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Adaptive Hybrid Mesh Refinement for Multiphysics Applications

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Abstract. The accuracy and convergence of computational solutions of mesh-based methods is strongly dependent on the quality of the mesh used. We have developed methods for optimizing meshes that are comprised of elements of arbitrary polygonal and polyhedral type. We present in this research the development of r - h hybrid adaptive meshing technology tailored to application areas relevant to multi-physics modeling and simulation. Solution-based adaptation methods are used to reposition mesh nodes (r -adaptation) or to refine the mesh cells (h -adaptation) to minimize solution error. The numerical methods perform either the r -adaptive mesh optimization or the h -adaptive mesh refinement method on the initial isotropic or anisotropic meshes to equidistribute weighted geometric and/or solution error function. We have successfully introduced r - h adaptivity to a least-squares method with spherical harmonics basis functions for the solution of the spherical shallow atmosphere model used in climate modeling. In addition, application of this technology also covers a wide range of disciplines in computational sciences, most notably, time-dependent multi-physics, multi-scale modeling and simulation.

1. Introduction.

Mesh generation is a crucial first step for the solution of multi-dimensional problems in field simulation. The accuracy and convergence of solutions using mesh-based numerical methods are strongly dependent on the quality of the mesh being used. Mesh generation lies at the core of many areas in advanced computational sciences and engineering and has emerged as an enabling technology and a major pacing item in computational modeling and simulation. In particular, adaptive mesh optimization and refinement plays an important role in complex high-fidelity simulation fields. Generation of a quality mesh to support these calculations is a challenging, multi-disciplinary problem.

Over the years, computational mesh discretization and optimizations have been intensely studied and a variety of approaches were developed for generating adaptive structured and unstructured computational meshes. However, not a great deal of effort in the field of mesh generation has been devoted to the study of the generation of adaptive high-quality hybrid meshes (i.e., mixed cell elements). Traditional approaches to mesh generation have utilized either structured quadrilateral/hexahedral or unstructured triangular/tetrahedral elements. The literature is rich with materials describing such methodologies and a survey of these techniques can be found in [1-5]. There are advantages and disadvantages to both approaches, and thus the approach selected has been dependent on the particular application. Structured meshes have simple connectivity and high computation efficiency but are time consuming to construct, and cannot be easily adapted to complicated geometries, whereas, unstructured meshes are easy to generate but have higher overhead, and, sometimes, lower accuracy. Unfortunately, employing a single type of mesh technology appears to be too restrictive in resolving complex multi-dimensional multi-scale fields accurately and efficiently.

Recently, an alternative new approach to the meshing problem has been the use of hybrid meshes. These meshes provide more flexibility than traditional approaches through the use varying cell topologies ranging from hexagons, pentagons, quads, to triangles in two dimensions and hexahedra,

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prisms, and pyramids, to tetrahedral in three dimensions. The hybrid mesh approach attempts to combine the advantages of both structured and unstructured approaches.

We have focused our efforts on developing technology to create and adapt high-quality hybrid meshes for climate modeling and nuclear reactor simulation. We have utilized algebraic algorithms and partial differential equations (PDE) methods for the generation of hybrid meshes. Our meshing efforts include methods for optimizing meshes that are comprised of elements of arbitrary polygonal/ polyhedral type. These methods provide the ability of focusing or refining mesh resolution over areas of particular interest yet strives to equidistribute the node density of the mesh while improving cell aspect ratios.

2. Adaptive Hybrid Mesh Optimization.

The principle objective of this paper is to present an overview of current meshing efforts and development at Oak Ridge National Laboratory. Our capability is geared for generating high-quality adaptive meshes for petascale applications. In this work, we have researched and developed tools and algorithms for the generation and optimization of adaptive hybrid meshes using finite-volume discretization approach. The hybrid mesh approach attempts to combine the advantages of both structured and unstructured meshing strategies. The prismatic and hexahedral elements are used in regions of high solution gradients, and tetrahedra are used elsewhere with pyramids used at the boundary between these two element categories to provide a transition region. In addition, the polyhedral/icosahedral meshes are often the best choice of solving symmetric computational problems (e.g., inertial confinement fusion and climate modeling). They have the properties of producing symmetric higher order orthogonal meshes and do not introduce artificial geometric interfaces. The geometry of the mesh and its symmetries are matched to the analytical and numerical methods used to solve the governing equations. Furthermore, hexahedral/prismatic layers close to wall surfaces exhibit good orthogonality and clustering capabilities characteristic of structured mesh generation approaches. The mesh example demonstration in figure 1 showcase the generation of hybrid surface and volume meshes on symmetric multi-region geometries. The geometry of the mesh and its symmetries are matched to the analytical and numerical methods used to solve the governing equations.

