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Parallel adaptive wavelet collocation method for PDEs

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ABSTRACT

A parallel adaptive wavelet collocation method for solving a large class of Partial Differential Equations is presented. The parallelization is achieved by developing an asynchronous parallel wavelet transform, which allows one to perform parallel wavelet transform and derivative calculations with only one data synchronization at the highest level of resolution. The data are stored using tree-like structure with tree roots starting at *a priori* defined level of resolution. Both static and dynamic domain partitioning approaches are developed. For the dynamic domain partitioning, trees are considered to be the minimum quanta of data to be migrated between the processes. This allows fully automated and efficient handling of non-simply connected partitioning of a computational domain. Dynamic load balancing is achieved via domain repartitioning during the grid adaptation step and reassigning trees to the appropriate processes to ensure approximately the same number of grid points on each process. The parallel efficiency of the approach is discussed based on parallel adaptive wavelet-based Coherent Vortex Simulations of homogeneous turbulence with linear forcing at effective non-adaptive resolutions up to 2048^3 using as many as 2048 CPU cores.

1. Introduction

The quest for highly scalable adaptive numerical methods is still ongoing despite more than three decades of extraordinary developments in supercomputing. Many attractive mathematical properties of the wavelet multi-resolution analysis such as compression, denoising, and multi-scale decomposition have made it a very promising tool in the challenging search for robust and computationally efficient multi-scale computational approach for modeling and simulation. Adaptive Wavelet Collocation Method (AWCM) is such a technique, which has been developed and thoroughly investigated for parabolic [1,2], hyperbolic [3], and elliptic [4] partial differential equations. It was successfully applied to a wide spectrum of problems including incompressible [5], compressible subsonic [6] and supersonic [3] flows, wavelet-based Adaptive Large Eddy Simulation [7–13], thermoacoustic wave propagation [14], Rayleigh–Taylor instability [15], ocean modeling [16], combustion [17], fluid–structure interactions [18,19], viscoelastic and poro-viscoelastic flows [20–22].

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Adaptive Wavelet Collocation Method [1–4] is based on the "second generation wavelets" [23,24]. In AWCM, the partial differential equations are solved in physical space on an adaptive nested (dyadic) computational grid. This prevents the major difficulties associated with adaptive wavelet Galerkin methods: challenging treatment of nonlinearities and general boundary conditions. The evaluation of the nonlinear terms in adaptive wavelet collocation methods is performed in a physical domain similar to pseudo-spectral methods. The grid adaptation in wavelet collocation methods is done similarly to other wavelet-based methods and is based on analyzing the wavelet coefficients. Despite enormous compression achieved by wavelets, e.g. 99%, very large-scale simulations cannot yet fit onto a single process and require highly scalable parallel algorithms.

Despite almost 30 year history of wavelets since their introduction by Grossmann and Morlet [25] and wide use in science and engineering, very little attention was paid to parallel adaptive wavelet methodologies. Until recently, most of the efforts were put into the development of parallelization strategies for non-adaptive wavelet algorithms, e.g., a communication-free parallel discrete wavelet transform [26], a communication efficient fast wavelet transform without distributed matrix transpose [27], a distributed parallel biorthogonal lifted wavelet transform [28], a parallel wavelet transform for distributed and shared memory architectures [29], and parallel GPU based discrete wavelet transforms [30–33]. The only noticeable attempts to develop parallel adaptive wavelet-based methods are multi-block adaptive wavelet method by Rossinelli et al. [34] and Adaptive Wavelet Multiresolution Representation (AWMR) method by Paolucci et al. [35], with the latter published while the manuscript was under review. Thus, the main objective of this paper is to present the extension of the AWCM [1–4] for massively parallel computers.[1]

The paper is organized as follows. The one- and multi-dimensional second generation wavelet transforms are reviewed thoroughly in Section 2. The challenges associated with the parallelization of the update-stage of the second generation wavelet transform are explained in Section 3, and a parallel asynchronous second generation wavelet transform is then introduced. The robust tree structure database utilized in this study is discussed in Section 4. The grid adaptation strategy based on wavelet-thresholding is reviewed in Section 5, where the concepts of reconstruction-check, safety/adjacent zone along with significant/adjacent masks are introduced. The finite difference based derivative algorithm for the adaptive wavelet collocation method and the use of ghost points are discussed in Section 6. After a short discussion of data migration in Section 7, the four different static and dynamic domain partitioning methods utilized in this study are explained in Section 8. The algorithm of the resulting parallel adaptive wavelet collocation method (PAWCM), based on the aforementioned components, is illustrated in Section 9. This versatile general parallel dynamically adaptive PDE solver is then used to perform a comprehensive strong-scalability study of the PAWCM for the velocity-based Coherent Vortex Simulations (CVS) of linearly forced homogeneous turbulence, Section 10. The challenges associated with the buffer zone size, the speedup slope and saturation are analyzed in detail and the numerical results are compared with an asymptotic parallel efficiency, which is derived. Finally, conclusions are given in Section 11.

2. Wavelet transform

In this section we briefly discuss the key aspects of the second generation wavelet construction, which are essential for understanding of the Parallel Adaptive Wavelet Collocation method. For more details we refer the reader to Refs. [1,2,4,23,24].

The one-dimensional second generation wavelets are constructed on an interval Ω with arbitrary distribution of grid (collocation) points. The construction is performed on an arbitrary set of interpolating points, $\{x_k^j \in \Omega\}$, which are used to form a set of nested grids

$$\mathcal{G}^j = \left\{ x_k^j \in \Omega : \; x_k^j = x_{2k}^{j+1}, \; k \in \mathcal{K}^j \right\}, \tag{1}$$

where x_k^j are the grid points of the j level of resolution.

The restriction $x_k^j = x_{2k}^{j+1}$ guarantees the nestedness of the grids, i.e. $\mathcal{G}^j \subset \mathcal{G}^{j+1}$. Following the construction of second generation wavelets described in [23,24], one-dimensional scaling functions $\phi_k^j(x)$ ($k \in \mathcal{K}^j$) and wavelets $\psi_l^j(x)$ ($l \in \mathcal{L}^j$) are constructed such that a function $u(x)$ can be decomposed as

$$u(x) = \sum_{k \in \mathcal{K}^0} c_k^0 \phi_k^0(x) + \sum_{j=0}^{+\infty} \sum_{l \in \mathcal{L}^j} d_l^j \psi_l^j(x), \tag{2}$$

where $\mathcal{K}^j$ and $\mathcal{L}^j$ are some index sets associated respectively with scaling functions and wavelets on level j. One may think of a wavelet decomposition as a multilevel or multiresolution representation of a function, where each level of resolution j (except the coarsest one) consists of wavelets ψ_l^j having the same scale but located at different positions. Note that scaling function coefficients represent smoothed version of the function at the current scale, while the wavelet coefficients represent the details of the function between the current scale and the next finest scale. An important property and strength

[1] PAWCM was first reported in Ref. [36].