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A priori mesh quality metrics for three-dimensional hybrid grids

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ABSTRACT

Use of general hybrid grids to attain complex-geometry field simulations poses a challenge on estimation of their quality. Apart from the typical problems of non-uniformity and non-orthogonality, the change in element topology is an extra issue to address. The present work derives and evaluates an *a priori* mesh quality indicator for structured, unstructured, as well as hybrid grids consisting of hexahedra, prisms, tetrahedra, and pyramids. Emphasis is placed on deriving a *direct* relation between the quality measure and mesh distortion. The work is based on use of the Finite Volume discretization for evaluation of first order spatial derivatives. The analytic form of the truncation error is derived and applied to elementary types of mesh distortion including typical hybrid grid interfaces. The corresponding analytic expressions provide relations between the truncation error and the degree of stretching, skewness, shearing, torsion, expansion, as well as the type of grid interface.

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1. Introduction

The need for field simulations that involve complex physics and geometries poses a formidable challenge to grid generation [1–3]. The distribution of points and elements can be quite irregular leading to inaccurate computations. The error is often assessed after the simulation is performed causing multiple grid generations and subsequent field simulations. It is desirable to have an assessment of the appropriateness (quality) of the mesh before performing the simulation.

Grid quality is affected by two primary factors: the local size of the computational elements, and the uniformity of the spatial distribution of the points/elements. A primary method for solving the issue of coarse mesh resolution has been adaptive refinement (e.g. [4–11]). Substantial work has been performed on mesh adaptation. However, relatively less work has been devoted to study the local distribution of the points which relates to the shape of the elements. The present work focuses on this contributor to the truncation error. The truncation error (TE) in a numerical discretization is an indicator of mesh quality. It is of significant importance to evaluate TE for realistic grids. The task is quite difficult given the complexity of hybrid meshes in three dimensions.

Two broad categories of mesh quality indicators involve: (i) *a priori* and (ii) *a posteriori* estimation. The first does not make use of solution field information and looks into the grid element metrics. The second “works” with the solution. The two

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approaches are basically complementary. *A priori* error evaluation can aid mesh generation, while the *a posteriori* estimation can provide guidance to mesh adaptation during the simulation [12]. Definition of a *priori* quality measures can result in (i) fewer grid iterations thus saving computational time, and (ii) more optimum initial grid yielding increased accuracy with reduced computing resources. Further, improving the quality of the grid *a priori* could lead to improved convergence of various flow solvers such as the ones that use "defect correction" techniques to account for bad grid properties.

The present work falls under the first category of *a priori* error estimation, which does not make use of the field solution. As a result, it could label elements as having bad quality in regions where the numerical error could be small, such as uniform flow areas. Previous work bases the *a priori* grid quality assessment on geometric characteristics of the elements such as ratios of sizes of neighboring elements, as well as on element shape measures, such as angles of the elements [13–17]. In the Finite Element method, the quality of a mesh is often given in terms of the element/mesh regularity. This type of approach has given measures that can be computed easily and are quite popular with practical applications.

A posteriori error estimation methods include the *Richardson* extrapolation [18–22]. Use is made of two or more grids with the difference in the yielded solution offering a measure of the local error distribution. Generating appropriately nested meshes can be quite difficult for general hybrid grids. However, use of the "error transport equation" [23] eliminates the need for multiple grids.

Another *a posteriori* method evaluates the error indirectly via tracking of the numerical solution variation (e.g. [24]). Local field features, such as boundary layers, shock waves and vortices are detected using indicators that are based on variations of the computed field parameters, such as the pressure and velocity. The assumption here is that the discretization error is large where the solution variations are high. The method has been primarily used for guiding grid adaptation and not for quantifying the numerical error.

Another school of *a posteriori* error estimation work employs Finite Element discretization and derives analytic expressions of error bounds [25–28]. Various model equations have been utilized in order to provide the estimates. Although, the error bounds do not yield grid quality measures directly, there is potential for such use.

The present work assesses grid quality by computing appropriate metrics of the elements. However, there are three distinguishing aspects of it: (i) the metrics indicating quality are derived *directly* from the analytic form of the truncation error, (ii) the true and not an approximation of the TE expression is employed, and (iii) it can give analytic expressions for a potential improvement of the mesh via re-shaping of the elements.

Truncation error (TE) analysis usually falls under the *a posteriori* estimation. Work in this area has been reported by several publications including the "τ-estimation" [29], and "adjoint" error estimation [30,31]. Recently, a quasi-*a priori* estimation of truncation error was carried out using numerical solutions before convergence [32]. The Finite Difference discretization method has offered a vehicle for calculating TE via performance of *Taylor* series expansions of the solution at the points forming the discretization stencil [33]. The complexity of the expressions has led the previous work to focus on simplified model field equations [34–36]. Nevertheless, those works expressed the dependence of the solution on the grid quality.

Direct relations between TE and mesh distortion parameters, such as departure from orthogonality, skewness and uniformity have been reported in [11] and [37,38]. Significantly less work exists for unstructured meshes [39] and for the Finite Volume (FV) method [40,41]. However, despite the large number of studies on the relation of TE to the numerical solution, there have been few derivations of mesh quality measures based on it.

The primary issue with TE analysis is the complexity of the related expressions, especially for multi-dimensions and for general hybrid mesh topologies. The present work addresses this complexity barrier via employment of symbolic mathematics software [42].

The present effort is based on prior work for two-dimensional hybrid grids [43]. This work was evaluated in [44], and presented favorable agreement between numerical error and the mesh quality indicators derived in [43]. This was a motivation for the present work in three-dimensions.

The following Section 2 derives the analytic form of the truncation error which corresponds to the evaluation of first order spatial derivatives. The main types of mesh distortion in three dimensions, including hybrid mesh interfaces, are defined in Section 3. Section 4 relates the truncation error to mesh distortion. In Section 5, the proposed mesh quality indicator is presented and evaluated. Section 6 deals with application of the proposed grid quality indicator to structured, unstructured and hybrid meshes. Finally, Section 7 contains the summary and the future work.

2. Truncation error for hybrid meshes in three dimensions

The goal of the present work is the creation of *a priori* quality measures for general hybrid three-dimensional meshes, consisting of prisms, hexahedra, tetrahedra, and pyramids. The approach is based on finding the analytic expression of the truncation error (TE) corresponding to the numerical evaluation of first order spatial derivatives. The discretization of first order derivatives is a common calculation not only for fluid flow governing equations, but also for other field equations. For the present study, the common Finite Volume (FV) method will be the discretization approach employed. Previous work [43] has studied the two-dimensional case.

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