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Commutative discrete filtering on unstructured grids based on least-squares techniques

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Abstract

The present work is concerned with the development of commutative discrete filters for unstructured grids and contains two main contributions. First, building on the work of Marsden et al. [J. Comp. Phys. 175 (2002) 584], a new commutative discrete filter based on least-squares techniques is constructed. Second, a new analysis of the discrete commutation error is carried out. The analysis indicates that the discrete commutation error is not only dependent on the number of vanishing moments of the filter weights, but also on the order of accuracy of the discrete gradient operator. The results of the analysis are confirmed by grid-refinement studies.

Keywords: Curve fitting; Interpolation; Numerical methods

1. Introduction

The technique of large-eddy simulation (LES) is perhaps the most promising approach to simulating turbulent flows of engineering interest with acceptable accuracy. Moin [7] summarized recent advances in LES with particular focus on flows typically encountered in engineering applications. Unstructured grids are often the only feasible method of discretizing the highly complex geometries relevant to engineers. Hence there is a great need to extend the applicability of LES to unstructured grids. The earliest LES on unstructured grids appears to be that of Jansen [5], who pointed out that the local control over grid spacing afforded by unstructured grids might lead to a saving in grid points and hence computational cost.

Despite the growing maturity and use of LES techniques, some fundamental issues remain unresolved. It can be argued that the most fundamental issue concerns the precise form of the equations governing LES, which are formally derived by applying a low-pass filter to the Navier–Stokes equations. In doing so, it is

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often tacitly assumed that the filtering and differentiation operations commute. This assumption is invalid if the filter width is not uniform – as in the case of wall-bounded flows – unless special filter operators are constructed, see, e.g. [8] (hereafter referred to as VLM). Because unstructured grids rarely satisfy smoothness constraints on the grid spacing, the assumption that the operations of filtering and differentiation commute may be violated even away from walls. The construction of commutative discrete filters for unstructured grids is thus a particularly pressing issue.

Recent work by Marsden et al. [6] (hereafter referred to as MVM) resulted in a framework for the construction of filters on unstructured grids which commute with differentiation to a potentially arbitrarily high order. The key concept in the construction of a commutative discrete filter is that the filter weights exhibit vanishing moments. Their analysis indicated that the larger the number of vanishing moments, the higher the order of the commutation error. MVM also demonstrated a filter operator with a second-order commutation error. However, because their method relies on the explicit construction of geometric simplices, it is quite complicated, particularly in three dimensions and near boundaries. It is also not immediately clear how their method can be implemented for higher orders of accuracy.

The goal of the present work is to develop a commutative filtering method which is simpler than that of MVM. The new filtering method is based on the following observation: The conditions derived by VLM for filtering a function to a given order of commutation error are formally identical to the conditions for reconstructing the gradient of a function to a given order of truncation error. In other words, the construction of commutative filter operators may be reinterpreted as the construction of – suitably reformulated – gradient-reconstruction operators. This apparently trivial observation has important consequences because the reconstruction of gradients is central to many flow-solution methods on unstructured grids and is well understood, see [4].

We formulate and validate the new filtering method in the framework of a vertex-centered discretization on a triangular grid. However, it is important to note that the method can be extended to other discretization methodologies and to grids with arbitrary cell types and combinations thereof in two and three dimensions in a straightforward manner.

This article is structured as follows. Section 2 describes least-squares gradient reconstruction, which serves as the basis for the new filtering method introduced in Section 3. The construction of appropriate stencils is outlined in Section 4. The transfer function of the new filter operators is investigated in Section 5. Discrete commutation errors are studied analytically and numerically in Section 6. Section 7 contains a comparison of the current analysis and results with those obtained with VLM and MVM. Conclusions and suggestions for further work are provided in Section 8.

2. Least-squares gradient reconstruction

Suppose we wish to reconstruct the gradient of a dependent variable at vertex 0 in Fig. 1. The running index i denotes the points which are included in the reconstruction stencil at vertex 0. The reconstruction will include at least the nearest neighbors of 0, namely those vertices which are linked by an edge to vertex 0. The stencil may be extended recursively to take into account mth-nearest neighbors, which are those vertices which are linked by an edge to $(m-1)$th-nearest neighbors of vertex 0 and are not already included in the $(m-r)$th-nearest neighbors, where $0 \leqslant r \leqslant 2 \leqslant m$. According to this definition, vertex 0 is its own 0th neighbor. In the following, we define by d_0 the degree of vertex 0, i.e., the number of neighbors included in the gradient reconstruction at vertex 0. Note that this definition is in general different from the topological degree of vertex 0, which is equal to the number of nearest neighbors of vertex 0.

The least-squares gradient-reconstruction procedure originally developed by Barth [1] is based on approximating the variation of a dependent variable ϕ along an edge linking vertices 0 and i by a truncated Taylor series, e.g., for a linear approximation,

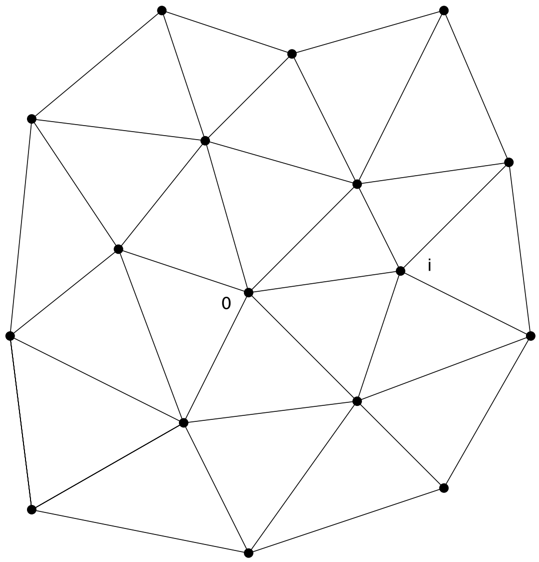

Fig. 1. Fragment of unstructured triangular grid illustrating gradient reconstruction at vertex 0.

