order spatial discretization methods as they can potentially give higher resolution accuracy at lower computational cost for the Direct Numerical Simulation (DNS) of vortex-dominated flows. Many of the modern high-order schemes use more degrees-of-freedom (DOF) in each cell to achieve high-order accuracy. This paper formulates and demonstrates a high-order (up to 4th order) correction method by using successive differentiation method. Unlike the popular Discontinuous Galerkin method, the present approach does not increase the degrees-of-freedom in each cell, but instead adds higher-order correction terms through a successive differentiation. As a result, the existing code structure and solution procedure can be maintained, and the high-order correction terms can be modularized. Verification cases using simple grids against analytical solutions demonstrate that the developed 4th order scheme can provide up to 5th order accuracy. Validation studies illustrate significant reduction in grid requirements using the high-order scheme in resolving near-wall turbulence down to the Kolmogorov scale. The present high-order method adds 20–50% CPU overhead in solving 3D problems, and can be applied to an existing CFD solver with minimal modification.

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1. Introduction

There has been a growing interest in higher-order spatial discretization methods due to their potential for providing high accuracy at reasonable computational cost for DNS of vortex dominated flows [1–9]. As the truncation error of a high-order method decreases more rapidly than that of a lower-order method if the flow field is sufficiently smooth, a high-order scheme is more cost effective. Visbal and Gaitonde [3,4] developed a high-order spatial accuracy method (up to 6th-order accurate) in curvilinear grid (structured grid) by using implicit compact finite-difference schemes. Robustness is achieved through a low-pass Pade-type non-dispersive spatial filter that regularizes the solution in flow regions where the computational mesh is not sufficient to fully resolve the smallest scales.

It is observed that almost all production unstructured CFD codes, such as USM3D, Loci/CHEM, and Fun3D, and commercial CFD codes, such Fluent, and CFD-ACE, all provide no better than 2nd order spatial accuracy. Unlike structured grid procedures where there is an implied structured connectivity between neighboring grid points, for unstructured grids it is more difficult to compute higher derivatives due to a lack of explicit connectivity beyond the first neighboring cells. This is true even for the regular Cartesian type of grid.
Recently there has been a great interest and activities in high-order scheme development for unstructured grids using variants of the Discontinuous Galerkin (DG) method [5–11]. In the DG method, one introduces extra degrees-of-freedom in each cell, as shown in Fig. 1 to fit a high-order polynomial to the solution within a given cell. In a sense, “structured” connectivity is recovered within each cell in the DG method. An excellent review for unstructured grid-based high-order schemes can be found in Wang [2]. Even with these advancements of high-order methods, the development of a new production code to take advantage of these new high-order schemes would be very expensive, considering the required implementation, verification and validation efforts.

This paper formulates a new high-order correction scheme that utilizes a successive differentiation approach. The goal is to find an alternative technique to improve spatial accuracy of the existing CFD solver without major modification. In this method, there is no increase in DOF within each cell, and the connectivity requirement is only the first neighbor points. Unlike the least squares method, which involves a large amount of extra storage [12,13], the higher-order accuracy in the current approach is achieved by adding higher-order correction terms. The present technique is innovative in that it can achieve high-order accuracy without using excessive storage. It can make use of either central or upwind schemes. More importantly, its implementation requires only minor modifications to an existing code making high resolution simulations possible for production problems.

We will take a building block approach. In the following, the high-order scheme using the successive differentiation approach will be first derived and verified for one-dimensional (1D) and three-dimensional (3D) regular Cartesian grid problems. A benchmark problem of turbulent flow over a cylinder employing a curvilinear grid will be used for the validation and demonstration of the high-order accuracy.

2. High-order formulation

To demonstrate the high-order scheme, we will start with problems in 1D.

2.1. Derivation of one dimensional high-order schemes

Let us consider the problem of 1D scalar advection:

\[
\frac{\partial f}{\partial t} + \frac{\partial uf}{\partial x} = 0
\]  \hspace{1cm} (2.1)

where \( u \) is the velocity and \( f \) is a scalar quantity. Integrating Eq. (2.1) over a control volume (number 2) and using Gauss’ theorem as shown in Fig. 2, one has:

\[
\frac{\partial f}{\partial t} V + (uf)_e A_e - (uf)_w A_w = 0
\]  \hspace{1cm} (2.2)
With known values at cell centers 1, 2 and 3, the task is to evaluate the value at cell faces, \( w \) and \( e \). Let us apply the following Taylor series expansions:

\[
\begin{align*}
    f_{w+}^2 &= f_1 + f_1'(x_w - x_1) + \frac{1}{2!} f_1''(x_w - x_1)^2 + \frac{1}{3!} f_1'''(x_w - x_1)^3 + O((x_w - x_1)^4) \\
    f_{w+}^2 &= f_2 + f_2'(x_w - x_2) + \frac{1}{2!} f_2''(x_w - x_2)^2 + \frac{1}{3!} f_2'''(x_w - x_2)^3 + O((x_w - x_2)^4)
\end{align*}
\]

