

DEALIASING STRATEGY FOR HIGHER-ORDER METHODS IN TURBULENT FLOW SIMULATIONS

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Abstract

Higher-order schemes have been proved to be very efficient in solving turbulent flows. A Compact fourth-order finite volume method was shown to be 10X faster than the second-order scheme. Recently, the author proposed a new discretization called Finite Surface Method (FSM). A sixth-order approximation of FSM was found to be 2.7X faster than the fourth-order FVM. However, FSM needs to dealias the convection term by means of low-pass filter. The low-pass filter used in the original work was sub-optimal. Therefore the 2.7X factor can be improved. In this work, we investigate several choices of the dealiasing strategy with the combination of different low-pass filters, namely i.) double six-order compact filter, ii.) double fourth-order compact filter, iii.) the mixed-order 6-4 compact filter and iv.) direct sixth-order compact filter. First, we introduce the aliasing error in the convection term and analyse its consequent and the intermingle role with the local truncation error in the Fourier space. After that we present a model spectrum which is used to evaluate the selected filters. We rule that the mixed-order is not as good as the other two filters, when they are at their best. Nonetheless, the mixed-order works satisfactory in every situation. Finally, we perform a careful grid independent study of a turbulent channel flow at Reynolds number = 5,600 from 323 grid to 1283 grid. The results from the turbulent simulations agree well with the analysis. The fourth-order filter work very well at underresolved regime while the convergence ceases after 803 grid. The sixth-order works very well on fine grid, but it cannot eliminate the aliasing error at the underresolved resolution. Overall, for a 1%-level error, the fourth-order filter improves the performance of the FSM to 73X faster than the second-order scheme.

Keywords: Finite volume method, turbulent flow, finite surface method, direct numerical simulation, Navier-Stokes equations, higher order method

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Introduction

Finite Volume Method (FVM) and Finite Difference Method (FDM) have been important tools for turbulence research. In the past three decades, numerous higher-order methods have been developed (Lele, 1992; Kobayashi, 1999; Moser *et al.*, 1999; Hokpunna and Manhart, 2009; Knikker, 2009; Sun *et al.*, 2016). Despite having significant higher cost, they outperformed the low-order methods in both accuracy and performance in three-dimensional problems. The main reason is because higher-order methods require a smaller number of grid points and this reduction is a quartic function (including time-step) while the cost function is a linear one. These advantages are well observed in convection and diffusion problems. Early applications of higher-order scheme to the incompressible Navier-Stokes equations (NSE) often improved the approximation of the convection and diffusion terms, but kept the approximation of pressure and the Poisson equation to second order. This was partly due to the pressure can be viewed as a Lagrange multiplier and thus it should not affect the accuracy of the momentum. Another reason is because higher-order treatment of the pressure is difficult. The new discrete Laplacians are wide and no efficient solver was known at the time. Later it was shown that the n -th order NSE solver must be used with the n -th order pressure treatment. This higher-order treatment of the pressure demands more computing power than the momentum equation.

Recently, the author proposed a new discretization called “Finite-Surface Discretization” (Hokpunna, 2019). A recent finding (Hokpunna *et al.*, submitted) indicates that this new type of discretization, coupled with sixth-order scheme can be much more accurate than the fourth-order finite volume method in Hokpunna and Manhart (2009). In that work, it is reported that the sixth-order FSM is 27X faster than, at the same accuracy level. However, it is noted that the performance can still be improved if aliasing error is managed in an optimal way. The aliasing error in Navier-Stokes equations stems from the

nonlinearity in the convection term where the convection process can generate high frequency structure beyond the Nyquist limit of the grid. These unresolved waves are perceived by the grid as a lower wave component with modulo N . This aliasing violates the energy conservation and could destabilize the numerical simulation. When the numerical simulation properly manages the aliasing error, a more accurate results can be obtained on coarse grids. The key difficulty, however, lies in the selection and management of the dealiasing process.

In this paper we investigate the effects of 3 different filters on the accuracy of the turbulent channel flow simulations. First, we present the basic concept of Finite Surface Method and then we discuss the aliasing error strategy and its effects on the flow accuracy and turbulent structures.