$$\phi_i = \phi_0 + (\nabla\phi)_0 \cdot \Delta\mathbf{r}_{0i}, \quad 1 \leqslant i \leqslant d_0, \tag{1}$$

where $\Delta\mathbf{r}_{0i} = \mathbf{r}_i - \mathbf{r}_0$ and $\mathbf{r}$ is the position vector. The application of Eq. (1), or corresponding higher-order approximations, to all edges incident to vertex 0 gives a system of linear equations for the derivatives at vertex 0,

$$\mathbf{A}\mathbf{x} = \mathbf{b}, \tag{2}$$

where $\mathbf{A}$ is a $d_0 \times n_0$ matrix of geometrical terms, $\mathbf{x}$ is an n_0-vector containing derivatives, $\mathbf{b}$ is a d_0-vector of function values, and n_0 is the number of derivatives reconstructed at vertex 0. Since the degree is usually larger than the number of derivatives reconstructed, Eq. (2) is solved for $\mathbf{x}$ in a least-squares fashion.

Through the QR-decomposition of $\mathbf{A}$ using the Gram–Schmidt process, see, e.g. [2], a general closed-form solution of Eq. (2) can be derived. In the following, we denote by $\mathbf{a}_i$ and $\mathbf{q}_i$ the ith column vectors of the matrices $\mathbf{A}$ and $\mathbf{Q}$, respectively, and by r_{ij} the ijth element of the upper triangular matrix $\mathbf{R}$. There is no summation over repeated indices throughout this article. The general closed-form solution can be written as [3]

$$\mathbf{x} = \mathbf{W}^{\mathrm{t}}\mathbf{b}, \tag{3}$$

where $\mathbf{W}$ is a $d_0 \times n_0$ matrix with column vectors $\mathbf{w}_i$ given by

$$\mathbf{w}_i = c_{ii}\mathbf{q}_i + \sum_{k=i+1}^{n_0} c_{ik}c_{kk}\mathbf{q}_k, \quad 1 \leqslant i \leqslant n_0 \tag{4}$$

with

$$\mathbf{q}_i = c_{ii}\left(\mathbf{a}_i - \sum_{j=1}^{i-1} r_{ji}\,\mathbf{q}_j\right) = c_{ii}\left(\mathbf{a}_i + \sum_{j=1}^{i-1} c_{ji}\,\mathbf{a}_j\right), \quad 1 \leqslant i \leqslant n_0. \tag{5}$$

The geometrical quantities c_{ij} are defined as

$$c_{ij} = \begin{cases} r_{ii}^{-1} & \text{if } i = j,\ 1 \leqslant i \leqslant n_0, \\ -\left(c_{ii} r_{ij} + \sum_{k=i+1}^{j-1} c_{ik} c_{kk} r_{kj}\right) & \text{if } i \neq j,\ i < j \leqslant n_0, \end{cases} \tag{6}$$

where

$$r_{ij} = \begin{cases} \sqrt{\|\mathbf{a}_i\|^2 - \sum_{k=1}^{i-1} r_{ki}^2} & \text{if } i = j,\ 1 \leqslant i \leqslant n_0, \\ \frac{1}{r_{ii}}\left(\mathbf{a}_i \cdot \mathbf{a}_j - \sum_{k=1}^{i-1} r_{ki} r_{kj}\right) & \text{if } i \neq j,\ i < j \leqslant n_0. \end{cases} \tag{7}$$

The general closed-form solution allows the reconstruction of derivatives to an arbitrarily high order of accuracy on arbitrary unstructured grids in two and three dimensions. If q denotes the degree of the highest derivative included in $\mathbf{x}$, the least-squares gradient-reconstruction method presented above gives an order of accuracy of $q - m + 1$ for derivatives of degree $m \leqslant q$ on asymmetric stencils. Cancellation may result in higher orders of accuracy for symmetric stencils, i.e., on uniform grids and away from boundaries. For example, $q = 1$, which gives only first-order accurate first derivatives on asymmetric stencils, leads to second-order accuracy on symmetric stencils.

In the remainder of this article, we shall make frequent use of the discrete first derivative given by

$$\left(\frac{\delta\phi}{\delta x}\right)_0 = \sum_{i=1}^{d_0} \omega_{0i} \Delta\phi_{0i}, \tag{8}$$

where $\omega_{0i} = w_{1,i}$ is the edge weight and it is noted that ω_{0i} has dimensions of inverse length. For linear gradient reconstruction in two dimensions, the edge weights for the discrete derivative in the x-coordinate direction are given by

$$\omega_{0i} = \frac{\Delta x_{0i}}{r_{11}^2} - \frac{r_{12}}{r_{11} r_{22}^2}\left(\Delta y_{0i} - \frac{r_{12}}{r_{11}} \Delta x_{0i}\right), \tag{9}$$

where the terms r_{ij} are given by Eq. (7). A similar expression can be derived for the discrete derivative in the y-coordinate direction.

In Section 1, we stated that the construction of commutative filter operators can be reinterpreted as the construction of suitably reformulated gradient-reconstruction operators. This statement is easily understood by examining the accuracy of Eq. (8). Upon expanding the term $\Delta\phi_{0i}$ using a Taylor series, the conditions for Eq. (8) to achieve a given order of accuracy q are

$$\sum_{i=1}^{d_0} \omega_{0i} \Delta x_{0i}^{r-s} \Delta y_{0i}^{s} = \delta_{1r}\delta_{0s}, \quad 1 \leqslant r \leqslant q,\ 0 \leqslant s \leqslant r,$$

where δ_{ij} is the Kronecker delta. These conditions require nothing but vanishing moments of the gradient reconstruction weights, and are thus identical in form to the conditions derived by VLM for commutative filter operators. The reformulation of the least-squares gradient reconstruction method into a least-squares filtering method is addressed in the following section.

