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High Order Finite Difference Discretization for Composite Grid Hierarchy and Its Applications

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Abstract. We introduce efficient approaches to construct high order finite difference discretizations for solving partial differential equations, based on a composite grid hierarchy. We introduce a modification of the traditional point clustering algorithm, obtained by adding restrictive parameters that control the minimal patch length and the size of the buffer zone. As a result, a reduction in the number of interfacial cells is observed. Based on a reasonable geometric grid setting, we discuss a general approach for the construction of stencils in a composite grid environment. The straightforward approach leads to an ill-posed problem. In our approach we regularize this problem, and transform it into solving a symmetric system of linear of equations. Finally, a stencil repository has been designed to further reduce computational overhead. The effectiveness of the discretizations is illustrated by numerical experiments on second order elliptic differential equations.

AMS subject classifications: 35J57, 47A52, 65M50, 65N06

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1 Introduction and preliminaries

Adaptive mesh refinement (AMR) is a simple and popular framework to reduce the computational overhead in dealing with large scale modern scientific computational problems. It is commonly used in a number of research areas, and there are several software packages available that implement AMR to solve problems on different scales. For

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example, APBS [2, 16] uses multilevel adaptive finite elements for solving the Poisson-Boltzmann equation in order to study the chemical properties of complex molecules or polymers and their microscopic behavior with implicit solvents. Macroscopic applications can be found in ENZO [7, 23], designed for multi-physics simulations in astrophysics and cosmology. General purpose packages such as CHOMBO [10], developed by a team at Lawrence Berkeley National Laboratory (LBNL), is designed for the solution of multidimensional elliptic equations and time-dependent problems. Packages such as PARAMESH [21] and AGRIF [12] are similar tools that have been developed for solving partial differential equations (PDEs) in a parallel environment.

Based on an adaptive mesh hierarchy, there are several approaches for transforming the partial differential equations into their discrete counterpart. Attempts that incorporate classical discretization methods like finite difference method (FDM), the finite element method (FEM), or the finite volume method (FVM) within the AMR framework have been very successful. It was introduced by Berger and Oliger for the study of hyperbolic partial differential equations using an adaptive finite difference method (AFDM) [5]. This same discretization framework was used by Berger and Colella to carry out simulations of hydrodynamic shocks [3]. More recently, this approach has been used for the study of the phase separation process using the Cahn-Hilliard equations [8], for the study of multiphase incompressible flows [9], and for simulating solid tumor growth [27], to name just a few examples. This approach also has a long history within the finite element community. It is a standard tool in elasticity theory computations, specially in the study of solid fracture [25]. In recent years it has also proved to be a very effective tool in electronic structure computations, within the orbital-free [15] or the Kohn-Sham [29] approaches to density functional theory. The finite volume method could also be formulated within an adaptive mesh refinement framework. In [19], the incompressible heat flow problem was studied using an adaptive finite volume method (AFVM); in [17] the authors investigated the multi-phase flow and transport in porous media based on the same framework; and in [28, 31] the authors developed an adaptive coupled level-set/volume-of-fluid (ACLSVOF) method for interfacial flow simulations on unstructured triangular grids.

High order numerical schemes are also a trend for development of high performance solvers and are necessary to simulate complex and large systems. There is also a large body of literature on the subject. For instance, in [20] the authors reported a parallel implementation of a solver for the Poisson-Boltzmann equation with periodic boundary conditions using a sixth order finite difference scheme. The three dimensional sixth order scheme is basically a Cartesian product of three one dimensional sixth order stencils. An alternative approach to implement and achieve high order accuracy can be found in compact schemes. For compact finite difference methods, explicit formulas have been presented in earlier works. A compact fourth order scheme can be found in [30], while a sixth order compact scheme is applied in [26]. Note that the sixth order compact discretization relies on derivatives of the right hand side. It is well known that compact schemes higher than sixth order on uniform grids do not exist, unless derivatives of the