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A dynamically optimized finite difference scheme for Large-Eddy Simulation

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ABSTRACT

A low-dispersive *dynamic finite difference scheme* for Large-Eddy Simulation is developed. The dynamic scheme is constructed by combining Taylor series expansions on two different grid resolutions. The scheme is optimized dynamically through the real-time adaption of a dynamic coefficient according to the spectral content of the flow, such that the global dispersion error is minimal. In the case of DNS-resolution, the dynamic scheme reduces to the standard Taylor-based finite difference scheme with formal asymptotic order of accuracy. When going to LES-resolution, the dynamic scheme seamlessly adapts to a dispersion-relation preserving scheme. The scheme is tested for Large-Eddy Simulation of Burgers equation. Very good results are obtained.

1. Introduction

The necessity for numerical quality in Direct Numerical Simulations (DNS) and Large-Eddy Simulations (LES) of turbulent flows, has been recognized by many researchers e.g. Ghosal [1], Kravchenko et al. [2] and Chow et al. [3]. In a fully resolved DNS, the smallest resolved scales are located far into the dissipation range. Since these scales have only a very small energy-content in comparison with the largest resolved scales in the flow, they are often considered to have a negligible influence on the mean flow statistics. In a Large-Eddy Simulation, however, where only the most important large scale structures are resolved, the smallest resolved scales are part of the inertial subrange and contain relatively more energy than those in the dissipation range. Hence, the smallest resolved scales in Large-Eddy Simulation are not negligible and have a significant influence on the evolution of the LES-flow. The accuracy with which these small scales are described is therefore expected to be important. Moreover, some advanced subgrid modeling techniques such as the dynamic procedure or multiscale modeling strongly rely on the smallest resolved scales in LES, making their accurate resolution even more important. Good numerical quality for an affordable LES is thus vital for accurate flow prediction, as it directly influences resolved physics as well as subgrid modeling.

Aside from aliasing errors, which should be prevented by eliminating scales beyond $\kappa_c = \frac{2}{3}\kappa_{\max}$, as motivated in [4], discretization errors are mainly responsible for the loss of numerical accuracy. Since it is highly desirable in LES to maximize the ratio between the physical resolution and the grid resolution $\kappa_c/\kappa_{\max}$, in order to lower computational costs, standard second-order central schemes may not be sufficient. Ghosal [1] and Chow et al. [3] recommend the filter-to-grid cutoff-ratio to be at most $\frac{\kappa_c}{\kappa_{\max}} = \frac{1}{4}$ when using a second-order central scheme. This ensures the magnitude of the discretization errors are smaller than the magnitude of the modeled force of the subfilter scales, but is prohibitively expensive for most 3D LES computations. Instead, one could apply higher-order discretizations allowing larger filter-to-grid cutoff-ratios.

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However, acceptable dispersion errors up to $\kappa_c = \frac{2}{3}\kappa_{\max}$, which is the maximum resolution that can be obtained when using the 2/3-dealiasing procedure, requires at least a standard tenth-order central scheme, or a sixth-order compact Padé scheme, which inevitably leads to increased complexity and computational costs.

In the present work, we develop a *dynamic* low-dispersive finite difference scheme for Large-Eddy Simulation. This scheme is constructed by combining Taylor series expansions on two different grid resolutions similar to Richardson Extrapolation. A first attempt of this technique has proved successful for obtaining higher accuracy in laminar flows in [5, 6]. Further, we show the agreements of the new dynamic scheme with the dispersion-relation preserving scheme of Tam et al. [7]. In contrast to their work, the constructed scheme is optimized dynamically during the simulation according to the flow's spectral properties and dispersion errors are minimized through the real-time adaption of a dynamic coefficient. In case of DNS-resolution, the dynamic scheme reduces to the standard finite difference scheme which has an asymptotic order of accuracy. However, going to LES-resolution, the dynamic scheme seamlessly adapts to a dispersion-relation preserving scheme. This could be particularly interesting for transient developing flows, or in case of grid refinement studies with fixed filter width.