Finite Surface Discretization of Navier-Stokes equations Materials and Methods

The integral form of the incompressible Navier-Stokes equations for incompressible Newtonian fluid can be written as

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

$$\frac{\partial}{\partial t} \int_{\Omega} u \, d\Omega + \oint_A (u \cdot n) u \, dA = \nu \oint_A T \, dA - \frac{1}{\rho} \oint_A p I \cdot n \, dA \quad (2)$$

Here, the variables and notations are velocity vector: u , pressure: p , strain rate tensor: T , identity matrix: I , density: ρ and the kinematic viscosity: ν . The unit vector (n) of an infinitesimal area dA is pointing outwards of the volume Ω FSM discretizes the continuous domain to a discrete domain where the momentum variables are defined on the area normal to its direction while the pressure is defined as the averaged quantity over the cells (Figure 1). Such arrangement allows an exact

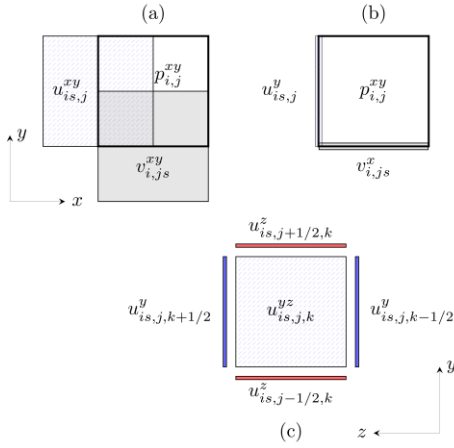


Figure 1. (a) Arrangement of flow variables on 2D staggered grids consisting of pressure (clear), u-momentum (dash) and v-momentum (gray) cells. (b) The finite surface discretization constricts the momentum control volumes on to the surfaces of the pressure cell. (c) The west-face momentum of 3D pressure cell and the edge momentums viewed from the right side of (b)

evaluation of mass imbalance over the pressure cell. This exact imbalance can be calculated easily and efficiently. It only costs 5 floating point operations (FP) while the standard sixth-order approximation of the divergence costs 35 FP. This advantage together with the reduction in the Poisson equation for the pressure enable the sixth-order FSM to be as fast as the fourth-order FVM, in term of computing time.

The special discretization of this method requires a special integral form of Equations (1) and (2) and the discrete form of the NSE under finite-surface method is displayed in Figure 2. The square brackets represent the average and its superscript is the plane of averaging. Note that the indices ijk indicates the center of the pressure cells. The staggered indices e.g. js is the midpoint between the j and $j+1$. Please note that the position of js and $js+1/2$ are the same. The finite surface method that will be investigated in this paper uses compact sixth-order schemes for convection and diffusion terms. The pressure term is

treated using the explicit fourth-order scheme. This fourth-order pressure treatment does not degrade the overall accuracy of the scheme. Further detail of the finite surface discretization can be found in Hokpunna (2019).

Aliasing Error in Convection Term Under Standard Finite Difference Method

During the solution process of NSE, numerical errors can come from different sources. In this work the main focus is the error in the convection term. Let us consider the standard conservative form of the convection term when the control volume in Equation (2) approaches zero:

$$\oint_A (u \cdot n) u dA = \frac{\partial u_i u_j}{\partial x_j} \quad (3)$$

The RHS of the above equation represents the physical convection process. The current form of this term is called divergence form in finite difference method and it can be written in different, but mathematically equivalent forms, such as:

$$\text{rotational form} \\ H_i = u_j \left(\frac{\partial u_i}{\partial x_i} - \frac{\partial u_j}{\partial x_j} \right) \quad (4)$$

