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Interoperable mesh components for large-scale, distributed-memory simulations

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Abstract. SciDAC applications have a demonstrated need for advanced software tools to manage the complexities associated with sophisticated geometry, mesh, and field manipulation tasks, particularly as computer architectures move toward the petascale. In this paper, we describe a software component — an abstract data model and programming interface — designed to provide support for parallel unstructured mesh operations. We describe key issues that must be addressed to successfully provide high-performance, distributed-memory unstructured mesh services and highlight some recent research accomplishments in developing new load balancing and MPI-based communication libraries appropriate for leadership class computing. Finally, we give examples of the use of parallel adaptive mesh modification in two SciDAC applications.

1. Introduction

Many simulations for solving partial differential equations (PDEs) require the ability to model complex geometries defined by CAD or other engineering design tools. Such geometries in turn require the generation of meshes that have high fidelity to both the computational domain description as well as to the features of interest in the numerical solution, e.g., regions of high gradients. This process is further complicated by the need to perform simulations on petascale computers where additional issues such as load balance, communication costs, and optimal data decompositions come into play. Because these operations are common to many simulations, reusable software for these tasks can be shared across many application codes which could reduce the time, effort, and expertise required to develop and maintain simulation software.

Reuse of scientific software has traditionally relied on the use of *frameworks* or *library-based* implementations and many useful tools have been developed over the years for both unstructured (e.g., [1, 2, 3, 4, 5]) and structured meshes (e.g., [6, 7, 8]). In addition, libraries that provide mesh quality improvement [9, 10], front tracking [11], mesh refinement [12], and parallel partitioning and load balancing [13] have been developed as well. However, the use of libraries or frameworks can significantly hamper experimentation with different software

instances that provide similar functionality. In particular, libraries of similar purpose often package functionality in very different ways. Consequently, data structures shared between the application and library and even the control flow between the application and library may need to be totally re-designed. This is especially true for meshing and geometry libraries where applications often directly access the underlying data structures, which can be quite different from implementation to implementation. Thus, using different libraries interchangeably or interoperably for this functionality has proven difficult at best and has hindered the wide spread use of advanced meshing and geometry tools developed by the research community.

Components represent a higher level of abstraction than libraries. Essentially, a component defines both a *specification* for an application programming interface (API) and an abstract *data model* defining the semantics of the data that is passed through the interface. There are several key advantages to using a component-based approach in that the focus is on interfaces rather than on data structures or file formats. This allows any application using a component to use another implementation of the same component API, because all implementations have substantially equivalent functionality.

In this paper, we describe a parallel unstructured mesh component developed by the Interoperable Technologies for Advanced Petascale Simulations (ITAPS) project (Section 2). As we have worked to scale the software that uses our mesh component implementations to 100,000 processors and beyond, several interesting research projects to improve load balance and reduce communication costs have arisen. We briefly describe our work in these areas and show both weak and strong scaling results for implicit finite element/volume solvers and adaptive mesh refinement services (Section 3). We conclude by showcasing the use of the adaptive mesh refinement service in accelerator and fusion SciDAC applications (Section 4).

2. The ITAPS parallel mesh component

The ITAPS parallel mesh component builds on previous work that resulted in the definition of a serial abstract data model and interfaces for serial mesh data. In this section, we briefly describe the key concepts from that earlier work that are germane to the current discussion, and describe the parallel data model (Section 2.1) and language- and data-structure-independent interface to support query and modification of meshes on distributed memory computers (Section 2.2). We then highlight several software implementations of the interface and services that use the serial and parallel interfaces to provide key functionality to application codes (Section 2.3).

2.1. The abstract data model

At a high level, the ITAPS data model divides the data required by a simulation into three *core data types*: the geometric data, the mesh data, and the field data. These core data types are associated with each other through *data relation managers*. The data relation managers control the relationships among two or more of the core data types, resolve cross references between entities in different groups, and can provide additional functionality that depends on multiple core data types. Key building blocks within these data models are the concepts of *entities*, *entity sets*, and *tags*.

