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Optimizing computational high-order schemes in finite volume simulations using unstructured mesh and topological data structures

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ABSTRACT

Many numerical methods are based in mesh files to represent the computational domain. Also, an efficient storage and retrieval of mesh information can be achieved by data structures. Moreover, the development of topological operators is one of the important goals of the geometric modeling research field. While it loads mesh files more efficiently, it also allocates less main memory, provides persistence and allows consistent query operations. This paper proposes an improving of the computational scheme of high-order WENO schemes by coupling a standard cell centered, unstructured mesh, finite volume method with an topological data structure. The solver module uses the finite volume technique with a formulation that sets the property values to the control volume centroids. The two dimensional Euler equations are considered to represent the flow of interest. Beyond experiments using the improved approach, the computational cost of the data structure was measured by comparing with the traditional representation, and the results showed that our approach provides scalable loading and managing of meshes, having less memory occupation rate when comparing meshes with an increasing number of elements.

1. Introduction

It is known that performing numeric simulations by using high values for Mach can produce discontinuities, which are shock waves present in the flow field of interest. There are some approaches proposed to deal with this feature, such as upwind schemes, proposed for the flow vector separation [1,2], and tested using the linear reconstruction scheme MUSCL [3], generating discretization with second order on the spatial precision.

Moreover, an effective reduction in the precision order in such second order of nominal precision is observed when dealing with non-structured meshes [4]. Then, reconstructions of MUSCL type lead to schemes of the total variation reduction TVD, where schemes showed a reduction of precision order when discontinuities occur caused by the use of flux limiters [5,6].

Another approach to deal with oscillations in compressible flow computation is the essentially non-oscillatory (ENO) family of schemes. They are uniformly accurate and prevent oscillations in the non-smooth regions by detecting discontinuity and modifying the reconstruction stencil from cell to cell and time level to time level. But, the ENO schemes are

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computationally expensive and can slow the convergence due to their dynamic stencils [7]. Weighted ENO (WENO) schemes were designed to target problems caused by dynamic stencils. WENO schemes remove the effect of non-smooth data near discontinuities in the reconstruction stencil by giving it an asymptotically small weight [8–10]. Furthermore, performance of ENO/WENO schemes in the context of implicit time advance, which is one of the most efficient solution strategies, has not yet been fully explored. The present work also presents some results in this context.

Several ENO and WENO schemes were proposed, because new applications trigger new challenges, which includes simulations with interactions between shock waves and turbulence [11], simulations of hydrodynamic equations [12], simulations with interactions between shock waves and vorticity [13,14], simulations of incompressible flows [15], simulations of viscous-elastic flows [16], spectral analysis of dispersive and dissipative properties [17], fifth-order mapped semi-Lagrangian WENO methods [18]. Therefore, the usage of ENO and WENO schemes wich non-structured meshes are still considered a challenging area [19]. A good study on this topic can be found on [20], where the author applied the ENO and WENO schemes in non-structured meshes through a finite volume technique, solving Euler equations in two dimensions.

This work is an extension of work presented in [21]. While most methods manipulates mesh cells and perform the operations needed when traversing nodes together with the logic of the simulation method, and propose to center all operations into a data structure, designed specifically for the simulation here studied. Therefore, we propose an improving of the computational scheme of high-order WENO schemes by coupling a standard cell centered, unstructured mesh, finite volume method with an implicit topological data structure. The data structure handles all mesh-related functions and operations. All the considered simulations assume the compressible flow of a perfect gas, modeled by the 2-D Euler equations, written in conservation law form. For the spatial discretization, we used a WENO scheme [7], implemented for a cell centered, finite volume method on general unstructured meshes. As for the solution advancement in time we used explicit Runge–Kutta schemes.

WENO is a version of ENO (Essentially Non-Oscillatory) schemes. The cell-average version of ENO schemes originally was introduced and developed by Harten and Osher [22,23]. Later Shu and Osher developed the flux version of ENO schemes and introduced the TVD Runge–Kutta time discretization in [24]. The only difference between these schemes and the standard cell-average version of ENO is how to define a reconstruction procedure which produces a high-order accurate global approximation to the solution from its given cell averages. The cell-average version of ENO schemes attempts to avoid growth of spurious oscillations by an adaptive-stencil approach, in which each cell is assigned its own stencil of cells for the purposes of reconstruction. For each cell the cell-average version of ENO schemes selects an interpolating stencil in which the solution is smoothest in some sense. Thus a cell near a discontinuity is assigned a stencil from the smooth part of the solution and a Gibbs-like phenomenon is so avoided [15]. The Weighted ENO schemes follow this basic idea by using a convex combination approach, in which each cell is assigned all corresponding stencils and a convex combination of all corresponding interpolating polynomials on the stencils is computed to be the approximating polynomial. This is done by assigning proper weights to the convex combination.

The used topological data structure is called Mate Face (MF), which is an implicit topological data structure developed to handle unstructured meshes. It supports management and query operators and also provides code iterators to ease the mesh manipulation. More details can be found on Section 5. The representation of cells is obtained by storing references to vertexes, edges (and faces in the three-dimensional case). Beyond that, mate cells can be retrieved through incident edges or faces. One consideration about the organization in memory of mesh elements in two-dimensional meshes is that for each cell, the number of vertexes is equal to the number of edges and neighbors. This feature eases the implementation and representation of relationships of neighborhood. Then, by using a counter clock orientation, every neighbor cells are indexed in the mesh.

Besides the available traverse queries, geometric operators are also available, and are very used in the simulation code, such as the distance between two points, the area of a cell, the localization of a given query point (like inside a triangle or on the edge of it), the coordinates of a centroid of a cell, among others. The MF supports loading many mesh file formats, such as VTK and VRML.

In this paper, a computational study of the integration of the topological data structure into the solver module was made, where the data structure controls all mesh access by providing operators and iterators that perform complex neighbor queries. We analyze memory and performance issues about Mate Face mesh indexing applied on a simulation using finite volume technique with a formulation that sets the property values to the control volume centroids, using high order methods - the ENO and WENO schemes.

The paper outline is defined as follows. Section 2 presents the theoretical formulation, while Section 3 presents the numerical formulation for the considered scope. Section 4 presents the ENO/WENO schemes and its reconstruction process. Section 5 presents the topological data structure used in this work, including the multi-code integration and challenges. Section 6 shows the experiments made and presents the results of computational performance and of simulations on particular problems. Finally, Section 7 draws conclusions and highlights the contribution of the this work.

2. Theoretical formulation

The 2D Euler equations in conservative form [25], can be written as