MESH DATA MANAGEMENT COMPONENTS FOR PETASCALE ADAPTIVE UNSTRUCTURED MESH BASED SIMULATIONS

By

Ting Xie

A Thesis Submitted to the Graduate

Faculty of Rensselaer Polytechnic Institute

in Partial Fulfillment of the

Requirements for the Degree of

DOCTOR OF PHILOSOPHY

Major Subject: COMPUTER SCIENCE

Approved by the
Examining Committee:

____
Dr. Mark S. Shephard, Thesis Adviser

____
Dr. Christopher D. Carothers, Member

____
Dr. Elliot Anshelevich, Member

____
Dr. Kenneth E. Jansen, Member

____
Dr. Seegyoung Seol, Member

Rensselaer Polytechnic Institute
Troy, New York

May 2012
(For Graduation August 2012)

ABSTRACT

The simulation of complex physics problems over general 3D geometries can be effectively done using unstructured meshes that in many cases will have millions or billions of elements that can be only solved on massively parallel computers. The objective of this thesis is to support specific new unstructured mesh functionalities required by large-scale adaptive simulations building on the Flexible and distributed Mesh DataBase (FMDB).

To extend FMDB's functionalities in a sustainable manner that FMDB can easily evolve to support future application requirements, this work introduces a set of generic programming components for sets, iterators and tags designed for use in adaptive simulation software tools.

FMDB is then extended to address three specific requirements from large scale adaptive simulations. First, the generic set component is extended to support mesh set functions for mesh entities in parallel and is applied to support boundary layer mesh adaptations. Second, to support specific applications where the mesh representation on specific unconnected geometric model entities must match, such as applications with periodic boundary conditions, the capability of mesh matching is developed. Third, since it is desirable to increase the number of processors in the simulation as the mesh size increases, the capability to have multiple parts per process is developed to define new mesh partitions with alternative partitioning strategies and migration algorithms, based on an enhanced partition model.

With the addition of these capabilities, FMDB has been able to support a large class of adaptive unstructured mesh simulations on petascale supercomputers, including IBM BlueGene (BG/P) and Cray system. Applications on meshes of billions of elements distributed over $O(100,000)$'s of processors demonstrate the effectiveness of the software components developed in this work.