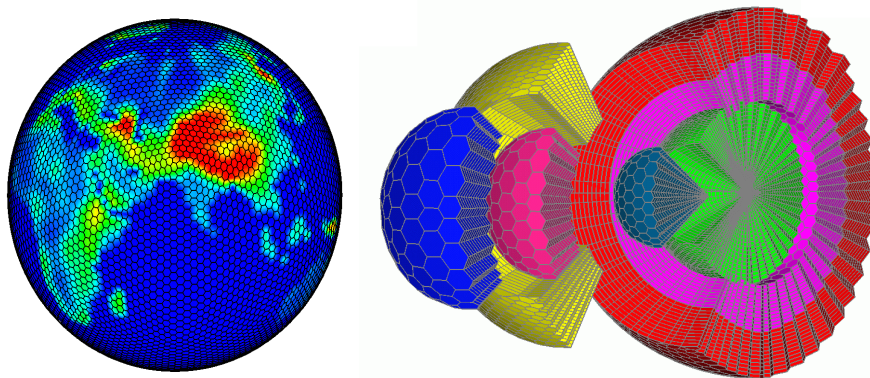


Figure 1. Hybrid icosahedra surface mesh (left) and multi-material hybrid volume mesh (right).

Our approach to the meshing problem is to utilize tools and technologies developed by the center of Interoperable Technologies for Advanced Petascale Simulations (ITAPS) into our integrated geometry, meshing and adaptivity server (GMAS). The ITAPS center is one of the mathematics Enabling Technologies Centers (CET) in the Department of Energy's Scientific Discovery through Advanced Computing (SciDAC) program. The center's focus is on developing advanced scalable interoperable software associated with geometry, mesh, and field manipulation. It also provides the necessary meshing tools to reach new levels of understanding through the use of high-fidelity calculations based on multiple coupled physical processes and multiple interacting physical scales.

GMAS is a code intended to integrate scientific software and provide geometry, meshing and adaptivity services for PDE solvers of coupled multiphysics applications without exposing details of the underlying libraries. GMAS is currently used to handle multiple meshes for multiple PDE solvers for a given geometry in a coupled application, and it provides the basic infrastructure to allow the application to evaluate fields over multiple meshes. It has been used in multiphysics applications to provide meshing services for a neutron transport simulation code and a solvent extraction fluid flow code in development. The following example (figure 2) exhibits coarse and refined anisotropic meshes generated using GMAS. The fine mesh is used to capture boundary layer flow and heat flux and the coarse mesh is needed for neutronics in the coolant channels of high-temperature test reactor (HTTR).

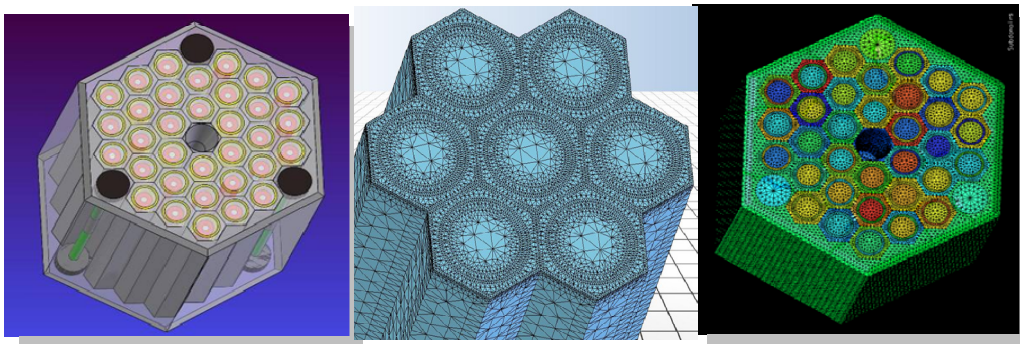


Figure 2. HTTR multi-material geometry (left), initial coarse mesh (middle), refined mesh (right).