- *Entities* are used to represent atomic pieces of information such as vertices in a mesh or edges in a geometric model. Entity adjacency relationships define how the entities connect to each other and both first-order and second-order adjacencies are supported.
- *Entity sets* are arbitrary collections of entities that may be an ordered list or unordered. The two primary supported relationships among entity sets are *contained in* and *parent/child* to allow for subsetting and hierarchical applications. In addition, entity sets also have “set operation” capabilities such as set subtraction, intersection, or union.

- *Tags* are used as containers to attach user-defined data to ITAPS entities and entity sets. Tags can be multi-valued which implies that a given tag handle can be associated with many different entities. We support specialized tag types for improved performance as well as the more general opaque case that allows any type of data to be attached.

To support many of the services that applications desire, such as adaptive mesh refinement, the data model includes the concept of modification to allow changes to geometry, topology, or set structure. In the case of the mesh, capabilities include changing vertex coordinates and adding or deleting entities. Modification often requires interactions between the mesh, geometry and field data models and is one of the primary uses for the data relations manager.

The parallel ITAPS data model extends the concepts described above to handle the requirements of distributed memory applications. In such applications, the unstructured mesh is typically divided or *partitioned* over the independent processor memories of the computer. To be useful to applications, we must maintain information about mesh entities and their adjacencies that is “shared”. In addition, applications require the ability to move mesh entities and their associated information between different processors to update the mesh partition while maintaining this shared information. Moreover, applications expect that the mesh data model defined previously will continue to work as expected within a process or for global address spaces and shared memory paradigms. These requirements are addressed through the following additional core concepts.

- A mesh *partition* is a decomposition of the mesh entities (e.g., vertices, edges, faces, and regions) into subsets called *parts*. The partition is responsible for mapping the entities to parts and for mapping the parts to processes. We note that each process may have one or more parts and that each part is wholly contained within a process. Parts are identified globally by unique part IDs and, within a process, by opaque part handles. A partition has a communicator associated with it. Thus “global” operations are performed with respect to data in all parts in the partition’s communicator and “local” operations are performed with respect to either a part’s or process’s data.
- Mesh entities are *owned* by exactly one part in the partition where ownership imbues the right to modify. It is important to note that ownership is not necessarily static during the course of a computation and can be changed due to a repartitioning of the mesh or due to local micro-migration operations. In addition, some entities will have read-only copies on other parts, for example, along part boundaries and for ghosting operations. No globally unique entity IDs are required or supplied by the data model although they can be constructed by the user as a pair [*part ID*, *entity handle*].
- Mesh entities can be further classified as an *internal entity* (an owned entity not on an interpart boundary), a *part-boundary entity* (an entity on an interpart boundary which are shared between parts), or a *ghost entity* (a non-owned, non-part-boundary entity); see Figure 1. *Copies* are defined to be all ghost entities plus all non-owned part-boundary entities. The data model defines rules for the amount of information about copies that an implementation must manage. For example, an entity’s owner must store information about all copies of the entity, and a copy must store information about the entity’s owner. Remote parts and entities are computed after mesh modification so that queries for remote data do not require communication.

2.2. The ITAPS iMeshP interface

Once the abstract data model is defined, the next step to creating interoperable technologies is to define common interfaces that support its functionality. A key aspect of the ITAPS approach is that we do not enforce any particular data structure or implementation with our interfaces,