$$\begin{aligned} [div]_{i,j,k}^{xyz} \Delta x_i \Delta y_j \Delta z_k &= \left([u]_{i+\frac{1}{2},j,k}^{yz} - [u]_{i-\frac{1}{2},j,k}^{yz} \right) \Delta y_j \Delta z_k \\ &+ \left([v]_{i,j+\frac{1}{2},k}^{xz} - [v]_{i,j-\frac{1}{2},k}^{xz} \right) \Delta x_i \Delta z_k \\ &+ \left([w]_{i,j,k+\frac{1}{2}}^{xy} - [w]_{i,j,k-\frac{1}{2}}^{xy} \right) \Delta x_i \Delta y_j \\ A_{j,k} \frac{\partial [u]_{i,j,k}^{yz}}{\partial t} &= -C_{is,j,k} + \nu D_{is,j,k} - \frac{1}{\rho} P_{is,j,k} \\ C_{is,j,k} &= \left[\frac{\partial u}{\partial x} \right]_{is,j,k}^{yz} \Delta y_j \Delta z_k + \left([v]_{i,j+\frac{1}{2},k}^{yz} - [v]_{i,j-\frac{1}{2},k}^{yz} \right) \Delta z_k \\ &+ \left([w]_{i,j,k+\frac{1}{2}}^{yz} - [w]_{i,j,k-\frac{1}{2}}^{yz} \right) \Delta y_j, \\ D_{is,j,k} &= \left[\frac{\partial^2 u}{\partial x^2} \right]_{is,j,k}^{yz} \Delta y_j \Delta z_k + \left(\left[\frac{\partial u}{\partial y} \right]_{i,j+\frac{1}{2},k}^{yz} - \left[\frac{\partial u}{\partial y} \right]_{i,j-\frac{1}{2},k}^{yz} \right) \Delta z_k \\ &+ \left(\left[\frac{\partial u}{\partial z} \right]_{i,j,k+\frac{1}{2}}^{yz} - \left[\frac{\partial u}{\partial z} \right]_{i,j,k-\frac{1}{2}}^{yz} \right) \Delta y_j \end{aligned}$$

Figure 2. Discrete Navier-Stokes equation of FSM

convective form

$$H_i = u_j \frac{\partial u_i}{\partial x_j} \quad (5)$$

skew symmetric form

$$H_i = \frac{1}{2} \left(\frac{\partial u_i u_j}{\partial x_j} + u_j \frac{\partial u_i}{\partial x_j} \right) \quad (6)$$

The forms in Equations (5)-(7) make use of the continuity equation $\partial u_i / \partial x_i = 0$. They have been used extensively in finite difference method. There are two main errors associated with the approximation of convective terms: the local truncation error and the aliasing error. The local truncation errors (LTE) manifest itself in dispersive and dissipative errors which can be analyzed using Fourier analysis. The aliasing errors requires the analysis of the nonlinear term. First let us take a look at the effects of the numerical approximation on the derivative under the Fourier space. Let $\delta u / \delta x$ be a numerical approximation of the first derivative ($\partial u / \partial x$):

$$\frac{\delta u}{\delta x} = \frac{\partial u}{\partial x} + LTE \quad (7)$$

Assuming that the approximation is symmetry, the dissipation error is zero and the error in Equation (7) would only appear as the dispersive error which is the retardant in the modified wave number function $k^*(k)$. in the Fourier space:

$$\frac{\delta u}{\delta x} = Ik^*(k)\hat{u}, \quad (8)$$

instead the actual wave number k (I is the imaginary number). Some examples of the modified wave number is displayed in Figure 3. In the linear convection, this modified wave number indicate how fast the wave would travel. The closer the modified wave number follow the exact curve, the more accurate the scheme. At high wave number, the modified wave numbers usually drop and the wave will be convected slower than it should. The sixth-order scheme provide a substantial improvement over the compact fourth-order scheme. However, as the accuracy at the far end of the spectrum increases, the aliasing error become increasingly problematic. Let follows the definition used by Kravchenko and Moin

Hokpunna *et al.* (submitted) and consider the convection of two velocity u and v whose Fourier expansions read:

$$u = \sum_{n=-N/2}^{N/2-1} \hat{u}_n e^{Ik(2\pi/N)} \quad (9a)$$

and

$$v = \sum_{m=-N/2}^{N/2-1} \hat{v}_m e^{Ik(2\pi/N)} \quad (9b)$$

The amplitude of the k -th wave component of the product of these two velocities ($w = uv$), written separately for the resolved and the non-resolved part is:

$$w_k = \sum_{n+m=k} \hat{u}_n \hat{v}_m + \sum_{n+m=k \pm N} \hat{u}_n \hat{v}_m \quad (10)$$