3. Hybrid Adaptive Meshing.

Our ongoing meshing research and development concentrates on hybrid mesh adaptation strategies, along with mesh optimization. In certain multiphysics applications, the size of mesh at a given location should be selected to resolve the smallest physics length scale at that point. Too few mesh elements result in a locally incorrect solution; whereas, too many mesh cells slow the calculation needlessly. The quality of the solution also depends on other mesh characteristics, such as, element shapes and connectivity, smoothness and “impedance” requirements, element orthogonality, anisotropic elements to match anisotropic physics, and boundary representation requirements.

We have developed a hybrid finite volume-based mesh generator for r -adaptivity with certain emphasis on climate modeling. We employ conformal mapping to derive the elliptic PDEs models for the optimization and adaptation of hybrid surface meshes, see [6]. However, an algebraic method is used in the case of combined h - p adaptivity wherein the degree p of the polynomial basis functions can be adapted to the features of the field quantities. The following demonstrated examples (figure 3) exhibit the generation of r - h adapted hybrid surface meshes for climate modeling. It has been shown that mesh adaptation can reduce simulation error in prediction of the dynamics of the climate system.

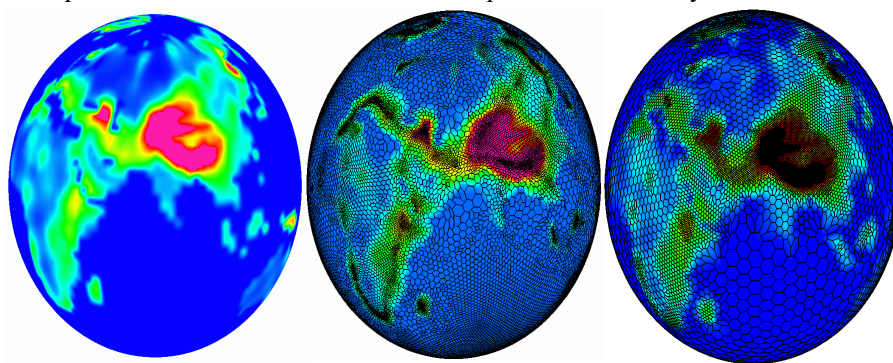


Figure 3. Orography field (left), r -adaptivity (center) and h -adaptivity (right) for climate modeling.

Applications to this capability also include field transformation and mapping across multiple meshes. In particular, the generation and smooth adaptive grid transformations for resolving orography (earth surface height) and fine-scale processes in climate modeling. Orography plays an important role in determining the strength and location of the atmospheric jet streams. Its impact is most pronounced in the numerical simulation codes for the detailed regional climate studies. In addition, orography is a crucial parameter for prediction of many key climatic dynamics, elements, and moisture physics, such as rainfall, snowfall, and cloud cover. The phenomenon of climate variability is sensitive to orographic effects and can be resolved by the generation of finer meshes in regions of high altitude. Resolving orography produces a more accurate prediction of wetter or dryer seasons in a particular region. And moreover, orography defines the lower boundary in general circulation models. The following example (figure 4) shows a very dense orography field on planar uniform mesh with two kilometer gridded resolution (figure 4-top). The initial field data size was two gigabits and it was obtained from <http://www.ngdc.noaa.gov/mgg/topo/globe.html>. We have successfully introduced *h-p* adaptivity to a least-squares method with spherical harmonics basis functions for field mapping and mesh adaptation. The end mesh (figure 4-bottom) is much coarser at the sea level (50-kilometers) and finer at the high altitude regions (1-kilometers) with only a fraction of the original field data size. Moreover, the orography field was globally preserved to very small accuracy. For a full detailed presentation of this adaptive meshing approach we refer the reader to [7,8].