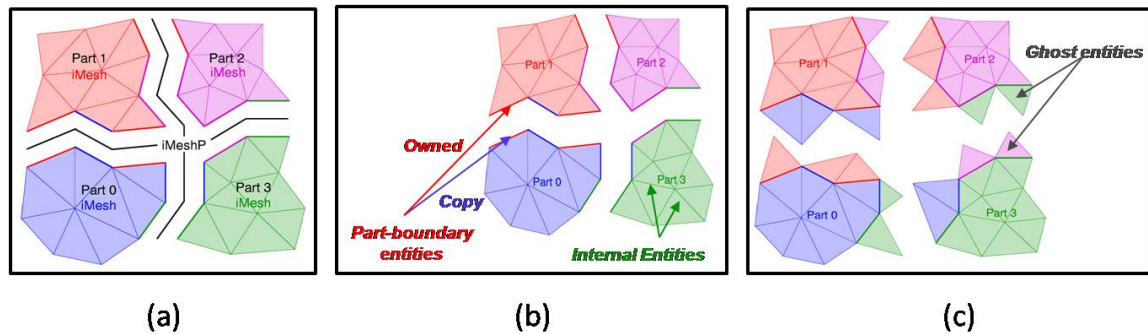


Figure 1. A simple example showing the iMeshP datamodel. Image (a) shows the relationship between iMesh and iMeshP, (b) shows entity classification, and (c) shows ghost entities.

requiring only that certain questions about the geometry, mesh, or field data can be answered through calls to the interface. All data passed through the interface is in the form of opaque handles to objects defined in the data model. One of the most challenging aspects of this effort remains balancing performance of the interface with the flexibility needed to support a wide variety of data types. Further challenges arise when considering the support of many different scientific programming languages which we address using a two-pronged approach. First, we provide a C-language binding for our interfaces that is compatible with most needs in scientific computing. Additional flexibility, albeit at a somewhat higher cost, is supported through the use of the SIDL/Babel technology [14] provided by the Common Component Architecture Forum.

In previous work, a full specification for the serial mesh interface, called iMesh, was completed and implemented by several institutions. The extension to iMeshP, the parallel mesh interface, required the definition of a number of additional functions; for example, functions to easily create and modify partitions, create ghost entities, retrieve ghost and owner entity tag data, and determine an entity's ownership status. To simplify the iMeshP interface, we allow part handles to be substituted for entity-set handles in all serial iMesh functions. Thus, operations such as adding entities to parts and querying the number of entities in a part can be achieved using the same interface as adding entities to and querying entity sets. Additional iMeshP functions provide information about part boundaries and neighboring parts. Furthermore, the iMeshP interface supports parallel operations needed for efficient computation, load balancing and mesh modification. By necessity, these operations involve parallel communication and both synchronous and asynchronous parallel operations are supported. This design enables such things as updates of tag data in ghost entities during computation, large- or small-scale entity migration for dynamic load balancing or edge swapping, updates of vertex coordinates in non-owned vertices for mesh smoothing, and coordination in the creation of new entities along part boundaries for mesh refinement. For more information see [15].

To illustrate iMesh and iMeshP interface usage, we provide a simple example of using the C-binding version in Figure 2. Line 14 shows the creation of a new mesh instance which creates the local opaque handle `mesh` that is used in later calls to refer to this instance of the interface on this process. Likewise, line 15 shows the creation of the `root_set` which contains all the mesh data on the processor once it is loaded. Line 20 shows the call to create the partition handle on all processors and associate the MPI communicator with it. Line 21 shows the use of the `iMeshP_load` function to populate the mesh and partition interface on all processors using a string name identifier. In this example, the data is loaded from file `125hex.vtk`, but `iMeshP_load` can also be used for on-the-fly mesh creation. Line 24 shows the global query to retrieve the number of parts in the partition. Line 25 shows the call to get the global number of

```

1  #include 'iMesh.h'
2  #include 'iMeshP.h'
4  #include <mpi.h>
5
6  int main( int argc, char *argv[] )
7  {
8      // create and populate the Mesh instance
9      iMesh_Instance mesh;
10     iBase_EntitySetHandle root_set;
11     iMeshP_PartitionHandle partition;
12     int num_parts, num_vtx, ierr;
13
14     iMesh_newMesh("", &mesh, &ierr, 0);
15     iMesh_getRootSet(mesh, &root_set, &ierr);
16
17     MPI_Init(&argc, &argv);
18
19     // create the partition and load the mesh
20     iMeshP_createPartitionAll(mesh, MPI_COMM_WORLD, &partition, &ierr)
21     iMeshP_load(mesh, partition, root_set, "125hex.vtk", "", &ierr, 10, 0);
22
23     // get the number of parts and number of vertices in the partition
24     iMeshP_getNumParts(mesh, partition, &num_parts, &ierr);
25     iMeshP_getNumOfTypeAll(mesh, partition, root_set, iBase_VERTEX, &num_vtx, &ierr);
26 }

```

Figure 2. Example use of the C-binding of the iMeshP interface.

vertices in the partition; this call may require global communication if it is not stored locally.

