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Accuracy-preserving source term quadrature for third-order edge-based discretization

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ABSTRACT

In this paper, we derive a family of source term quadrature formulas for preserving third-order accuracy of the node-centered edge-based discretization for conservation laws with source terms on arbitrary simplex grids. A three-parameter family of source term quadrature formulas is derived, and as a subset, a one-parameter family of economical formulas is identified that does not require second derivatives of the source term. Among the economical formulas, a unique formula is then derived that does not require gradients of the source term at neighbor nodes, thus leading to a significantly smaller discretization stencil for source terms. All the formulas derived in this paper do not require a boundary closure, and therefore can be directly applied at boundary nodes. Numerical results are presented to demonstrate third-order accuracy at interior and boundary nodes for one-dimensional grids and linear triangular/tetrahedral grids over straight and curved geometries.

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1. Introduction

Node-centered edge-based discretization methods are widely used in practical Computational Fluid Dynamics (CFD) solvers [1–12]. The approach has recently been shown to achieve third-order accuracy for first-order systems of conservation laws on arbitrary triangular [13–15] and tetrahedral grids [16–18] with quadratic least-squares (LSQ) gradients and linearly-extrapolated fluxes. The third-order edge-based discretization scheme is extremely efficient in that the spatial residual can be computed over a single loop over edges with a single numerical flux evaluation per edge. Another striking feature of this scheme is the ability to deliver third-order accurate solutions on linear triangular/tetrahedral grids even for curved geometries [16,19]. Therefore, the third-order edge-based method does not require generating high-order grids. Although high-order surface normal vectors are still needed at boundary nodes to provide formal third-order accuracy for some boundary conditions (e.g., slip wall), the scheme requires only normal vectors at nodes on solid bodies. Practical three-dimensional computations indicate that third-order accuracy is observed without high-order normals for some realistic geometries [16]. A high-order surface representation is required for evaluating integral quantities such as drag, but it is a matter of post-processing and thus does not affect the solution algorithm and the linear computational grid. Because of these attractive low-cost features, the third-order edge-based method has become a subject of great interest to CFD developers and practitioners; see Refs. [16–18,20–22] for recent developments.

The third-order edge-based discretization scheme relies on a special error elimination mechanism. On a regular grid, the truncation error of this scheme has a leading second-order error term proportional to the derivatives of the target equation,

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which thus vanishes and leads to third-order accuracy. This is a well-known mechanism, often called the residual property, common to low-cost high-order methods such as the residual-compact method [23] and the residual-distribution method [24]. In these methods, any additional term added to the target equation must be carefully discretized in order to preserve the residual property and guarantee the design accuracy. This paper focuses on source terms, which arise, for example, in reaction equations, the method of manufactured solutions, and implicit time-stepping schemes [25]. General compatible discretization formulas for source terms are derived and demonstrated by numerical experiments.

In node-centered edge-based methods, source terms are typically evaluated directly at nodes. This placement of the source terms does not generate any truncation error in the Taylor expansion of the residual. To achieve third-order accuracy, the source term discretization must generate a second-order truncation error in the form compatible with that of other terms. Two techniques are currently available to meet the compatibility condition. One is an extended Galerkin source discretization formula [25,26], and the other is a divergence formulation [27]. In the latter, a source term is cast in the form of a conservation law and thus allows a straightforward source term discretization by the third-order edge-based discretization. The compatibility condition is automatically met since all terms are discretized by the same algorithm. Both approaches have been successfully employed in the construction of third-order edge-based schemes. However, a major drawback of these approaches is the requirement for computations and storage of second derivatives of the source term. The additional cost associated with the source term discretizations can be substantial in three dimensions and even more so in unsteady computations where second derivatives need to be stored for all variables at all physical times required to approximate the physical time derivative. For example, in the three-dimensional Euler or Navier-Stokes equations, even with a symmetry assumption, six second derivatives are required for each of five variables at four time-levels with the third-order backward difference formula. In order to generate a truly efficient third-order edge-based scheme for practical three-dimensional unsteady computations, therefore, it is desirable to eliminate the second derivatives from the algorithm. This paper presents a new approach to deriving source term quadrature formulas that do not require second derivatives at all.

A detailed analysis on compatible source discretizations in two and three dimensions has not been reported in the literature. In Refs. [25,26,28], a one-dimensional truncation analysis is given, but it discusses mainly the elimination of first-order error terms and does not discuss the compatible discretization on regular grids in details for the third-order edge-based scheme considered here. In Ref. [27], the compatibility issue is discussed, but discretization details are not provided because the issue is resolved in the differential equation level to make the compatible discretization trivial. In this paper, we provide a detailed account for the compatible source term discretizations, and derive general formulas, demonstrating that previously reported formulas are only a small subset of a general three-parameter family of formulas. In particular, we derive a special subset that does not require second derivatives of source terms. These formulas completely eliminate the additional expense of computations and storage of second derivatives, and dramatically reduce the cost of the third-order edge-based scheme. Furthermore, a unique formula is identified, which does not require any derivative at the neighbor nodes, leading to a source term discretization with a significantly smaller stencil.

The paper is organized as follows. In Section 2, the third-order edge-based discretization is described for a general conservation law. In Section 3, the requirements for compatible source discretizations are discussed. In Section 4, previously reported formulas are reviewed. In Sections 5, new source quadrature formulas are derived. In Section 6, source discretizations at boundary nodes are discussed. In Section 7, numerical results are presented. Finally, the paper concludes with remarks.

2. Third-order edge-based discretization

Consider a scalar conservation law with a source term:

 $div \mathbf{f} = s$,

where **f** is a flux vector function of the solution u, and s is a source term. It is a steady conservation law, but directly relevant to unsteady equations, where physical time derivatives can be discretized in time and treated as a source term as is often done for implicit time-stepping schemes (see, e.g., Ref. [25]). Note also that all discussions are applicable to each component of a more general system of equations. For systems of equations, the flux **f** is a tensor and the source term is a vector **s**.

The target conservation law is discretized on a triangular/tetrahedral grid by the node-centered edge-based method, where a dual control volume is defined around each node by connecting the edge midpoints and the element centroids (and the centroids of the element faces in three dimensions). The discretization at a node j is given by

$$0 = -\sum_{k \in \{k_j\}} \phi_{jk}(\mathbf{n}_{jk}) + \int_{V_j} s \, dV, \qquad (2.2)$$

where V_j is the measure of the dual control volume around the node j, $\{k_j\}$ is a set of neighbor nodes of the node j, ϕ_{jk} is a numerical flux, and \mathbf{n}_{jk} is the directed area vector, which is a sum of the directed-areas corresponding to the dual faces associated with all elements sharing the edge [j, k]. In two dimensions, the directed area vector is defined as a sum of two face normal vectors \mathbf{n}_{jk}^{ℓ} and \mathbf{n}_{jk}^{r} as illustrated in Fig. 1. In three dimensions, it is defined as a sum of the surface normal

(2.1)

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