2. Construction of the dynamic finite difference scheme

We start by writing the Taylor series expansion for the nth-order derivative, $n = 0, 1, 2, \ldots$, for a kth-order central discretization scheme ($k = 2, 4, 6, \ldots$) on two grid resolutions, characterized by grid spacings $\Delta_1 = \Delta$ and $\Delta_2 = 2\Delta$

$$\overline{\frac{\partial^n u}{\partial x^n}}(x) = \left.\frac{\delta^n \overline{u}}{\delta x^n}\right|^{\Delta} + c_{k,n}\Delta^k \overline{\frac{\partial^{k+n} u}{\partial x^{k+n}}} + \mathcal{O}\left(\Delta^{k+2}\right) \tag{1}$$

$$\overline{\frac{\partial^n u}{\partial x^n}}(x) = \left.\frac{\delta^n \overline{u}}{\delta x^n}\right|^{2\Delta} + c_{k,n}\left(2\Delta\right)^k \overline{\frac{\partial^{k+n} u}{\partial x^{k+n}}} + \mathcal{O}\left(\Delta^{k+2}\right) \tag{2}$$

$\overline{u(x)}$ denotes the discrete representation of a continuum physical field $u(x)$ to the discrete grid, while the finite difference approximation of the partial derivative is denoted as $\overline{\frac{\partial}{\partial x}} = \frac{\delta}{\delta x}$. The coefficient $c_{k,n}$ is actually known from the Taylor series expansion. However, suppose that the leading order truncation terms in (1) and (2) are discretized with a minimal order $\mathcal{O}(\Delta^2)$ and that the Taylor series are truncated to order $\mathcal{O}(\Delta^{k+2})$. Then it would be possible to obtain a new value of $c_{k,n}$ by combining (1) and (2). The new $c_{k,n}$ will not necessarily have the same value as the one obtained from identification of the Taylor series, as it is a function of $\overline{u}(x)$, and its derivatives. Moreover, we expect the value of $c_{k,n}$ to be optimized with respect to $\overline{u}(x)$, such that deficiencies of the finite difference approximation, e.g. dispersion errors are minimized. This will be explained later. We first proceed by writing the truncated Taylor series with the discretized leading order truncation terms and we introduce a blending factor f in the second equation

$$\overline{\frac{\partial^n u}{\partial x^n}}(x) = \left.\frac{\delta^n \overline{u}}{\delta x^n}\right|^{\Delta} + c_{k,n}\Delta^k \left.\frac{\delta^{k+n} \overline{u}}{\delta x^{k+n}}\right|^{\Delta} + \mathcal{O}\left(\Delta^{k}\right) \tag{3}$$

$$\overline{\frac{\partial^n u}{\partial x^n}}(x) = \left.\frac{\delta^n \overline{u}}{\delta x^n}\right|^{2\Delta} + c_{k,n}\left(2\Delta\right)^k \left\{ f \left.\frac{\delta^{k+n} \overline{u}}{\delta x^{k+n}}\right|^{2\Delta} + (1-f)\left.\frac{\delta^{k+n} \overline{u}}{\delta x^{k+n}}\right|^{\Delta}\right\} + \mathcal{O}\left((2\Delta)^{k}\right). \tag{4}$$

To explain the purpose of this blending factor $f \in [0, 1]$ we illustrate the cases $f = 0$ and $f \neq 0$. Remark that, unless $c_{k,n}$ has the exact Taylor value, the order of accuracy in both expressions remains $\mathcal{O}(\Delta^k)$.

2.1. Asymptotic high-order scheme for $f = 0$

For $f = 0$, the coefficient $c_{k,n}$ can be obtained by subtracting the truncated expressions (3) and (4), leading to

$$\left.\frac{\delta^n \overline{u}}{\delta x^n}\right|^{\Delta} - \left.\frac{\delta^n \overline{u}}{\delta x^n}\right|^{2\Delta} = c_{k,n}\left(2^k - 1\right)\Delta^k \left.\frac{\delta^{k+n} \overline{u}}{\delta x^{k+n}}\right|^{\Delta}. \tag{5}$$

Although the left-hand-side and the right-hand-side finite difference approximations do not necessarily have identical stencils, they represent the same derivative. This relation will be used further in this work for simplifications. Substitution of (5) into (3), eliminating $c_{k,n}$, finally leads to the finite difference approximation of order $k + 2$

$$\overline{\frac{\partial^n u}{\partial x^n}}(x) = \frac{2^k \left.\frac{\delta^n \overline{u}}{\delta x^n}\right|^{\Delta} - \left.\frac{\delta^n \overline{u}}{\delta x^n}\right|^{2\Delta}}{2^k - 1} + \mathcal{O}\left(\Delta^{k+2}\right) \tag{6}$$

which is the well-known Richardson's Extrapolation formula. It should be emphasized that the same result is obtained by combining (1) and (2) which proves that expression (6) is an approximation with formal asymptotic order of accuracy $k+2$. Since the aim is to construct optimized finite difference schemes with good Fourier characteristics, abandoning the concept of formal asymptotic order of accuracy, obviously f needs to be different from zero.