(2.3)

(2.4)

If we first consider a uniform mesh, then we have \( h = (x_w - x_1) = -(x_w - x_2) \), and:

\[
\begin{align*}
    f_{w+}^2 &= f_1 + f_1' h + \frac{1}{2!} f_1'' h^2 + \frac{1}{3!} f_1''' h^3 + O(h^4) \\
    f_{w+}^2 &= f_2 - f_2' h + \frac{1}{2!} f_2'' h^2 - \frac{1}{3!} f_2''' h^3 + O(h^4)
\end{align*}
\]

(2.5)

(2.6)

Apparently, once we know the derivatives of a variable at the cell center, \( f' \), \( f'' \), and \( f''' \), we can potentially achieve high-order accuracy of the solution.

The next question is how to determine the derivatives at the cell centers. For a structured grid topology, it is possible to compute the high derivatives by using the known connectivity in the grid data structure. For the unstructured grid, one only knows the next neighbor points, and it is very difficult to compute the high derivatives. Our current approach is to use Gauss–Green theory, which states that:

\[
\int \nabla f dV = \oint f d\mathbf{A} \quad \text{or:} \quad \nabla f = \frac{1}{V} \sum f f \Delta \mathbf{n}
\]

(2.7)

Where \( A \) is the surface area and \( \mathbf{n} \) is the surface normal. Based on the above definition, the computed gradient of \( f \) is a volume-averaged value, rather than a local value as in typical 2nd-order approaches. For the 1D problem, the above expression leads to:

\[
f_2' = \left. \frac{\partial f}{\partial x} \right|_2 = \frac{1}{2h} (f_e - f_w) = \frac{1}{2h} \left[ \frac{1}{2} (f_3 + f_2) - \frac{1}{2} (f_2 + f_1) \right] = \frac{1}{4h} (f_3 - f_1)
\]

(2.8)

For unstructured grids, one can only compute the first derivative from the above formulation. We will compute the second derivative using the same procedure as:

\[
f_2'' = \left. \frac{\partial f'}{\partial x} \right|_2 = \frac{1}{2h} (f_e' - f_w') = \frac{1}{2h} \left[ \frac{1}{2} (f_3' + f_2') - \frac{1}{2} (f_2' + f_1') \right] = \frac{1}{4h} (f_3' - f_1')
\]

(2.9)

One observes that once the first derivative field is built, it is also possible to compute the field of the second derivative. The same is true for the third derivative:

\[
f_2''' = \left. \frac{\partial f''}{\partial x} \right|_2 = \frac{1}{2h} (f_e'' - f_w'') = \frac{1}{2h} \left[ \frac{1}{2} (f_3'' + f_2'') - \frac{1}{2} (f_2'' + f_1'') \right] = \frac{1}{4h} (f_3'' - f_1'')
\]

(2.10)

Interestingly, all of the derivative computations follow the same recipe, and can be used recursively. Indeed, by continuously applying Gauss–Green theory, one can potentially reach a high-order of accuracy.

2.2. Explicit expression for 1D problems

We can explicitly express the higher derivatives from the above procedure for 1D case:

1. 2nd order upwind (assuming velocity \( u \) is positive):

\[
f_{w+}^{2u} = f_1 + f_1' h = f_1 + \frac{1}{4h} (f_2 - f_0) h = f_1 + \frac{1}{4} (f_2 - f_0)
\]

(2.11)

2. 2nd order central (regardless of velocity sign)

\[
f_{w+}^{2c} = \frac{1}{2} \left( f_{w+}^{2u} + f_{w+}^{2d} \right) = \frac{1}{2} (f_1 + f_2) + \frac{1}{2} (f_1' h - f_2' h) = \frac{1}{2} (f_1 + f_2) + \frac{1}{8} (-f_0 + f_1 + f_2 - f)
\]

(2.12)
3. **3rd order upwind:** the third order scheme can be built by adding high-order correction terms to the 2nd order scheme:

\[
f^{3+}\! = \! f^{2+} \!+ \! \frac{1}{2!} f'' h^2 = f^{2+} \!+ \! \frac{1}{2!} \frac{1}{4h} (f''_2 - f''_0) h^2 = f^{2+} \!+ \! \frac{1}{32} (f_3 - 2f_1 + f_{-1})
\] (2.13)