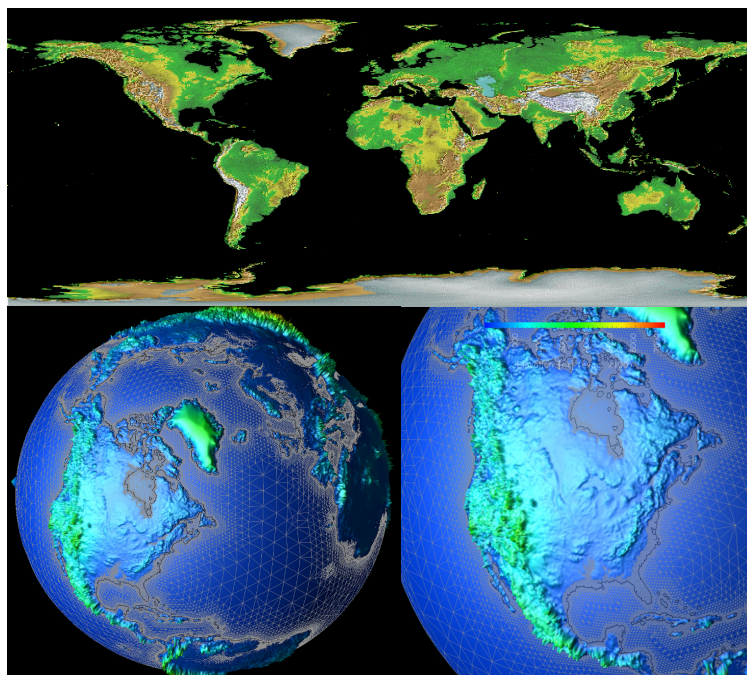


Figure 4. Coupled orography field transfer with *h*-adaptivity. Planar orography field (top), *h*-adapted surface mesh (bottom-left) and closeup view of the mesh (bottom-right).

4. Meshing and Load Balancing.

The advent of petascale computing creates new opportunities for representation of realistic geometries via meshing at an unprecedented fidelity. Fine meshes also have a beneficial impact on the accuracy of the PDE's solution if they can be generated with sufficient quality. One central effort is the generation of meshes with large number of elements that truly represent complex multi-region geometries and adapt (*h*-adaptivity) to areas of steep solution gradient, notably at the walls of the vortex generator. Such very large meshes can only be created with the help of parallel computing. Our approach is to

generate an initial mesh that resolves the surface geometry at any practical tolerance in a single processor while keeping the interior volume mesh coarse. In practice, such meshes can only be of unstructured type and there is a risk that many elements will become singular or of unacceptable aspect ratio. Next, we leverage tools from the ITAPS center into GMAS to partition the mesh, distribute the data, refine/improve the quality of the distributed mesh in parallel, and balance the load of the new mesh. Existing functionality of GMAS already provides the partition and distribution of the data (figure 5), we are currently concentrating on developing of the parallel mesh refinement, data distribution and load balancing.

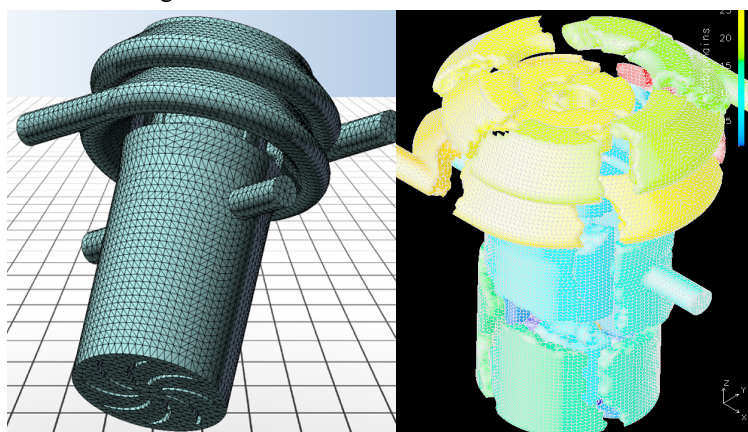


Figure 5: Meshing and partitioning of Centrifugal contactor.

5. Conclusions.

The paper presents an overview of the current tools being developed by ITAPS and GMAS for the generation, optimization, and adaptation of hybrid meshes. In addition, the research in this paper is involved in the development of r - h - p adaptive technology tailored to application areas relevant to other simulation fields. The r - h - p adaptive meshing approach and its underlying methods can be attractive to many application areas when solving three-dimensional, multi-physics, multi-scale, and time-dependent PDE's. This method builds on r - h -refinement/coarsening, p -refinement, interpolation, and error estimation applied to climate modeling and astrophysics simulation.

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