Thus, the multiplication creates structures finer than the original ones. These new fine structures are not resolvable by the grid and they alias back as lower wave component which have totally different effects on the flow field. It is consensus that the non-resolved components should be removed from the calculation. Otherwise, it must be made sure that this error is controlled such as through the filtering methods or the usage of conservative scheme. Thus when there are substantial amount of the high-wave component, the aliasing error can be larger than the local truncation error. In early days where we used low-order methods, the high-wave parts are multiplied by the modified wavenumber and the aliasing error is less severe. As the approximation method is improved, the

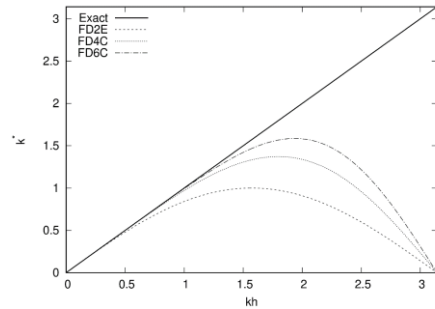


Figure 3. Modified wave number of some approxaition of the first derivative: classical second-order method (FD2E), compact fourth-order scheme (FD2C) and compact sixth-order scheme (FD6C)

aliasing errors become larger and it can be as important as the truncation error.

Aliasing Error in Finite Surface Method

In FSM, the convections of u_i in j -direction ($j \neq i$) are performed by finite volume method. In this direction, the FVM deconvolve the field using a process similar to interpolation which possesses an inherent filtering property. Therefore, the aliasing errors in this direction is less problematic. This is one of the reasons why dealiasing error is almost not discussed in the FVM. In i -direction, the convection is carried out by finite difference method and thus it is generally not conservative and the aliasing errors play an important part in this problem. The convective form of the convection under FSM in this direction reads:

$$\frac{\partial u_i u_i}{\partial x_i} = u_i \frac{\partial u_i}{\partial x_i} + u_i \frac{\partial u_i}{\partial x_i}. \quad (11)$$

In FDM, the second term on the RHS is usually ruled out as zero due to the incompressibility and yields Equation (4). However, since the other two directions in FSM does not provide these terms, thus FSM uses the following approximation for the convection in i -direction:

$$N_c = 2u_i \frac{\partial u_i}{\partial x_i} \approx \frac{\partial u_i u_i}{\partial x_i} = N, \quad (12)$$

which is the multiplication of a transported quantity (u_i) and the transporting derivative ($\partial u_i / \partial x_i$). The Fourier transform of the above equation reads:

$$\hat{N}_c(k) = 2 \sum_{n+m=k} (i \hat{u}_n k^*(m) \hat{v}_m) + 2 \sum_{n+m=k \pm N} (i \hat{u}_n k^*(m) \hat{v}_m) \quad (13)$$

Here one can see that the damping on the modified wave number is only applied to the derivative: $k^*(m)$. In order to reduce the aliasing errors, one can apply a filter to the transported u before commencing the multiplication in Equation (11), that is to compute the convection from:

$$\frac{\partial u_i u_i}{\partial x_i} \approx 2 \overline{u_i} \frac{\partial u_i}{\partial x_i}, \quad (14)$$

where the overline denotes a filter quantity. This leads to the following Fourier coefficients:

$$\hat{\bar{N}}_c(k) = 2 \sum_{n+m=k} (i \hat{\bar{u}}_n k^*(m) \hat{v}_m) + 2 \sum_{n+m=k \pm N} (\hat{\bar{u}}_n k^*(m) \hat{v}_m). \quad (15)$$

Here, the Fourier coefficient of the transported velocity is altered by the transfer function $T(n)$ of the filter i.e. $\hat{\bar{u}}_n = T(n) \hat{u}_n$. Substitute this relationship to Equation (15) and compute the error w.r.t. the Fourier coefficient of N in Equation (12), delivers

$$\hat{E}(k) = \hat{\bar{N}}_c(k) - \hat{N}(k) = \hat{E}_{LTE} + \hat{E}_{ali}, \quad (16)$$

$$\hat{E}_{LTE, n+m=k} = T(n) k^*(m) \quad \text{and} \quad \hat{E}_{ali, n+m=k \pm N} = T(n) k^*(m), \quad (17a \text{ \& } 17b)$$