4. **3rd order central:** again, we add a high-order correction term to the 2nd order central scheme:

\[
f^{3c}\! = \! f^{2c} \!+ \! \frac{1}{2!} \frac{1}{2} (f''_2 + f''_0) h^2 = f^{2c} \!+ \! \frac{1}{2!} \frac{1}{8h} (f''_2 - f''_0 + f''_3 - f''_1) h^2
\]

\[
= f^{2c} \!+ \! \frac{1}{64} (f_3 - 2f_1 + f_{-1} + f_4 - 2f_2 + f_0)
\] (2.14)

It is observed that using the above procedure, a larger stencil of grid cells can be linked in the computation. Fig. 3 shows the cells involved in computing higher derivatives for a triangular mesh. It should be noted that the connectivity for the high-order derivatives are built implicitly and our correction method will only add the high-order terms to the right-hand side. The current method does not change the implicit time integration but rather it takes the advantage of the iterative feature of solving nonlinear Navier–Stokes equations to reach high-order accuracy.

There are several merits of the present high-order schemes:

- Since there are no additional DOFs added to extend the scheme to higher orders of accuracy, existing code structure can be maintained. The technique is also applicable to any CFD code; and
- There is very small overhead. One only needs to add the high-order correction terms to extend to higher orders of accuracy.
2.3. Verification of high-order interpolation by hand

In order to verify that the above interpolation between cell and face centers indeed gives the designed order accuracy, an one dimensional problem is considered, with

\[ f = \sin(\pi x), \quad 0 < x < 2 \]  

(2.15)

The computational domain is first divided into 10, 20, 40 and 80 cells, and the interpolated face values are compared with the analytical solution as given in Table 1.

One notices that:

- The proposed high-order interpolation method to obtain the face value indeed gives the designed order of accuracy; and
- For the 3rd order central scheme, the accuracy can be as high as 4th order.

2.4. Implementation and verification in a CFD solver

The high-order scheme described above has been implemented in a coupled fluid-structure code, CoBi, developed at CFDRC. CoBi uses pressure-based unstructured grid topology. The general conservations of mass, momentum and energy are written as:

\[ \frac{\partial \rho f}{\partial t} + \frac{\partial (\rho u_j f)}{\partial x_j} = \frac{\partial}{\partial x_j} D f T f + S f, \]

(2.16)

with \( f = 1 \) for the continuity equation, \( f = u_i \) for the momentum equations, and \( f = T \) for the temperature equation. By integrating Eq. (2.16) over a control volume, one has:

\[ \int_V \frac{\partial \rho f}{\partial t} dV + \oint_A \rho u_j n_j f dA = \int_V D f T f n_j dA + \oint_V S f dV \]

(2.17)

It should be noted that in the high-order interpolation of Eq. (2.5):

\[ f = f_1 + f_1'(x - x_1) + \frac{1}{2!} f_1''(x - x_1)^2 \]

(2.18)

\( f_1 \) is a local value, not the volume-averaged value. However, in the simulation using control volume approach, all solution quantities are the volume-averaged values. To convert the local values from the volume-averaged values, one can integrate Eq. (2.18) over a control volume. This gives:

\[ f = f_1 + f_1' \bar{x}_1 + \frac{1}{2!} f_1'' \bar{x}_1^2 \]

(2.19)

where

\[ \bar{x}_1^2 = \frac{1}{V} \int (x - x_1)^2 dV; \quad \frac{1}{V} \int f dV = \bar{f}_1; \quad \bar{x}_1 = \frac{1}{V} \int (x - x_1) dV \]

(2.20)

Now, we have:

\[ f = \bar{f}_1 + f_1' [(x - x_1) - \bar{x}_1] + \frac{1}{2!} f_1'' [(x - x_1)^2 - \bar{x}_1^2] \]

(2.21)

We again use the 1D scalar transport equation as an example to verify the implementation. The 1D equation is the same as Eq. (2.1) with an initial condition given by Eq. (2.15). To ensure that the computed errors are dominated by the spatial...
discretization, the 4th order backward differentiation formula (BDF4) is used for temporal discretization of Eq. (2.17) with a CFL number of 0.5.

The results are shown in Fig. 4. One can see that:

• The conventional 2nd order scheme, either central or upwind, has the highest L2 error compared to the other schemes;
• The 3rd order upwind scheme exhibits its formal order-of-accuracy of 3rd order;
• The 3rd order central scheme has an observed order-of-accuracy of 4th order;
• The 4th order upwind scheme exhibits 4th order accuracy as expected; and
• The 4th order central scheme exhibits 5th order accuracy. This is not a surprise considering the regularity of the grid.

To ensure $10^{-3}$ L2 error, one only requires ten points when using the 4th order central scheme, while it will take 40 points using the 3rd order upwind scheme. This requirement is in contrast to the 80 points that would be required when using the 2nd order schemes. Thus, the savings in required cell count for the 4th order central scheme over the 2nd order schemes is a factor of 8 for this 1D problem.