2.3. ITAPS software using iMesh and iMeshP

The ITAPS consortium has produced four implementations of the iMesh interface based on pre-existing mesh databases. Each of the four has its own particular strengths and so are useful in different application settings. In addition, two of the four iMesh implementations also have at least partial iMeshP implementations available. These implementations are listed in Table 1. In addition, the ITAPS team is developing a number of *component services* that use the iMesh and iMeshP interfaces to support simulations involving complex domains, adaptive techniques, and high-order methods. Specific tools include mesh quality improvement through smoothing with Mesquite [9] and swapping [10], high-order mesh curve correction tools [16], adaptive mesh refinement through MeshAdapt [12], front tracking through FronTier [11], dynamic load balancing services through Zoltan [13], and visualization plug-ins into VisIt [17]. These component services can be used directly by applications and can also be integrated to form higher-level integrated services such as shape-optimization and AMR-Front tracking technologies. Each of these services has been demonstrated to work with multiple implementations of the iMesh and iMeshP component APIs. We generally see little reduction in the overall efficiency of an application using the iMesh or iMeshP interfaces compared to using native data structures when following the ITAPS “best practices” implementation guidelines. For example, we tested the time to partition a MOAB mesh using Zoltan through the MOAB native interfaces and compared this with the time required to partition the same mesh through the iMesh interface. We found the overhead ranged from under 1% for small problem sizes to about 2% for larger problems sizes. Similarly, when building a stiffness matrix associated with

a simple finite element solver, the overhead costs associated with the use of iMesh ranged from 2% to 11% depending on the access pattern chosen.

Table 1. iMesh and iMeshP Implementations

Implementation	Emphasis	Parallel Capability	Applicaitons
FMDB: Flexible Mesh Database [1, 2] (iMesh/iMeshP)	Adaptively changing meshes (entity addition or removal)	Scalable to 32K procs; 2B elements	fusion, accelerators CFD, solid mechanics multiphase flow
MOAB: Mesh Oriented dAtaBase [3] (iMesh/iMeshP)	Low memory usage first; then CPU time	Up to 64 procs	nuclear reactors, accelerators, rad. transport, inertial confinement fusion
GRUMMP: Generation and Refinement of Mixed-Element Meshes in Parallel [4] (iMesh)	Fast adjacency retrieval for mesh generation and improvement, adaptation	In development	CFD, biological systems, structural mechanics
NWGrid: Northwest Grid Generation Code [5] (iMesh)	Simplicial meshes; parallel generations of unstructured, hybrid, meshes	Parallelism based on Global Arrays; Scalable to at least 10K procs	CFD, subsurface transport, biological systems

3. Scalability of ITAPS software

In this section, we highlight recent results on the scalability of ITAPS tools that use the iMeshP interface. In particular, in this paper we focus on the combination of the FMDB mesh database, Zoltan dynamic load balancing, and MeshAdapt services used in implicit finite element and finite volume applications. We are interested in both strong and weak scaling to minimize run time and maximize resolution, respectively. This has driven the need to research new load balancing technologies and communication tools; particularly as we scale to $O(100,000)$ processors and beyond. We describe these research efforts in some detail and highlight the resulting scalability of our tools and solvers that use our tools on a number of different leadership class computers.