3. Least-squares filtering

3.1. Formulation

The least-squares gradient-reconstruction method can be turned into a filtering method by modifying Eq. (1), so that ϕ_0 is no longer a point value, but represents an interpolated or a filtered value $\overline{\phi}_0$,

$$\phi_i = \overline{\phi}_0 + (\nabla\phi)_0 \cdot \Delta\mathbf{r}_{0i}. \tag{10}$$

The effect of this modification is that the filtered value $\overline{\phi}_0$ is affixed to the vector of unknowns $\mathbf{x}$. The resulting system of equations can be solved using the method described in Section 2. This leads to an expression for the filtered value in the form of a weighted sum,

$$\overline{\phi}_0 = \sum_{i=1}^{d_0} \overline{\omega}_{0i}\phi_i, \tag{11}$$

where we have used the following notation: $\overline{\omega}_{0i} = w_{n_0,i}$.

To characterize the discrete filter operator, it is more convenient to refer of its order of accuracy p rather than to the number of vanishing moments of its weights. This is because the number of vanishing moments $\overline{N}$ depends on the number of spatial dimensions D through

$$\overline{N}(p, D) = \frac{1}{D!}\prod_{i=0}^{D-1}(p+i) - 1.$$

Furthermore, since we are interested in the order of the commutation error, it is more natural to identify filter operators through their order of accuracy.

The order of accuracy of the filter operator is determined by the degree of the highest derivative included in $\mathbf{x}$. If q denotes the degree of the highest derivative included in $\mathbf{x}$, the least-squares filtering method gives an order of accuracy of $p = q + 1$ on asymmetric stencils. Cancellation may result in higher orders of accuracy for symmetric stencils, i.e., on uniform grids and away from boundaries. For example, $q = 2$ gives a filtering method with fourth-order accuracy on symmetric stencils.

To illustrate the form of the filter weights, we can consider linear gradient reconstruction, which leads to a second-order accurate expression for the filtered variable. In two dimensions, the corresponding filter weights are given by

$$\overline{\omega}_{0i} = \frac{1}{r_{33}^2}\left[1 - \left(\frac{r_{13}}{r_{11}} - \frac{r_{12}r_{23}}{r_{11}r_{22}}\right)\Delta x_{0i} - \frac{r_{23}}{r_{22}}\Delta y_{0i}\right], \tag{12}$$

where r_{ij} is given by Eq. (7). Eq. (12) leads to two vanishing moments,

$$\sum_{i=1}^{d_0} \overline{\omega}_{0i}\Delta\mathbf{r}_{0i} = \mathbf{0},$$

as is easily verified by direct substitution and use of Eq. (7).

3.2. Implementation

One advantage of the new filtering method is that it allows reusing data structures and geometric weights already employed to compute gradients in the flow-solution method. Therefore, the implementation of the new filtering method in an existing program based on least-squares gradient reconstruction entails little additional effort: Code to compute and store the weights can be adapted, the data structure to loop over edges is already in place, and routines to compute filtered values closely follow those computing gradients.

It should be noted that the reuse of weights is dependent upon *affixing* the filtered value $\overline{\phi}_0$ to the vector of unknowns $\mathbf{x}$. If $\overline{\phi}_0$ were *prefixed* to $\mathbf{x}$, the weights for filtering would be different from those for gradient reconstruction, and reuse would not be possible. Further advantages of the new filtering method are that it is easily extended to three dimensions and does not require special treatment at boundaries beyond ensuring

– as for interior vertices – that the degree of a given vertex is greater than the number of derivatives reconstructed at that vertex.

4. Stencil construction

The least-squares filtering method described above requires the construction of a suitable stencil. Two conditions must be satisfied for a stencil to be suitable.

First, the stencil must include at least $d_0 \geqslant d_{0,\min}$ distinct, noncollinear/noncoplanar vertices, where $d_{0,\min}$ is given by

$$d_{0,\min} = \frac{1}{D!} \prod_{i=1}^{D} (q+i),$$

where q denotes the degree of the highest derivative included in $\mathbf{x}$. The selection of the vertices is governed by two considerations. The first consideration is that the stencil extent should be kept as small as possible to minimize the truncation error constants for a given order of accuracy. The second consideration is that the stencil should be as symmetric as possible to ensure cancellation of terms in the truncation error, a real-valued amplification factor on uniform grids, and minimization of the imaginary part of the amplification factor on nonuniform grids. In general, the first and second considerations are contradictory, because a symmetric stencil usually includes more vertices than the minimum.

The second condition is that the matrix $\mathbf{A}$ must be nonsingular. This requires the matrix $\mathbf{R}$ to be nonsingular, which in turn means that its diagonal elements r_{ii} must be nonzero. In contrast to one spatial dimension, the first condition is necessary but not sufficient to guarantee a nonsingular matrix $\mathbf{A}$. Fig. 2 depicts some of the stencils for which the matrix $\mathbf{A}$ is singular. In the present work, we circumvent singular matrices by increasing the support of the stencil by an entire additional layer of neighbors in order not to destroy the symmetry of the stencils.

In further work, we plan to use compact gradient reconstruction and filtering to reduce the stencil extent for a given order of accuracy.

For notational convenience, we introduce the notion of a neighbor set for the remainder of this article. The neighbor set of vertex 0 is denoted by $\mathscr{S}_0$. This allows the summations over neighbors to be rewritten in the following form

$$\sum_{i=1}^{d_0} (\cdot) = \sum_{i \in \mathscr{S}_0} (\cdot).$$

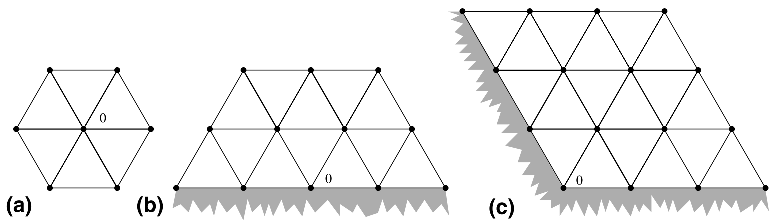

Fig. 2. Stencils for which the matrix $\mathbf{A}$ is singular. Gray shading indicates the presence of a boundary. The stencil shown in (a) is nonsingular for quadratic gradient reconstruction, but becomes singular for quadratic filtering. The stencil depicted in (b) is singular for cubic gradient reconstruction. The stencil displayed in (c) is singular for quartic gradient reconstruction.

