The Terascale Simulation Tools and Technology Center

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The TSTT Center aims to eliminate the barriers associated with using sophisticated meshing and discretization tools in DOE scientific applications that involve complex geometry. To accomplish this goal we are working directly with a number of SciDAC application partners to insert TSTT technology directly into their codes. We are also creating new technology to ease the development of powerful hybrid solution strategies that employ multiple meshing and discretization techniques in an interoperable and interchangeable way.

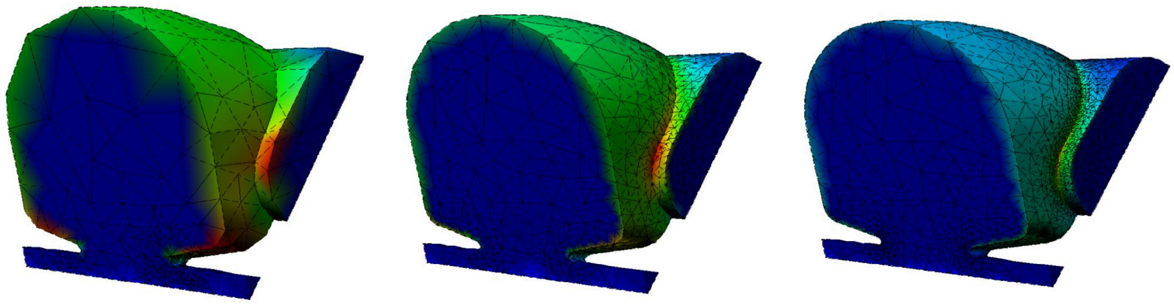
The TSTT Vision. Terascale computing environments provide an unprecedented opportunity to perform numerical simulations at levels of detail and accuracy previously unattainable. The Terascale Simulation Tools and Technology (TSTT) center aims to help application scientists exploit this opportunity by allowing them to more easily use high-order, adaptive, parallel mesh and discretization tools. By working directly with a number of SciDAC application teams to introduce these technologies into their application domains, TSTT is making a near term impact on the SciDAC applications, ensuring that new TSTT technology will remain relevant to a broad range of DOE science applications. In addition, by developing new technologies, we will eliminate the technical and human barriers preventing the effective use of powerful meshing and discretization techniques in large-scale scientific simulations. A key goal of these efforts is to enable existing techniques to be used in an interoperable and interchangeable way, thus laying the groundwork for the development of new application codes that employ powerful hybrid solution techniques.

TSTT and SciDAC Applications. We have invested a significant portion of our resources in meeting with scientists from each of the SciDAC application areas, analyzing their needs for advanced meshing and discretization technologies, and working with them to demonstrate the promise of such techniques in their application domains.

Accelerator Design: TSTT is helping to improve the computational efficiency of electromagnetic simulation codes by inserting adaptive technologies into an existing frequency domain code. (See Figure). This has enabled highly accurate solutions using only a fraction of the comparable fine resolution mesh. TSTT mesh generation technology is being used to shorten the time required to generate high quality meshes for complex accelerator geometries.

Climate: TSTT has investigated mesh generation strategies that create high-quality meshes with mesh points focused over regions of high altitude. TSTT and the members of the climate modeling community have jointly developed a new preconditioner for spectral element simulations, accelerating the solution of an important test problem for climate scientists.

Diesel spray formation: TSTT is applying advanced front-tracking technology to create a simulation code modeling spray formation in diesel engine injection systems.



Adaptive simulation results for the Trispal cavity reliably gives more accurate predictions of magnetic field distribution than solutions using a conventional mesh.

Fusion: TSTT is investigating the use of high-order spectral elements and adaptive finite element methods to improve the accuracy of MHD fusion simulations.

Computational Biology: TSTT is applying meshing and solver technology to develop a virtual microbial cell simulator.

TSTT Technology Developments. The TSTT center is working on new technology developments in three primary areas.

1) We are defining a common software interface for mesh and geometry access that all support. This allows application scientists and tool developers to use any compliant TSTT technology in a consistent, uniform way.

2) We are demonstrating interoperability through one-on-one tool interfaces. The most notable of these efforts is the combination of front-tracking techniques with adaptive refinement techniques to create a new, highly accurate and computationally efficient technique for modeling sharp interfaces.

3) We are developing new solvers and technologies to demonstrate or enable hybrid solution processes in SciDAC application areas. For example, we are creating a stand-alone mesh quality improvement toolkit and a discretization library that will work with all TSTT mesh management software packages through the TSTT interface.

Future Work. The TSTT team will continue to work closely with all our SciDAC application partners to ensure that advanced meshing and discretization strategies can be used to their fullest extent. We will continue to develop common interfaces for TSTT meshing and discretization technology and demonstrate the utility of a software environment that supports interoperability for hybrid solution strategies.

The TSTT Team. The TSTT partners, representing six DOE national laboratories (ANL, BNL, LLNL, ORNL, PNL, SNL) and two universities (RPI and SUNY SB), bring extensive expertise in structured, unstructured, and hybrid meshing and discretization technologies into one Center with the goal of delivering advanced, mesh-based simulation capabilities to scientific applications.

Benefits from Teaming. The SciDAC team approach has transformed the manner in which the Center members conduct science by increasing the emphasis placed on collaboration, end use relevance, and integration. New technology based on interface development effort and interoperability of tools would not be possible without SciDAC support.

Further Information: *http://tstt-scidac.org*

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