2.5. Implementation in 2D and 3D

To extend the above high-order scheme to multiple dimensions, we can employ a 3D Taylor series expansion as follows:

$$f(x, y, z) = f(x_{\text{center}}, y_{\text{center}}, z_{\text{center}}) + \sum_{q=1}^{n} \frac{1}{q!} \left( \Delta x \frac{\partial f}{\partial x} + \Delta y \frac{\partial f}{\partial y} + \Delta z \frac{\partial f}{\partial z} \right)^q f$$

(2.22)

For the 4th order scheme, one can write the above expression in a compact form as:

$$f(x, y, z) = f_{\text{center}} + \Delta x_i \frac{\partial f}{\partial x_i} + \frac{1}{2} \Delta x_i \Delta x_j \frac{\partial^2 f}{\partial x_i \partial x_j} + \frac{1}{6} \Delta x_i \Delta x_j \Delta x_k \frac{\partial^3 f}{\partial x_i \partial x_j \partial x_k}$$

(2.23)

where $\Delta x_i = x_i - x_{i,\text{center}}$.

Now, the Gauss–Green theory will be applied to $f$, $\frac{\partial f}{\partial x_j}$, and $\frac{\partial^2 f}{\partial x_i \partial x_j}$.

Again, the key to extending the current high-order scheme to multiple dimensions is in recovering the cell-centered solution values from the cell averages. In multiple dimensions, Eq. (2.23) is written as:

$$f(x, y, z) = f_{\text{center}} + (\Delta x_i - \bar{x}_{i,\text{center}}) \frac{\partial f}{\partial x_i} + \frac{1}{2} (\Delta x_i \Delta x_j - \bar{x}_{ij,\text{center}}) \frac{\partial^2 f}{\partial x_i \partial x_j} + \frac{1}{6} (\Delta x_i \Delta x_j \Delta x_k - \bar{x}_{ijk,\text{center}}) \frac{\partial^3 f}{\partial x_i \partial x_j \partial x_k}$$

(2.24)

So, to evaluate Eq. (2.24), we need an efficient and accurate method for computing the cell moments shown below in Eq. (2.25).

$$\bar{x}_{i,\text{center}} = \frac{1}{V} \int (x_i - x_{i,\text{center}}) dV$$

$$\bar{x}_{ij,\text{center}} = \frac{1}{V} \int (x_i - x_{i,\text{center}})(x_j - x_{j,\text{center}}) dV$$

$$\bar{x}_{ijk,\text{center}} = \frac{1}{V} \int (x_i - x_{i,\text{center}})(x_j - x_{j,\text{center}})(x_k - x_{k,\text{center}}) dV$$

(2.25)
One common approach is to use Gauss’s theorem to convert the above volume integral into a surface integral:

$$\bar{x}_{ij,center} = \bar{y}^{m} = \frac{1}{V} \int \frac{1}{n+1} (x - x_{center})^{n+1} (y - y_{center})^{m} n_{x} dA$$  (2.26)

In the above expression, \(x\) and \(y\) can be switched. Thus, it is the same as a regular Gaussian gradient, except we only use the \(x\) component [12]. The function is:

$$\frac{1}{n+1} (x - x_{center})^{n+1} (y - y_{center})^{m}$$  \(2.27\)

The numerical flux in Eq. (2.17) can now be written as:

$$\int_{A} \rho u_{i} n_{j} f dA = \sum_{i=1}^{N} (\rho u_{i} n_{j} A_{i}) \frac{\int f(x, y, z) dA_{i}}{A_{i}} = \sum_{i=1}^{N} C_{i} \frac{\int f(x, y, z) dA_{i}}{A_{i}}$$  (2.28)

In Eq. (2.28), \(i\) is for each surface enclosing the control volume, \(C\) is the averaged connective mass flux over the surface, and \(N\) is the total number of the surfaces. As \(f\) is a high-order polynomial, the surface integral will be conducted using an \(n\)-point Gaussian quadrature rule such that the integration of a function becomes a weighted sum of the function value at specified points within the domain of integration.

### 2.6. Verification in 3D

The high-order schemes (3rd and 4th order upwind and central schemes) developed above have been extended and verified for 3D problems. The 3D scalar advection under consideration can be written as:

$$\frac{\partial f}{\partial t} + \frac{\partial f}{\partial x} + \frac{\partial f}{\partial y} + \frac{\partial f}{\partial z} = 0; \quad 0 \leq x \leq 2; \quad 0 \leq y \leq 2; \quad 0 \leq z \leq 2.$$  (2.29)

The initial condition is shown Fig. 5 with \(16 \times 16 \times 16\) hexahedral cells, and has a functional form of:

$$f = \sin \pi (x + y + z)$$  (2.30)

Periodic boundary conditions in the \(x\), \(y\) and \(z\) directions are imposed. The simulation errors are computed after 0.1 s.