5. Investigation of filter transfer functions

The transfer function of the discrete filter operators is given by

$$G(k_x, k_y) = \sum_{i \in \mathscr{S}_0} \overline{\omega}_{0i} \, e^{\mathbf{i}\mathbf{k}\cdot\Delta\mathbf{r}_{0i}}, \tag{13}$$

where i is the imaginary unit and $\mathbf{k} = \{k_x, k_y\}^t$ is the wave-number vector. In investigating the filter transfer functions, we use a modified version of Eq. (11) to improve the spectral behavior,

$$\overline{\phi}_0 = \omega_{00}\phi_0 + (1 - \omega_{00}) \sum_{i=1}^{d_0} \omega_{0i}\phi_i, \tag{14}$$

where ω_{00} is a coefficient which influences primarily the high wave-number components of the function being filtered. This modification does not degrade the accuracy of Eq. (11).

The transfer functions of the linear and quadratic filter functions are depicted in Fig. 3 for uniform triangular grids. The linear filter function with $\omega_{00} = 1/5$ damps high wave-number components well, but

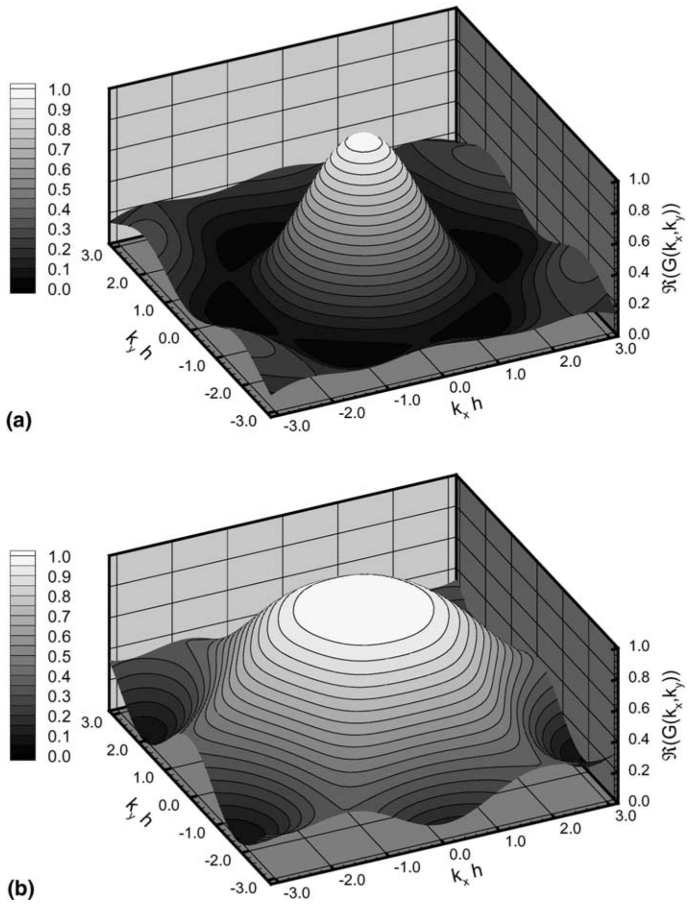

Fig. 3. Transfer functions for filter operators on uniform grids of spacing h. (a) Linear filter operator with $\omega_{00} = 1/5$ and (b) quadratic filter operator with $\omega_{00} = 1/2$.

deviates quickly from unity for low wave-numbers. The quadratic filter function with $\omega_{00} = 1/2$ exhibits better behavior for low to moderate wave-numbers, but high wave-number components are not damped uniformly well.

6. Investigation of commutation error

6.1. Derivation of discrete commutation error

In previous work, VLM and MVM studied the commutation error due to continuous differentiation and filter operators in computational and physical spaces, respectively. By contrast, the present work considers the commutation error arising from discrete differentiation and filter operators. As the following analysis demonstrates, this difference is crucial in understanding the interaction of the two operators.

We first derive the discrete commutation error for uniform and nonuniform grids in one dimension, and then extend the derivation to multiple space dimensions.

6.1.1. Derivation in one dimension

The discrete commutation error in one dimension is

$$E_{\mathrm{c}} = \overline{\frac{\delta\phi}{\delta x}} - \frac{\delta\overline{\phi}}{\delta x}, \tag{15}$$

which is expressed at vertex 0 as

$$E_{\mathrm{c}} = \sum_{i\in\mathscr{S}_0} \overline{\omega}_{0i}\left(\frac{\delta\phi}{\delta x}\right)_i - \sum_{i\in\mathscr{S}_0} \omega_{0i}\Delta\overline{\phi}_{0i}, \tag{16}$$

or as

$$E_{\mathrm{c}} = \sum_{i\in\mathscr{S}_0} \overline{\omega}_{0i} \sum_{j\in\mathscr{S}_i} \omega_{ij}\Delta\phi_{ij} - \sum_{i\in\mathscr{S}_0} \omega_{0i}\left(\sum_{j\in\mathscr{S}_i} \overline{\omega}_{ij}\phi_j - \sum_{j\in\mathscr{S}_0} \overline{\omega}_{0j}\phi_j\right), \tag{17}$$

through repeated applications of Eqs. (8) and (11).