Thus the best filter must minimize both terms. This which means, $T(n)$ should be close to unity for $N/2 < n+m < N/2-1$, and it should be close to zero elsewhere. In practice, it is very difficult to find such a sharp filter in the physical space. Therefore, most of the filter aiming at removing high-wave components, inevitably remove part of the low wave ($-N/2 < k < N/2-1$). In order to find an optimal filter, we also need to assume the shape of the velocity spectra, because the Equations (17a) and (17b) only identify the error of each mode, but the final error is the cumulative of this error convoluted with the amplitude of every mode. To this end, we use the following model spectrum:

$$\Psi_u(kh) = kh^{-a}, \quad (18)$$

with a spectral decay rate a . Thus, when a is relatively small, the flow will appear rough and complicated, relative to the numerical grid (high-wave contents are relatively large). At this stage, it is sufficient to consider the uni-wave mode i.e. $k = n+m$ with $n = m$. We could make a distinction between the low- and high-wave components ($|n/h| < \pi/2$ and $|n/h| > \pi/2$). As a is decreased from 7/3 to 5/3 and 1/3, the ratio of the energy between the non-resolved

part ($n+m>N$) and resolved part ($n+m<N$), increases from 3.8% to 9.5%, and 46%, respectively. Thus, when the flow becomes relatively rough to the underlying grid, the aliasing become more and more important. Furthermore, when these aliasing errors get back to the flow field, they will become low-wave components which are damped very slowly by the viscosity. They will be piling up and the numerical simulation will fail.

Dealiasing Strategy

In large-eddy simulation (LES), the high-wave component of the flow is explicitly filtered out and the simulation can be kept stable, regardless of the approximation of the convective term. This filter explicitly removes high-wave components from the velocity field. In direct numerical simulation (DNS), the explicit filtering is usually avoided because it can be reformulated as the diffusion which can be considered as a kind of turbulence modeling. Our approach, however, filters only the convection term. This is not considered as a model because it is applied directly to the convection term. The diffusion, and the original velocity fields are not altered in anyway. This filtering approach acts in the same way as the dealiasing procedure in spectral method.

In this work, we use a double half-cell interpolation as the low pass filter. This double interpolation is chosen instead of the direct filter because a direct filter needs a large stencil which requires very wide ghost cells. This extra wide ghost cells translates to a major CFD code restructure which is undesirable by many practitioners. This double interpolation

is done in two steps: i.interpolation to the middle point between the grid and ii.reverse interpolation which we interpolate the value from the fictitious middle point back to the original position. Two types of interpolation are selected, the compact fourth- and sixth-order interpolation (Lele, 1992). Therefore, there are three type of filter considered in this work: i.the double fourth-order filter (4-4) ii.the double sixth-order filter (6-6) and iii.the mixed (6-4)-filter. The sum of the total error with different filters and decay rates are shown in table 1, along with the magnitude of the exact aliasing error (non-resolved convection). Due to the limited space we report only the total error numerical errors (aliasing + LTE) in Table 1. It clearly shows that, when the flow is smooth to the grid, the aliasing error is small and using the sixth-order is the best choice. At the top three rows of the table, the flows appear very rough to the grid and the decay rates are small. Here the aliasing error is larger than the local truncation error and using fourth-order filter strongly damps these errors. The total errors are 55%, 34%, and 40% under the fourth-, sixth- and the mixed-order filters. At $a = 7/3$, the sixth-order filter reduce the total error by 28% of the aliasing error. The fourth-order filter, introduces too much local truncation error and raise the total error by 30%. The mixed-order introduces the LTE as much as it damps the aliasing error and the total error remains similar to the aliasing error. There could be a range where the mixed-order would perform best, but we did not try to find it. According to this analysis, we can hypothesize that the fourth-order should deliver a more accurate result when the flow is underresolved and the sixth-order should be the best choice when the flow is sufficiently