The comparison of error convergence with number of cells is plotted in Fig. 6. The equivalent cell size is represented by the cube root of the total degrees-of-freedom (DOFs). For the hexahedral grid, the present 2nd order central and upwind schemes all show a 2nd order convergence rate. The 3rd order upwind scheme has lower error than the 2nd order schemes and shows a 3rd order convergence rate. The 4th order upwind and the 3rd order central schemes all display the 4th order convergence. The 4th order central has the lowest error with a 5th order convergence rate.

Previous studies have found that for a good grid resolution using 2nd order scheme, 16 points per wavelength will be necessary. As illustrated by the dotted line in Fig. 6, one needs only 6 points per wavelength using the 5th order central scheme to achieve the same L2 error. The saving in the total cell number is a factor of 19 for this 3D problem. Table 2 lists the equivalent cell numbers per wavelength for different high-order schemes and the saving in the total cell accounts.
Fig. 6. Solution error convergence for 3D sinusoidal wave using 2nd, 3rd and 4th order upwind and central schemes for hexahedral cells.

Table 2
Equivalent points per wavelength and total saving for the same L2 error.

<table>
<thead>
<tr>
<th>Schemes</th>
<th>2nd Order Upwind</th>
<th>3rd Order Upwind</th>
<th>3rd Order Central</th>
<th>4th Order Upwind</th>
<th>4th Order Central</th>
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</tbody>
</table>

3. Verification for Navier–Stokes equations

3.1. 2D vortex transport problem

Now we can turn to the verification of the high-order schemes for Navier–Stokes equations. We will use the transport of a vortex in an incompressible fluid as the test as there is a well-known analytical solution available. The ability to conserve the vortex shape and strength is important in many cases in which a shed vortex interacts with bodies well downstream of the vortex origin. The present inviscid vortex transport study will examine the relative dissipation and dispersion errors for different schemes. The computational domain has a size of \((x, y) = (0, L_x)(0, L_y)\). The initial velocity field is given as:

\[
\begin{align*}
  u &= u_\infty - \beta u_\infty \frac{y - y_c}{R} \exp\left(-\frac{r^2}{2}\right) \\
  v &= v_\infty + \beta u_\infty \frac{x - x_c}{R} \exp\left(-\frac{r^2}{2}\right) \\
  r &= \sqrt{(x - x_c)^2 + (y - y_c)^2}/R \\
  \beta &= 1/50 \\
  x_c &= 0.05 \\
  y_c &= 0.05 \\
  u_\infty &= 0.05 \\
  v_\infty &= 0 \\
  L_x &= L_y = 0.1
\end{align*}
\]  

(3.1)

\(x_c\) and \(y_c\) are cell center coordinates. If the computational domain extends to infinity, the exact solution with the above initial condition will be the passive convection of the vortex with the mean velocity of \(u = 0.05\). In this study, the computational domain is taken as \([0, 0.1] \times [0, 0.1]\), with periodic boundaries in both directions. The 4th order BDF4 scheme is used with a CFL number of 0.5 for the 128 \(\times\) 128 quadrilateral grid.
To study the spatial accuracy of different schemes, a series of increasingly fine grids from $16 \times 16$, $32 \times 32$, $64 \times 64$ to $128 \times 128$, are employed. Fig. 7 shows the error convergence rate for the 2nd, 3rd and 4th order schemes. It is observed that the 3rd order accuracy has been recovered by the 3rd order upwind scheme, and 4th order accuracy has been recovered by the 3rd order central scheme. The present 4th order upwind shows 4th order convergence and the 4th order central gives a fifth order error convergence. In general, the accuracy of the 3rd and 4th order schemes is far superior to that of the 2nd order schemes, with significantly reduced dissipation and dispersion errors. Using the 4th order scheme with $45 \times 45$ cells results in an error that is comparable to the 2nd order schemes with $192 \times 192$ cells.

A difficult test for a spatial scheme is to let the vortex travel for a long period. A comparison showing the horizontal velocity component after 50 cycles for various spatial schemes is given in Fig. 8. For the 2nd order scheme, the original vortex has split into multiple vortices. There is some twist to the vortex component for the 3rd order upwind scheme, but the 3rd order central scheme gives excellent results. These findings are confirmed in Fig. 9 where the $u$ component distribution along the vertical direction is displayed.

### 3.2. 3D Taylor–Green vortex transition to turbulence

The spatial and temporal evolution of the incompressible, Taylor–Green vortex flow in a three-dimensional periodic domain is a good model to investigate the accuracy of high-order schemes. The problem involves the nonlinear transfer of kinetic energy among eddies with a range of spatial scales. When the flow has a finite Reynolds number, the kinetic energy generated by velocity shear is dissipated by the smallest scales, which provides a simple model for the development of a turbulent flow and the cascade of energy from larger to smaller scales. The Taylor–Green vortex is a fundamental case
that has been traditionally used as a prototype for vortex stretching and consequent production of small scale eddies, to investigate the basic dynamics of transition to turbulence based on DNS [14].