Uniform grid. The analyses of VLM and MVM indicate that the commutation error is identically zero on a uniform grid. To demonstrate that the discrete commutation error is also identically zero on a uniform grid, it is convenient to express the Taylor-series expansion in operator form. Using the abbreviation $d_x(\cdot) = d(\cdot)/dx$, we can write

$$\phi_j = \mathrm{e}^{\Delta x_{ij} d_x}\phi_i = \mathscr{T}_{ij}\phi_i, \tag{18}$$

where $\mathscr{T}_{ij}$ is the shift operator. The gradient and filter operators become

$$\left(\frac{\delta\phi}{\delta x}\right)_0 = \sum_{i\in\mathscr{S}_0} \omega_{0i}(\mathscr{T}_{0i} - 1)\phi_0 \tag{19}$$

and

$$\overline{\phi}_0 = \sum_{i\in\mathscr{S}_0} \overline{\omega}_{0i}\mathscr{T}_{0i}\phi_0. \tag{20}$$

By substituting Eqs. (19) and (20), and their equivalent equations at vertex i, into Eq. (17), we arrive at the following expression for the discrete commutation error

$$E_{\mathrm{c}} = \sum_{i\in\mathscr{S}_0}\left(\sum_{j\in\mathscr{S}_i}\overline{\omega}_{0i}\omega_{ij}\left(\mathscr{T}_{ij}-1\right)\mathscr{T}_{0i} - \sum_{j\in\mathscr{S}_i}\omega_{0i}\overline{\omega}_{ij}\mathscr{T}_{ij}\mathscr{T}_{0i} + \sum_{j\in\mathscr{S}_0}\omega_{0i}\overline{\omega}_{0j}\mathscr{T}_{0j}\right)\phi_0. \tag{21}$$

Eq. (21) can be rearranged into a form which is more convenient for the error analysis,

$$E_{\mathrm{c}} = \sum_{i\in\mathscr{S}_0}\overline{\omega}_{0i}\left(\sum_{j\in\mathscr{S}_i}\omega_{ij}(\mathscr{T}_{ij}-1) - \sum_{j\in\mathscr{S}_0}\omega_{0j}(\mathscr{T}_{0j}-1)\right)\mathscr{T}_{0i}\phi_0 - \sum_{i\in\mathscr{S}_0}\omega_{0i}\left(\sum_{j\in\mathscr{S}_i}\overline{\omega}_{ij}\mathscr{T}_{ij} - \sum_{j\in\mathscr{S}_0}\overline{\omega}_{0j}\mathscr{T}_{0j}\right)\mathscr{T}_{0i}\phi_0. \tag{22}$$

In the case of a uniform unbounded (i.e., infinite or periodic) grid, the relationships

$$\begin{aligned}
\sum_{i\in\mathscr{S}_0}\omega_{0i} &= \sum_{j\in\mathscr{S}_i}\omega_{ij},\\
\sum_{i\in\mathscr{S}_0}\omega_{0i}\mathscr{T}_{0i} &= \sum_{j\in\mathscr{S}_i}\omega_{ij}\mathscr{T}_{ij},\\
\sum_{i\in\mathscr{S}_0}\overline{\omega}_{0i}\mathscr{T}_{0i} &= \sum_{j\in\mathscr{S}_i}\overline{\omega}_{ij}\mathscr{T}_{ij},
\end{aligned} \tag{23}$$

together with the fact that the summations over j become independent of i mean that the terms in parentheses on the right-hand side of Eq. (22) reduce to zero. Thus the discrete commutation error on a uniform unbounded grid is identically zero.

For bounded uniform grids, the commutation error near boundaries will be nonzero because of partially or entirely biased stencils.

Nonuniform grid. In order to analyze the commutation error on a nonuniform grid, we make use of the following identity

$$\mathscr{T}_{ij} = \mathrm{e}^{\Delta x_{ij} d_x} = \sum_{k=0}^{\infty}\frac{1}{k!}\,\Delta x_{ij}^k\,d_x^k. \tag{24}$$

We are interested in the form of the commutation error if the discrete gradient and filter operators are assumed to be accurate to orders q and p, respectively. With this assumption, the moments of the gradient and filter weights obey the relations

$$\sum_{j\in\mathscr{S}_i}\omega_{ij}\Delta x_{ij}^k = \delta_{1k} \quad \text{for } 1\leqslant k\leqslant q, \tag{25}$$

$$\sum_{j\in\mathscr{S}_i}\overline{\omega}_{ij}\Delta x_{ij}^k = \delta_{0k} \quad \text{for } 0\leqslant k\leqslant p-1. \tag{26}$$

Using Eqs. (24)–(26), Eqs. (8) and (11) can be recast as,

$$\left(\frac{\delta\phi}{\delta x}\right)_0 = \left[d_x + \sum_{k=q+1}^{\infty}\frac{1}{k!}\left(\sum_{i\in\mathscr{S}_0}\omega_{0i}\Delta x_{0i}^k\right)d_x^k\right]\phi_0, \tag{27}$$

and

$$\overline{\phi}_0 = \left[1 + \sum_{k=p}^{\infty} \frac{1}{k!}\left(\sum_{i\in\mathscr{S}_0} \overline{\omega}_{0i}\Delta x_{0i}^k\right) d_x^k\right]\phi_0, \tag{28}$$

respectively. VLM proved that the radius of convergence of the series in Eq. (28) is infinite. Note that Eq. (27) indicates that the gradient reconstruction is of order q – and not $q+1$ – because $\omega_{0i} \propto \Delta x_{0i}^{-1}$.

By substituting Eq. (24) into Eq. (22) and making use of Eqs. (25) and (26), we obtain the following expression for the commutation error

$$\begin{aligned} E_c = {} & \sum_{i\in\mathscr{S}_0} \overline{\omega}_{0i}\left[\sum_{k=q+1}^{\infty} \frac{1}{k!}\left(\sum_{j\in\mathscr{S}_i} \omega_{ij}\Delta x_{ij}^k - \sum_{j\in\mathscr{S}_0} \omega_{0j}\Delta x_{0j}^k\right) d_x^k\right] e^{\Delta x_{0i} d_x}\phi_0 \\ & - \sum_{i\in\mathscr{S}_0} \omega_{0i}\left[\sum_{n=p}^{\infty} \frac{1}{n!}\left(\sum_{j\in\mathscr{S}_i} \overline{\omega}_{ij}\Delta x_{ij}^n - \sum_{j\in\mathscr{S}_0} \overline{\omega}_{0j}\Delta x_{0j}^n\right) d_x^n\right] e^{\Delta x_{0i} d_x}\phi_0. \end{aligned} \tag{29}$$

The terms in parentheses may be interpreted as differences of truncation-error constants. These terms will vanish only for uniform unbounded grids. For nonuniform grids, the first term is $\mathrm{O}(q)$, and the second term is $\mathrm{O}(p-1)$. Therefore the upshot of this analysis is that the discrete commutation error on a nonuniform grid is given by

$$\mathrm{O}(E_c) = \min(p-1, q). \tag{30}$$

For discrete gradient and filter operators, it is thus not possible to reduce the commutation error by increasing the order of the filter operator arbitrarily. Given a particular filter operator with $p > q+1$, the order of the discrete gradient operator places a limit on the maximum order of accuracy of the commutation error. The influence of the discrete gradient operator on the discrete commutation error was not detected in previous analyses because the differentiation operators were assumed to be continuous.