The ability to scale implicit finite element and finite volume computations such as those used in the accelerator and fusion SciDAC application efforts, requires ensuring both the system formulation and solution are effectively load balanced. Graph-based partitioners are well known to produce a partitioning of the mesh into parts that are well balanced in terms of the specified partition object type while also minimizing inter-part communications. However, traditional graph-partitioners consider a single objective optimization subject to a single balance constraint. In the case of mesh-based analysis, the defined graph nodes are often mesh regions. This selection does an excellent job of balancing the number of regions (elements) and therefore the workload for the construction of the part-level finite element system. However, in the case of C^0 interpolating basis functions, for example, the workload balance for the iterative solution (e.g. matrix vector product and vector norms) of the resulting system is proportional to the number of mesh vertices per part. Since mesh vertices are not the objects in the original partitioning, the balance may not be optimal, particularly when the numbers of mesh entities per part is relatively low (e.g., a few thousand). We are developing two multiple compute-object based partition improvement algorithms to reduce the vertex imbalance thereby improving the overall balance of two mesh entities as required by a scalable implicit solve. They are referred to as local iterative inter-part boundary modification (LIIPBMod) and heavy part split (HPS).

- *The LIIPBMod Algorithm.* LIIPBMod locally migrates small numbers of mesh regions from parts that are relatively heavily loaded with respect to mesh vertices to neighboring parts

which are relatively lightly loaded with respect to mesh entities. On the heavily loaded part, the mesh vertices on the part boundary are traversed and the ones bounding a small number of elements are identified. If the neighboring part is lightly loaded, the whole “cavity” (all the adjacent elements of the picked vertex) is migrated to the neighboring part. By this minor inter-part boundary adjustment, the vertex imbalance is improved while only modestly perturbing the good element balance. This procedure may need to be repeated for several iterations to achieve desired vertex balance.

- *The HPS Algorithm*, Our studies of the mesh partitions given by a graph-based partitioner show that the percentage of heavily loaded parts (more than 10% imbalance) is usually less than 1%. The idea of HPS is that, if the desired number of parts is numP, first distribute the mesh to $99\% \cdot \text{numP}$ parts by a graph-based partitioner and leave the other $1\% \cdot \text{numP}$ parts empty. Then, select the $1\% \cdot \text{numP}$ parts with the highest vertex load and split them into two parts (i.e. migrate roughly half of the mesh entities from them to one of the empty parts). The splitting makes the heavily loaded parts become lightly loaded. Since the peak of the imbalance determines the scalability, HPS lowers the peak and hence improves the performance.

Figure 3 shows the results of applying the two algorithms to a 16.7M element anisotropically adapted mesh used in the simulation of an abdominal aorta aneurism (left image). The two graphs (center for LIIPBmod and right graph for HPS) indicate the number of vertices per part divided by the average per part before (red dots) and after (blue dots) application of the algorithms. Note in both cases the spikes (red dots in the upper parts of the graphs) that reduce scalability are dramatically lowered after the algorithms have been applied.

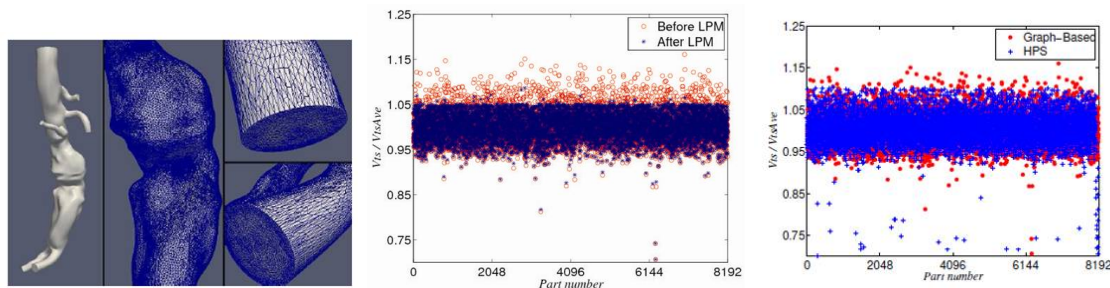


Figure 3. Vertex imbalance before and after LIIPBMod and HPS.