3.2.1. Computational model

The Taylor–Green vortex configuration considered here involves triple-periodic boundary conditions enforced on a cubic domain with box side length of $2\pi$. The initial condition is smooth and consists of a first-degree trigonometric polynomial in all three directions as:

\[
\begin{align*}
  u &= \cos(x) \sin(y) \sin(z) e^{-2\nu t}, \\
  v &= -\sin(x) \cos(y) \sin(z) e^{-2\nu t}, \\
  w &= 0; \\
  p &= -\frac{1}{4} (\cos 2x + \cos(2y)) e^{-4\nu t}
\end{align*}
\] (3.2)
The pressure is given by a solution of the Poisson equation for the above given velocity field. Here the density is chosen to be 1.0 kg/m³. The initial condition is illustrated in Fig. 10. The surfaces are the iso-surfaces of vorticity. Enclosed within each surface are regions of positive or negative vorticity.

For a long-time duration, a numerical scheme should capture the behavior of the flow field accurately as long as possible. The second order temporal scheme and 2nd and 3rd order spatial schemes will be used to simulate the dynamic process of the vortex transition. The Reynolds number is 1600 for this flow and is defined as:

\[
\text{Re} = \frac{1}{\nu}
\]  

Our simulations were carried out for the space of \( \pi \) rather than standard 2\( \pi \). The grid resolution varies from \( 60^3 \) (0.25 M), \( 80^3 \) (0.5 M), \( 100^3 \) (1 M) to \( 160^3 \) (4 M).

The evolution in time of the kinetic energy dissipation \( -dK/dt \), where \( K = \langle \frac{1}{2} v^2 \rangle \), with \( \langle \rangle \) denoting mean volume average is shown in Fig. 11 for the 2nd and 3rd order spatial central schemes. It is observed that for the 2nd order central, the accuracy improves with an increase in grid resolution from 0.25 M to 1 M and eventually to 4 M. On the other hand, for the 3rd order central scheme, the solution using 0.25 M cells is as good as that obtained using 1 M cells with the traditional 2nd order scheme. One can also observe that when using 1 M cells, the solution from the 3rd order scheme is comparable to that obtained when using 4 M cells with the 2nd order scheme.

To illustrate the impact of spatial schemes, Fig. 12 gives the iso-Q surface at \( t = 20 \) dimensionless time. It is clear that the 3rd order scheme produces finer vortical structures.
4. Validation: flow past a circular cylinder at Reynolds number 3900

Flow over cylinders has been studied extensively, both numerically and experimentally, in order to gain a better understanding of steady and unsteady flows at various Reynolds numbers. Excellent reviews have been given by Beaudan and Moin [15], Kravchenko and Moin [16], and Ma et al. [17]. Studies of the flow phenomena in the cylinder wake are conducted for many reasons, from direct application in industrial process to validation of numerical schemes. Based on Beaudan and Moin [15], at Reynolds numbers less than about 40, the flow is steady, laminar and symmetrical. Between 40 and 150 the flow remains laminar and is associated with a regular vortex shedding frequency, which increases with Reynolds number. At approximately 180 the flow becomes three-dimensional in the near wake. Between 300 and $2 \times 10^5$ the flow around the surface of the cylinder is laminar, and there is a transition to turbulence in the separated free shear layers. The range between 300 and $2 \times 10^5$ is known as the subcritical range. For lower Reynolds numbers in this range, the wake is fully turbulent 30 to 40 diameters downstream of the cylinder, and for the higher Reynolds numbers, the wake is fully turbulent close to the rear of the cylinder. Reynolds numbers between $2 \times 10^5$ and $3.5 \times 10^6$ are classified as the critical range.

The flow past circular cylinders at a subcritical Reynolds number of 3900 is the subject of this study. The flow in this subcritical range features several interesting phenomena, including a laminar boundary layer with unsteady separations and reattachments; flow reversals at the cylinder surface and in the near wake; adverse pressure gradients; transitioning free shear layers; and a turbulent wake with random and periodic Reynolds stresses [15]. The cases have been used to validate LES models by numerous researchers [15–23]. There are data from two separate experiments, which provide measurements of the velocity and Reynolds stresses in the cylinder wake. Lourenco and Shih [18] performed Particle Image Velocimetry (PIV) measurements to obtain mean and phase-averaged data within three diameters downstream, and Ong and Wallace [19] made single sensor measurements of mean velocities and Reynolds stresses in the wake between the closure point of the recirculation bubble and ten diameters aft of the cylinder. The rich physics of the flow and a large amount of experimental data make it an ideal test case for the validation of high-order numerical schemes. Results from the traditional 2nd order schemes and the present 3rd order schemes under development will be presented and compared to the experimental data of Ong and Wallace [19], and Lourenco and Shih [18] to demonstrate the improved accuracy of high-order schemes and their importance for efficiently resolving complex flows.