Table 1. Total error of Nonlinear convection with different filter subjected to the model spectra with different decay rate (a). The best method is underlined and the second best is italicized

a	Aliasing Error	Total Error		
		(4-4)	(6-6)	(6-4)
1/3	0.388770	0.214344	0.257882	<i>0.232611</i>
2/3	0.245905	0.142910	0.162340	<i>0.150437</i>
3/3	0.155002	0.097658	0.102242	<i>0.098601</i>
4/3	0.098708	0.069647	0.065426	<i>0.066708</i>
5/3	0.062642	0.051630	0.042069	<i>0.046354</i>
7/3	0.025312	0.032767	0.018156	<i>0.025305</i>

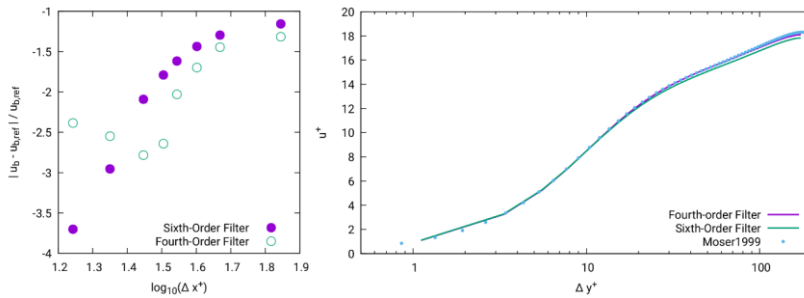


Figure 4. Left: convergence of FSM with fourth- and sixth-order filters. Right: the mean streamwise profile on 64^3 grid

resolved. In order to test these hypotheses, we perform a series of channel flow DNS in the next section.

Results and Discussion

In this test case we use direct numerical simulation of a turbulent channel flow with friction Reynolds number = 180 (bulk flow Reynolds number 5,600). The computation domain is $(L_x, L_z, L_y) = (4\pi H, 4\pi H/3, 2H)$ in which x , y , and z are the streamwise-, spanwise- and wall-normal directions and H is the channel's half-width. The flow is carried out by fixing the pressure gradient corresponding to the friction Reynolds number and let the flow develop. At the statistically steady state, the averaged bulk flow rate will be determined by the accuracy of the numerical scheme. The ratio of the bulk flow velocity to the friction velocity is in the range of 15.52-15.63 when the flow is solved with spectral method.

The grid convergence studies are performed for the fourth-order and the sixth-order filter. The mixed-order is omitted as it should behave second best as we have seen in the table. Figure 4 shows that using the fourth-order filter indeed improves the result on coarse grids. As the resolutions are improved, the fourth-order filter gradually pollutes the sixth-order scheme with the fourth-order LTE. The convergence eventually stops on 80^3 grid. Nevertheless on 64^3 grid, FSM delivers a solution with less-than-1%-error. The similar accuracy is achieved by the sixth-order filter

on 80^3 grid. In our separate study (Hokpunna *et al.*, submitted) FSM can use 64^3 grid to deliver the same result as the fourth-order FVM on 80^3 grid. We knew that the fourth-order FVM is 10X faster than the standard second-order scheme (Hokpunna and Manhart, 2009). Thus, for the overall error larger around $10^{-2.5}$, FSM with 4-4 filter is 73X faster than the second-order FVM. Therefore, when the sixth-order FSM is used with a proper filter. It is almost two-order of magnitude faster than the classical scheme.

Conclusions

We have analyzed the role of the simple low-pass filter in the dealiasing process of the convection term. This simple double compact fourth-order interpolation only requires two ghost cells which is very convenient. Despite the fact that this fourth-order is less accurate than the other parts of the scheme, it functions very well. Note that, in underresolved simulations, the local truncation errors are smaller than the aliasing errors. Thus, choosing the fourth-order filter, to eliminate the aliasing errors and accept some trade-off from the LTE, is perfectly justified and this choice significantly reduce the cost of the numerical simulation. Thus, we can argue that, moving to finite surface method, together with a proper dealiasing method, the solution process of turbulent flow can be two-order of magnitude faster than the second-order scheme. The simulation which would have taken over two

months to complete, can now be solved in a day.

Acknowledgments

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