Using the results of the multi-compute object load balancer, we showed that unstructured mesh solvers based on implicit methods can scale to very large numbers of processors [18]. Table 2 illustrates the parallel efficiency of PHASTA, a parallel, unstructured and implicit flow solver developed at RPI on up to $O(100,000)$ cores of IBM BG and Cray XT systems [19]. PHASTA uses FMDB and the MeshAdapt service for refinement on up to 32K processors and iMeshP and iZoltan to partition the resulting meshes into 128K parts for distribution to almost the full machine for the analysis step. Near-perfect (linear) strong scaling of the analysis step over multiple doublings of cores can be clearly seen on various systems with a slight decrease in parallel efficiency on the largest core counts due to the fact that computational load per core becomes insignificant (for a fixed-size problem). More information on PHASTA’s scaling studies can be found in [20].

We have also examined the scaling of the MeshAdapt service in both the weak and strong sense. Mesh adaptation is characterized by small, but variable, work per operation which implies that achieving “perfect scaling” can be very costly. In particular, our research has found that

Table 2. Strong scaling results of PHASTA up to O(100,000) cores on IBM BlueGene (BG) and Cray XT systems (1 implies perfect scaling with 100% parallel efficiency)

105 Million Elements				1 Billion Elements	
Core Count	BGL-CCNI RPI	BGP-ALCF ANL	XT4-NERSC LBNL	Core Count	BGP-ALCF ANL
512	1.00	1.00	1.00	16,384	1.00
1,024	1.01	1.02	1.03	32,678	0.99
2,048	1.00	0.99	1.16	65,536	0.97
4,096	0.99	0.99	1.00	131,072	0.89
8,192	1.02	0.95	0.77		
16,384	1.03	0.95			
32,768	0.93	0.88			

we can run adaptive mesh refinement algorithms on the large numbers of parts typically used in a simulation analysis, and the overall time will still be a small percentage of the overall total solution time. For example, for the weak scaling results shown in Table 3 for uniform adaptive refinement, the time required by the adaptivity algorithms for the largest case on 32768 processors is only 0.04% of the total time.

That said, the scaling efficiency is clearly decreasing as the number of processors increases, and to improve the scaling characteristics of the MeshAdapt and other services, we are developing a new general-purpose, MPI-based communication package called the Inter-Processor Communication Manager (IPComMan). This package aims to reduce data exchange costs by exploiting communications in a local neighborhood for each processor. The neighborhood is the subset of processors exchanging messages with each other during a specific communication round, which in many applications is bounded by a constant, typically under 40, independent of the total number of processors. Strong scaling of uniform adaptive mesh refinement using the IPComMan Message Passing library for a mesh starting with 4.3M elements and ending with 2.2B elements is shown in the right of Table 3. Significant improvements in scaling efficiency compared to the weak scaling case are evident due to decreased communication costs.

Table 3. Uniform adaptive mesh refinement: weak scaling using the AutoPack Message Passing library and strong scaling using the IPComMan library

Weak Scaling					Strong Scaling		
Number of Parts	Initial Mesh	Adapted Mesh	Time (s)	Scaling Factor	Number of Parts	Time (s)	Scaling Factor
2048	17M	128M	5.0	1.0	2048	21.5	1.0
4096	34M	274M	4.8	1.05	4096	11.2	0.96
8192	65M	520M	5.1	0.97	8192	5.67	0.95
16384	520M	1.1B	6.1	0.82	16384	2.73	0.99
32768	274M	2.2B	7.4	0.68			

4. Use of ITAPS parallel adaptive software in SciDAC applications

ITAPS technologies have impacted DOE applications in a number of ways including direct use of the services and software described in this paper (adaptive algorithms, mesh quality improvement, partitioning, front tracking), technology advancement through the demonstration and insertion of key new technology areas (shape optimization and petascale mesh generation), and by looking ahead and anticipating the needs of application teams through the development

of new services (mesh to mesh transfer for coupling multiphysics applications). In this section we highlight a few key examples of the use of ITAPS software in SciDAC applications. While we focus on our interactions with accelerator and fusion applications to insert adaptivity into their codes in this paper, more extensive interactions funded under the auspices of the SciDAC and other DOE programs include work with multiple accelerator and fusion teams along with subsurface flow and nuclear energy application teams.