4.1. Simulation model

The mesh used for the simulations is shown in Fig. 13 and contains 3.4 million hexahedral cells. It has more cells than those used in the LES study of Kravchenko and Moin [15] (1.3 M), but fewer cells than those used by Young and Ooi [23] (4.3 M). The mesh consists of 300 points in the circumferential direction, and hyperbolic tangent expansion is used in the radial direction away from the cylinder. The smallest cell spacing in the radial direction is $\Delta r_{\text{min}}/D = 1.25 \times 10^{-3}$. This spacing is the same as what Beaudan and Moin [15] used for their finest mesh. The spanwise extent of the domain is chosen to be $L_z/D = \pi$ in accordance with many previous studies [15,17,21]. Ma et al. [17] varied the spanwise extent as $L_z/D = \pi/2$, $3\pi/2$, and $2\pi$ and found no significant improvement in results beyond $L_z/D = \pi$, provided the resolution remained the same [17]. The domain extends 9D in the vertical (or cross-flow) direction, 7D in the inflow, and 20D in the outflow. In accordance with Beaudan and Moin [15], Mittal and Moin [21] and Kravchenko and Moin [16], 48 grid points are used in the spanwise direction.

The inflow condition is specified to be equal to the freestream velocity. The outflow condition is specified to change the velocity between the freestream value and zero gradients depending on its direction to allow for free recirculation at the boundary. The pressure at the outflow is specified as the freestream value. The front and back faces of the mesh in the
spanwise direction are given a periodic boundary condition, and the top and bottom surfaces are specified as symmetry boundaries. A non-slip condition is applied to the cylindrical wall.

The 3rd-order implicit time-accurate backward Euler method is used for time discretization, with a non-dimensional time step of 0.2. The simulations are first allowed to reach a statistically steady-state before any data is collected. The data are then averaged in time for statistics.

It should be pointed out that the high-order DG schemes are compact and hold multiple degrees-of-freedom (DOF) per element. As a consequence, meshes for use with compact high-order schemes are typically far coarser than those for use with low-order schemes (for an equivalent total number of DOF) [24]. The requirement of relatively large elements and the existence of multiple DOF per element lead to the need for the use of elements with curved surfaces. The purpose is to ensure that a coarse mesh can conform to (or at least reasonably approximate) complex boundaries. In comparison, the current approach uses the existing low order grid without coarsening, and hence has less sensitivity to the curved boundary requirement.

4.2. General flow features

The instantaneous streamwise, transverse and spanwise velocities in the wake of a circular cylinder obtained by the 3rd-order central scheme are shown in Fig. 14. The negative streamwise velocity next to cylinder wall shows the unsteady recirculation zone. For the transverse velocity (shown in Fig. 14b), the alternating positive and negative regions along the streamline direction correspond to the von Karman vortices. The flow becomes turbulent and three-dimensional as evident in the presence of both the small and large-scale structures in Fig. 14. The vorticity contours in Fig. 15 indicates that the flow structures increase in size with increasing streamwise distance and there are noticeable small scale structures even far away from the cylinder.

The 3D instantaneous Q iso-surfaces presented in Fig. 16 show a more comprehensive picture of the flow structures. The shear layer from the cylinder surface starts to break down into three dimensional vortices and the flow near the trailing edge of the cylinder is essentially turbulent. In the wake of the cylinder, the composition of the small-scale von Karman vortices is visible.

4.3. Comparison with experimental data

Next, we present results from CFD runs with the following schemes: 2nd order upwind, 2nd order central, 3rd order upwind, and 3rd order central. The comparisons will be made with experimental measurements of streamwise velocity and its r.m.s. at different locations along the streamwise direction. The streamwise data are significantly more reliable than the cross-flow velocity measurements [17]. For example, the experimental uncertainty in the measurements of the streamwise velocity is about 5% while for the cross-flow velocity it is more than 50% according to Beaudan and Moin [15]. As there are no established means by which to define the different regions in the cylinder wake, the convention adopted by Ma et al. [17] will be employed. Here, the near wake, defined as less than ten diameters aft of the cylinder (i.e. $x/D < 10$), is subdivided into the very near wake ($x/D < 3$) where the dynamics of the shear layer dominate, and the near wake ($3 < x/D < 10$).