It is worth noting that with the present filtering method, the order of accuracy of the commutation error is effectively only dependent on the order of accuracy of the gradient reconstruction. This is because, as already mentioned, the order of accuracy of the filtering operation is $p = q+1$ on nonuniform grids, so that Eq. (30) gives $\mathrm{O}(E_c) = q$. Thus the present filtering ensures that the order of accuracy of the commutation error is not lower than the order of accuracy of the spatial discretization.

6.1.2. Generalization of derivation to multiple dimensions

The derivation of the discrete commutation error in one dimension may be generalized to multiple dimensions in a straightforward manner. The following outlines the generalization to D dimensions, in which we define the discrete commutation error as

$$E_c = \overline{\boldsymbol{\delta}\cdot\boldsymbol{\phi}} - \boldsymbol{\delta}\cdot\overline{\boldsymbol{\phi}}, \tag{31}$$

where $\boldsymbol{\phi} = \{\phi_1, \ldots, \phi_D\}^{\mathrm{t}}$ represents the D-dimensional unfiltered field and $\boldsymbol{\delta}$ is the discrete analogue of the D-dimensional gradient operator ∇. We note that ϕ_k with $k \in \{1, \ldots, D\}$ denotes a component of $\boldsymbol{\phi}$, whereas $\boldsymbol{\phi}_k$ or ϕ_k with $k \in \{0, i, j\}$ stand for the corresponding variable evaluated at the indicated spatial location.

Uniform grid. The analysis is formally identical to the one-dimensional case, except that the D-dimensional shift operator is now defined as,

$$\boldsymbol{\phi}_j = e^{\Delta\mathbf{r}_{ij}\cdot\nabla}\boldsymbol{\phi}_i = \mathscr{T}_{ij}\boldsymbol{\phi}_i. \tag{32}$$

By using the operator approach, we can apply the previously derived results for one dimension on a term-by-term basis. Thus the discrete commutation error on uniform unbounded grids in two and three dimensions will also be identically zero. Numerical results which corroborate this conclusion are presented in the following subsection.

Nonuniform grid. The analysis for nonuniform one-dimensional grids can be extended to D dimensions in a straightforward manner. In particular, Eq. (24) can be rewritten as

$$\mathscr{T}_{ij} = \mathrm{e}^{\Delta \mathbf{r}_{ij}\cdot\nabla} = \sum_{k=0}^{\infty} \frac{1}{k!}(\Delta \mathbf{r}_{ij}\cdot\nabla)^k, \tag{33}$$

and Eqs. (27) and (28) can be recast as

$$\boldsymbol{\delta}\phi_0 = \left[\nabla + \sum_{k=q+1}^{\infty} \frac{1}{k!}\left(\sum_{i\in\mathscr{S}_0} \boldsymbol{\omega}_{0i}(\Delta\mathbf{r}_{0i}\cdot\nabla)^k\right)\right]\phi_0, \tag{34}$$

and

$$\overline{\phi}_0 = \left[1 + \sum_{k=p}^{\infty} \frac{1}{k!}\left(\sum_{i\in\mathscr{S}_0} \overline{\omega}_{0i}(\Delta\mathbf{r}_{0i}\cdot\nabla)^k\right)\right]\phi_0, \tag{35}$$

respectively, where ϕ is an arbitrary component of $\boldsymbol{\phi}$, and $\boldsymbol{\omega}_{ij}$ denotes the vector of weights for the discrete gradient operator. In deriving Eqs. (34) and (35), the discrete D-dimensional gradient and filter operators were assumed to be accurate to orders q and p, respectively, which implies the existence of relations in D dimensions equivalent to Eqs. (25) and (26). With this in mind, it can be shown that the commutation error in D dimensions becomes

$$\begin{aligned} E_{\mathrm{c}} = &\sum_{i\in\mathscr{S}_0} \overline{\omega}_{0i} \sum_{k=q+1}^{\infty}\left(\sum_{j\in\mathscr{S}_i} \boldsymbol{\omega}_{ij}(\Delta\mathbf{r}_{ij}\cdot\nabla)^k - \sum_{j\in\mathscr{S}_0}\boldsymbol{\omega}_{0j}(\Delta\mathbf{r}_{0j}\cdot\nabla)^k\right)\frac{\mathrm{e}^{\Delta\mathbf{r}_{0i}\cdot\nabla}}{k!}\cdot\boldsymbol{\phi}_0 \\ &- \sum_{i\in\mathscr{S}_0} \boldsymbol{\omega}_{0i} \sum_{n=p}^{\infty}\left(\sum_{j\in\mathscr{S}_i} \overline{\omega}_{ij}(\Delta\mathbf{r}_{ij}\cdot\nabla)^n - \sum_{j\in\mathscr{S}_0}\overline{\omega}_{0j}(\Delta\mathbf{r}_{0j}\cdot\nabla)^n\right)\frac{\mathrm{e}^{\Delta\mathbf{r}_{0i}\cdot\nabla}}{n!}\cdot\boldsymbol{\phi}_0. \end{aligned} \tag{36}$$

It can be seen that the previously derived results still hold, and that the order of the commutation error in D dimensions is also given by Eq. (30). Numerical results which corroborate this conclusion are presented in the following subsection.