Accelerator Design. The ITAPS team is working extensively with the “Community Petascale Project for Accelerator Science and Simulation (COMPASS)” SciDAC project, and in particular researchers at the SLAC National Accelerator Laboratory, to provide high-order mesh generation and adaptive control methods to improve the processes for the design and optimization of accelerator cavities. For example, in calculating the short-range wakefield inside an accelerator structure, only the small region in the vicinity of the moving particle beam is required to have a highly refined mesh in the simulation. The moving curved mesh adaptation procedure, which refines a small region of interest near the beam (see Figure 4), greatly reduces the computational effort required for a given level of accuracy. In particular, using such techniques has resulted in a tenfold reduction in the computational cost of these simulations [21, 22].

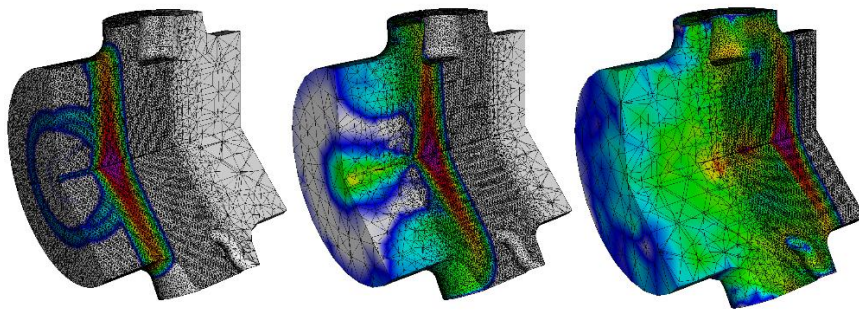


Figure 4. The electric fields on tree-refined curved meshes around the moving beam

Fusion. The SciDAC-funded “Center for Extended MHD modeling (CEMM)” has extensively used a 3D MHD code to simulate global instabilities in magnetic fusion devices. The ITAPS team is working with CEMM fusion scientists to extend the MHD high-order finite element software (M3D-C1) to interface with unstructured mesh adaptation technologies. This enables them to gain the efficiencies of using adaptive meshes (see Figure 5 for isotropic and anisotropic adapted meshes [23, 24]) and allows them to model general curved reactor domains (see the rightmost image in Figure 5).

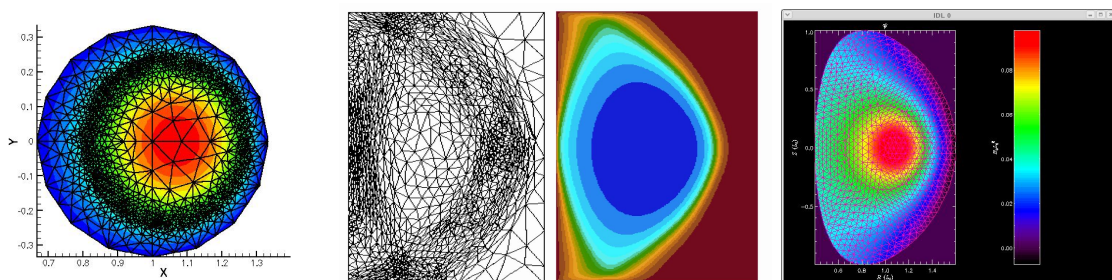


Figure 5. Isotropic and anisotropic mesh adaptation to increase computational efficiency in fusion applications. On the far right we show the vorticity contours in a curved reactor domain.

More information about ITAPS

More information on the ITAPS project including detailed descriptions of the ITAPS services, interfaces, software, and interactions with SciDAC application teams can be found at <http://www.itaps-scidac.org>.

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