PIV experimental data for $x/D < 3$ at $Re = 3900$ had been obtained by Lourenco and Shih and were published in Beaudan and Moin [15]. Fig. 17 shows the mean streamwise velocity predictions using several different 2nd order and 3rd order schemes at $x/D = 1.06$. One sees that very good agreement is obtained for the 3rd order central scheme. The central schemes do better than the upwind schemes. Both central schemes compare well with the V-shaped profile of the data. But the U-shaped and W-shaped profiles of the upwind scheme are not consistent with the data. In particular, a pronounced feature of the 2nd and 3rd order central schemes is the V-shaped velocity profile at $x/D = 1.06$ in contrast with the U-shaped (flat) profile of the 2nd and 3rd order upwind schemes. The U-shaped velocity profile was obtained in the LES studies of Moin and co-workers [15,16,21], while the V-shaped profile was obtained by Ma et al. in the DNS study [17]. In general, the agreement improves as the order of the scheme increases from 2nd to 3rd.
To investigate the results from different schemes, the r.m.s. values of streamwise velocity are displayed in Fig. 18. As one can see, the velocity fluctuations from the 2nd order upwind scheme are very small compared to the experimental data. The 3rd order upwind scheme exhibits larger fluctuations than the 2nd order upwind scheme, but they are still much smaller than those observed in the measured data. Previously, Mittal and Moin [21] reported that nondissipative finite-difference calculations were able to match the experimental data much better than the simulations of Beaudan and Moin [15] using upwind biased schemes. That is indeed the case observed here as well. The 2nd and 3rd order central schemes match with experimental data better than their upwind counterparts both in terms of mean velocity and r.m.s. values. Fig. 19(a) and Fig. 19(b) show the Q iso-surfaces for the 2nd and 3rd order upwind schemes. In comparison to the 3rd order central scheme results shown in Fig. 16, it is clear the numerical dissipation of the upwind-biased schemes, both 2nd and 3rd order alike tends to suppress the medium to small scale vortices in the cylinder wake. Due to the numerical dissipation, the flow features are similar to those at lower Reynolds numbers. To demonstrate this effect, the Q iso-surfaces, computed using the 3rd order central scheme at a lower Reynolds number of 1000, are given in Fig. 19(c). One can see that at Re = 3900, the upwind based schemes give the similar sizes of flow features as those from 3rd order central scheme at a lower Reynolds number of 1000.

Even with the inherent numerical dissipation, one observes from Fig. 18 that the 3rd order upwind scheme has less dissipation and shows larger velocity fluctuations and better agreement than the 2nd order upwind scheme. On the other hand, the 3rd order central scheme shows very good agreement with the measurements. Even though the 2nd order central scheme has some overshoot in the velocity fluctuations, the higher velocity fluctuations of the central schemes leads to
Fig. 17. Streamwise velocity comparison at $x/D = 1.06$ for different spatial schemes.

Fig. 18. r.m.s. streamwise velocity comparison at $x/D = 1.06$ for different spatial schemes.

better flow mixing locally, which promotes the corresponding V-shape of the velocity profile computed from the central schemes.

The comparison at another location of $x/D = 1.54$ is given in Fig. 20 for the mean velocity, and in Fig. 21 for the r.m.s. values. Again, results for the 3rd order central scheme agree very well with the experiment. Due to the dissipation present in the upwind schemes, a U-shaped velocity profile is observed.

To further prove the accuracy of the current simulations, Figs. 22 and 23 show a comparison with DNS of Ma et al. [17] and experiment data for streamwise mean and r.m.s. values. One can see that the agreements with other DNS solution are very good at all locations.

It is to be pointed out that throughout the simulations, we find that the present high-order method adds 20–50% CPU overhead in solving this 3D problem.

5. Conclusion

A novel high-order CFD scheme using successive differentiation has been presented in this paper. The present method does not introduce any extra degree-of-freedom in each grid cell. Instead, the high-order accuracy is achieved by using Taylor series expansions, and by finding high-order derivatives as a function of lower order ones. This approach adds 20–50% overhead in CPU time and can be implemented into an existing production CFD code. Several verification problems for regular grids prove that the scheme can achieve the designed accuracy. Application to turbulence transition problems shows that the high-order scheme can capture and resolve the detailed small flow scales while the traditional 2nd order schemes fail to do so.
Fig. 19. Iso-surfaces for 2nd and 3rd order upwind schemes at $Re = 3900$ and 3rd order central scheme at $Re = 1000$.

Fig. 20. Streamwise velocity comparison at $x/D = 1.54$ for different spatial schemes.
Fig. 21. r.m.s. streamwise velocity comparison at $x/D = 1.54$ for different spatial schemes.

Fig. 22. DNS mean streamwise velocity comparison at $x/D = 1.06, 1.54, 2.02$.

Fig. 23. DNS r.m.s. streamwise velocity comparison at $x/D = 1.06, 1.54, 2.02$. 
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References


