Rensselaer Component of the
Terascale Simulation Tools and Technologies

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1. Introduction

The Terascale Simulation Tools and Technologies (TSTT) SciDAC center focused on the development and application on SciDAC applications of advanced technologies to support unstructured grid simulations. As part of the TSTT team the RPI group focused on developing automated adaptive mesh control tools and working with SciDAC accelerator and fusion applications on the use of these technologies to execute their simulations. The remainder of this report provides a brief summary of the efforts carried out by the RPI team to support SciDAC applications (Section 2) and to develop the TSTT technologies needed for those automated adaptive simulations (Section 3). More complete information on the technical developments can be found in the cited references and previous progress reports.

2. Applications Developments:

2.1 Accelerator Modeling with SLAC National Accelerator Laboratory

In order to perform the analyses needed in the design of next generation accelerators, researchers at the SLAC National Accelerator Laboratory have been developing higher order parallel finite element methods. High-order methods are well known to provide higher rates of convergence, which can provide SciDAC applications with an effective means to address critical applications with dramatically reduced levels of computational effort. Two areas where the RPI TSTT team bas contributed to SLAC efforts are the development of parallel adaptive mesh control loops and tool to produce curved finite element mesh entities as needed to properly apply high order methods on domains defined as CAD models.

The combination of high required accuracy and geometric complexity of full accelerator cavity assemblies requires the execution of automated mesh adaptation that operates in parallel. The RPI TSTT team developed parallel adaptive tools to integrate with the parallel version of OMEGA3P. The key tools/developments included a parallel mesh database [25-27,29], parallel dynamic load balancing [29], and parallelization of mesh adaptation procedures [1,24], solution transfer functions and error estimation modules. These procedures effectively supported simulations providing accurate solution results [11,15,18].

A complexity that arises when applying higher order finite elements to complex 3-D domains is the need to have curved finite elements. The common approach to the construction of such meshes is to take advantage of available mesh generators that perform straight-sided mesh generation and then curve the mesh edges and faces adjacent to curved domain boundaries to conform to the boundaries. However, the resulting meshes often contain invalid elements because curving the mesh entities to conform to boundaries can lead to negative Jacobian determinants in the closures of elements. To address this problem, the RPI TSTT team has been developing mesh curving techniques that to be able to produce and control curved meshes [19,20,37]

2.2 Fusion Modeling with PPPL

The RPI TSTT team has been working with the Steve Jardin's group at PPPL to create accurate MHD simulation technologies. Initial efforts looked into extending adaptive discontinuous Galerkin formulations to solve MHD problems [14]. As the PPPL group moved more heavily to the use of high order finite element methods we investigated the potential advantages of stabilized high-order finite element formulations [9]. As the PPPL group began to develop their new high-order code M3D-C1, the RPI TSTT became directly involved with developing the structures needed to support parallel mesh adaptation and to construct the 2-D parallel adaptive mesh control tools needed [2,12].

3. TSTT Technology Development

3.1 Mesh Interface

The TSTT team has defined a mesh interface to support unstructured meshes based on entities and their adjacencies [5]. The RPI team was involved in its design and implementation [8,22]. The RPI implementation of the TSTT mesh interface builds on its research and development of flexible mesh databases that can store the desired mesh adjacencies [26]. The RPI implementation was fully implemented to support parallel distributed meshes [25,27,29,33].

3.2 Geometry Interface

The geometric domain is a central part of the high level definition of a simulation problem. In today's environments the key sources of these domain definitions are CAD models, meshes (simulation meshes and STL files) and image data. To effectively support general simulation capabilities, including automated adaptive analysis and evolving geometry problems, it is necessary that a high level understanding of the domain definition be used. The concept of geometric model topological entities and their adjacencies provide a natural abstraction for supporting these needs. A set of functions have been defined and implemented to support the interactions of the simulation process with general non-manifold geometric domains [3,4,31].

3.3 Mesh Adaptation Service

Adaptive methods are central to ensuring the reliability of the simulations used for SciDAC applications. An area of emphasis of the RPI TSTT team has been the development a service to that can be directly integrated with SciDAC analysis procedures to provide adaptive simulations that can greatly increase the reliability of the results obtained. The service that has been developed to support generalized mesh adaptation by controlling the mesh size through the domain of interest [16]. To ensure the ability to deal with general curved geometries that can come from CAD systems, the procedures build on a generalized interaction with the geometric model and ensure the mesh can properly represent the domain of interest [17,19,20,30]. The mesh adaptation service, which fully operates in parallel [1,29,32], has been used to develop adaptive simulations for accelerator and fusion simulations as discussed in Section 2. It has also been uesd to support several other applications including ones with evolving geometries [35,36], and ones requiring anisotropic mesh adaptation [6,21,28]. Some of methods and ideas used in the development of the mesh adaptation service are being used to support adaptive multiscale simulations [7,34].

4. Publications:

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