6.2. Demonstration of discrete commutation

To confirm the theoretical results, a dedicated computer program was written. The program determines the commutation error due to gradient and filter operators whose orders of accuracy can be specified independently. The order of accuracy of the commutation error is computed by carrying out a grid-refinement study using an analytic function for the unfiltered field on a hexagonal domain centered on the origin with edge-length unity. Six uniform triangular grids were generated, whose characteristics are listed in Table 1; it is noted that the finest grid is approximately 1100 times finer than the coarsest grid. The grids were distorted by displacing the interior vertices by random amounts of a given fraction of the grid spacing in both coordinate directions. In the results presented below, this fraction was taken to be 0.35. The distorted grid with 1141 vertices is shown in Fig. 4.

Table 1
Number of vertices contained in the six grid levels

Grid	Vertices
1	271
2	1141
3	4681
4	18,961
5	76,321
6	306,241

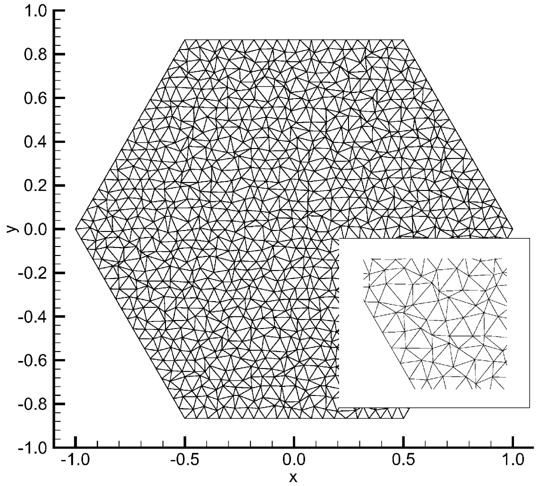

Fig. 4. Distorted grid with 1141 vertices. Inset shows detail of distorted grid.

In the present study, the function representing the unfiltered field is

$$\boldsymbol{\phi} = \left\{ \begin{matrix} \phi_1 \\ \phi_2 \end{matrix} \right\} = \left\{ \begin{matrix} \cos(4\pi x)\sin(4\pi y) \\ \sin(4\pi x)\cos(4\pi y) \end{matrix} \right\}. \tag{37}$$

The commutation error is defined in terms of the discrete divergence according to Eq. (31). We have chosen this definition in terms of local quantities to avoid the use of integration which might complicate the study and the interpretation of the results. To verify the accuracy of the filter and gradient operators, we also track the behavior of the filter truncation error defined by

$$E_\mathrm{f} = \overline{\phi}_1 - \phi_1, \tag{38}$$

and the divergence truncation error defined by

$$E_\mathrm{d} = \boldsymbol{\delta} \cdot \boldsymbol{\phi} - \nabla \cdot \boldsymbol{\phi}. \tag{39}$$

The order of accuracy of these errors is then inferred from a linear least-squares curve fit to the error norms on the finest three grid levels.

6.2.1. Uniform grids

To verify that the discrete commutation error is identically zero on a uniform unbounded grid, we carried out a grid-refinement study in which only the vertices unaffected by boundaries were included in the error norms. For a linear filter function and quadratic gradient reconstruction, the results are shown in Fig. 5. It can be seen that the discrete commutation error is close to machine precision regardless of the grid spacing. Corresponding results were obtained for other combinations of orders of accuracy of the filter function and the gradient reconstruction.

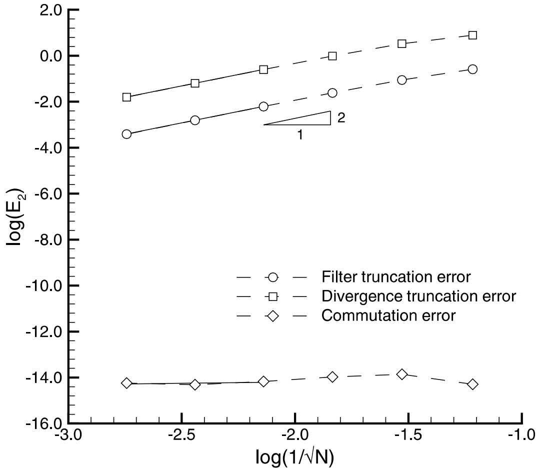

Fig. 5. Variation of L_2-norm of errors with grid refinement on uniform unbounded grids, demonstrating a discrete commutation error close to machine precision. Solid lines represent linear least-squares curve fits to data used to determine order of accuracy.

The ultimate test for commutation will be to specify a uniform filter width on a randomly distorted grid and to check whether the commutation error vanishes. This is an objective of future work.

6.2.2. Nonuniform grids

Figs. 6(a) and (b) depict the variation of the L_2-norms of the filter truncation error, the divergence truncation error, and the commutation error on nonuniform grids for different combinations of p and q. In either case, the order of the commutation error is approximately 2, as predicted by Eq. (30).

Table 2 summarizes the computed orders of accuracy of the filter truncation error, the divergence truncation error, and the commutation error. The results shown in this table also verify the conclusion that the order of the commutation error is given by $\min(p-1, q)$.

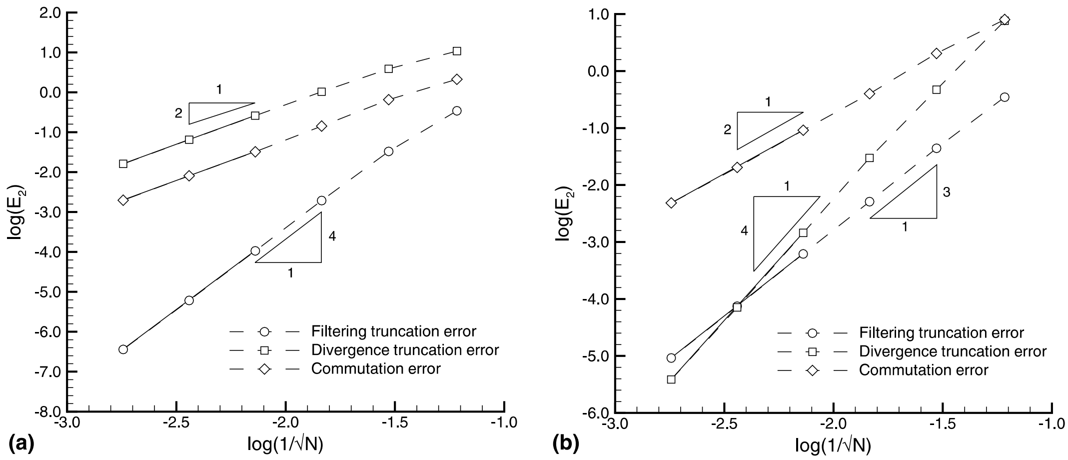

Fig. 6. (a) Variation of L_2-norm of errors with grid refinement on nonuniform grids for $p = 4$ and $q = 2$. Solid lines represent linear least-squares curve fits to data used to determine order of accuracy. (b) Variation of L_2-norm of errors with grid refinement on nonuniform grids for $p = 3$ and $q = 4$. Solid lines represent linear least-squares curve fits to data used to determine order of accuracy.

Table 2
Computed orders of accuracy in L_1-, L_2-, and L_∞-norms of filter truncation error, divergence truncation error, and commutation error on nonuniform grids

			q											
			1			2			3			4		
			L_1	L_2	L_∞	L_1	L_2	L_∞	L_1	L_2	L_∞	L_1	L_2	L_∞
p	2	E_f	2.01	2.01	2.15	2.01	2.01	2.15	2.01	2.01	2.15	2.01	2.01	2.15
		E_d	1.01	1.01	0.98	2.00	2.00	1.96	3.05	3.10	3.04	4.01	4.02	3.85
		E_c	0.98	0.99	0.88	1.35	1.38	1.00	1.10	1.14	0.98	1.22	1.33	1.06
	3	E_f	3.03	3.02	2.81	3.03	3.02	2.81	3.03	3.02	2.81	3.03	3.02	2.81
		E_d	1.01	1.01	0.98	2.00	2.00	1.96	3.05	3.10	3.04	4.01	4.02	3.85
		E_c	0.98	0.99	0.96	2.10	2.10	1.90	2.04	2.05	2.03	2.17	2.23	1.95
	4	E_f	4.04	4.09	4.00	4.04	4.09	4.00	4.04	4.09	4.00	4.04	4.09	4.00
		E_d	1.01	1.01	0.98	2.00	2.00	1.96	3.05	3.10	3.04	4.01	4.02	3.85
		E_c	0.98	0.99	0.94	2.01	2.01	1.60	3.03	3.03	2.80	3.38	3.41	2.98
	5	E_f	5.05	5.06	4.94	5.05	5.06	4.94	5.05	5.06	4.94	5.05	5.06	4.94
		E_d	1.01	1.01	0.98	2.00	2.00	1.96	3.05	3.10	3.04	4.01	4.02	3.85
		E_c	0.99	0.98	1.00	2.01	2.01	1.78	3.01	3.01	2.83	4.08	4.12	3.81

7. Discussion of results

It is instructive to compare the analytical and numerical results presented by VLM and MVM with those obtained in the present work.

The analysis of VLM indicates that the commutation error is $O(n)$ for a filter with n vanishing moments in one dimension. Numerical experiments carried out by VLM confirmed this result. The main differences between the present analysis and that of VLM are that their filter operator was defined in computational space and that their gradient operator was assumed to be continuous. In fact, it can be proved that performing the filtering operation in computational space means that the influence of the gradient operator – be it continuous or discrete – is removed from the commutation error: If a filter operator of order p is used in computational space, the commutation error is of order p regardless of the order of accuracy of the gradient operator. This theoretical result was verified numerically during the present study for quadrilateral grids generated using a tensorial mapping. Thus there is a clear advantage to performing the filtering in computational space.

Regarding the numerical results presented by MVM, it can be demonstrated easily that they are consistent with Eq. (30). Their filter operator is second-order accurate on nonuniform grids because it exhibits vanishing first moments. On nonuniform grids and with the low-order integration scheme, the truncation error of the gradient operator is first order; hence Eq. (30) predicts that the commutation error is also of order one, as observed by MVM. On uniform grids, the high-order integration scheme leads to a second-order accurate approximation of the curl and a third-order accurate approximation of the circulation. However, the commutation error is not identically zero despite the uniform grids, because the stencil of the filter operator changes shape. As a result, the second moments of the filter weights are constant, but the third moments are not. Hence the second term in Eq. (29) vanishes for $n = p = 2$, but not for $n = p + 1 = 3$. Eq. (30) thus predicts the commutation error to be of order two, as observed by MVM. Therefore, the present theory demonstrates that the orders of accuracy of the commutation error observed by MVM were not affected spuriously by the approximation of the gradient operator, but represented a genuine and unavoidable effect.

8. Conclusions and further work

A new filtering method for unstructured grids based on least-squares techniques was presented. Closed-form expressions were given which allow the construction of filtering operators of arbitrarily high order. The new filtering method is easily constructed, does not require special treatment at boundaries, and allows reusing data structures and geometric terms needed by the flow-solution method without filtering.

A new analysis of the discrete commutation error demonstrated that the order of the commutation error is not only dependent on the number of vanishing moments of the filter weights. Instead, the order with which the spatial derivatives are approximated also influences the discrete commutation error. The analytical results were corroborated by grid-refinement studies in two dimensions.

We envisage possible uses of the new filtering method to include explicit filtering of nonlinear terms to prevent generation of high-frequency errors and test filtering for dynamic subgrid-scale models. Furthermore, the new filtering method may be used for filtering of experimental data or direct numerical simulation results for consistent comparisons with LES results.

Further work will focus on the determination of the filter width on nonuniform grids, and the creation of filter weights which result in a specified filter width. We are also developing a compact filtering operator for unstructured grids to reduce the stencil extent for a given order of accuracy.

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