TSTT

SciDAC
Scientific Discovery through Advanced Computing

Terascale Simulation Tools and Technology Center

Vision

Terascale computing provides an unprecedented opportunity to achieve numerical simulations at levels of detail and accuracy previously unattainable. Scientists in many different application areas can reach new levels of understanding through the use of adaptive, composite, hybrid approaches. Unfortunately, the lack of easy-to-apply, interoperable meshing, discretization, and adaptive technologies severely hampers the utilization of these advanced methods. The Department of Energy Office of Science, through the program for Scientific Discovery through Advanced Computation (SciDAC), has recently funded the Terascale Simulation Tools and Technologies (TSTT) Center to address this critical gap. The TSTT Center's central goal is to eliminate the technical and human barriers preventing the effective use of powerful adaptive, composite, and hybrid methods in large-scale scientific simulations for application areas of interest to the Department of Energy.

Current State-of-the-Art

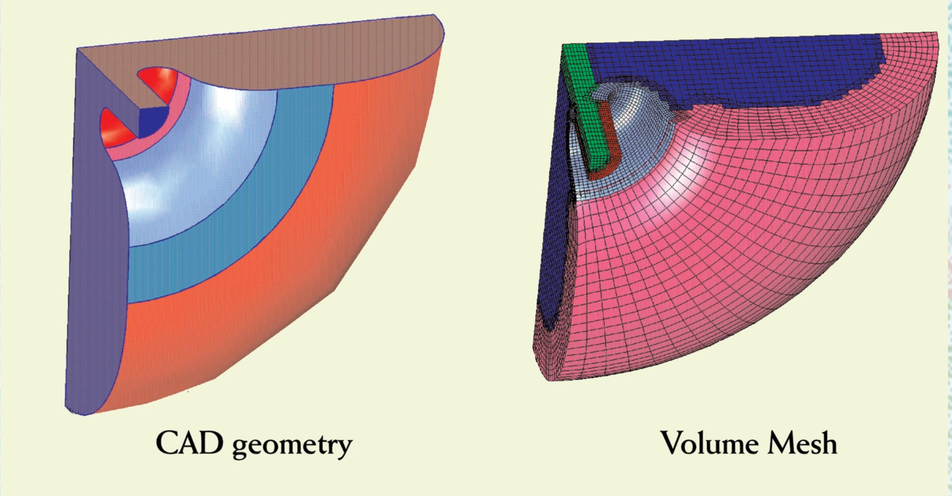
There are many combinations of mesh generation and approximation technologies that can be used to solve problems that are formulated as a system of partial differential equations (PDEs). The fundamental concepts are the same for all approaches: a discrete representation of the geometry, called a mesh, is used to approximate the physical domain, and some discretization procedure is used to represent approximate solutions and differential operators on the mesh. In addition, the concepts of adaptive mesh refinement, data transfer between different meshes, and parallel decomposition of the mesh for computation on advanced computers are the same regardless of their implementation. In each case, the software tools providing these advanced capabilities are increasingly accepted and used in the scientific community, but their application interfaces are not always compatible. Thus, interchanging technology is often a labor-intensive and error-prone code modification process that must be endured by the application scientist. This typically results in a lengthy diversion from the central scientific investigation and severely inhibits experimentation with improved mesh and discretization technologies.

Major Technical Goals

The TSTT Center aims to provide application scientists with a set of powerful, flexible, and easy-to-use tools by developing the technologies needed to create interoperable and interchangeable meshing and discretization software. Our efforts focus on three primary areas:

Advanced meshing technologies

The TSTT Center will build upon advanced structured and unstructured meshing capabilities developed by TSTT partners. Our goal is to create common interfaces for these meshing and discretization technologies that will allow them to interoperate with each other, providing fundamentally increased capabilities, and allowing application scientists to easily switch among them. We will develop new capabilities as needed within these tools to provide compatible functionality and to support complex geometries, high-order discretization techniques, and adaptive methods.



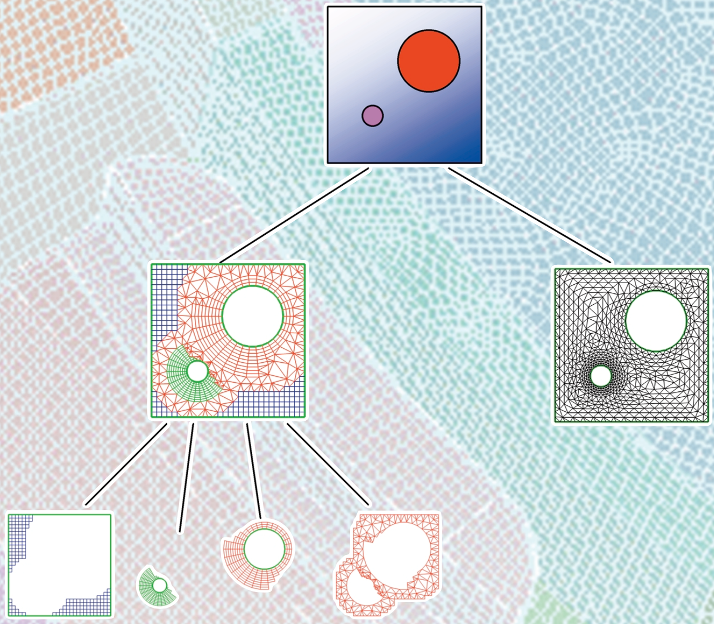
Technology from TSTT partners will be used to provide higher quality meshing capabilities for SciDAC applications such as the 21st Century Accelerator Science & TechnologyCenter. CAD-to-mesh technology, shown here applied to the TRISPAL accelerator cavity geometry, will be used to produce hybrid meshes for this and other SciDAC applications. (Images courtesy of LLNL.)

High-order discretization techniques

The TSTT Center will use extensive experience with a number of different types of discrete operators to create a Discretization Library. This library will support commonly used operators and boundary conditions, will be extensible to provide application-specific customization, and will be independent of the underlying mesh type and therefore interoperable with all TSTT meshing technology. Low-level interfaces will be provided to allow the insertion of new discrete operators as kernels into existing applications, and high-level interfaces will be provided to ease the development of new applications by allowing access to discrete operators over the entire mesh.

Terascale computing issues

The TSTT Center will develop the algorithms necessary for efficient performance on terascale architectures. Our focus will be on dynamic partitioning strategies for hybrid, adaptive computations, and the use of preprocessing tools to achieve optimized single processor performance.



TSTT will provide common interfaces to multiple meshing technologies. Different mesh types and data structures may be produced from the same geometry, but high-level access to these meshes occurs through the same interface.

TSTT Center software

TSTT research will encapsulate software components with well-defined interfaces that enable different mesh types, discretization strategies, and adaptive techniques to interoperate in a "plug and play" fashion. The interface design will be driven by application scientists'requirements and the need for intuitive, easy–to-use interfaces at multiple levels of sophistication. All software developed as part of the TSTT Center will be freely available in the public domain. To ensure the relevance of our research and software developments to the SciDAC goals, we will collaborate closely with both SciDAC application researchers and other software infrastructure centers.

Interaction with SciDAC application teams

TSTT technologies will be inserted into the SciDAC application areas of fusion, accelerator design, climate modeling, chemically reacting flow, and astrophysics. To ensure significant near-term impact on these efforts and to receive the necessary feedback for the success of our long-term goals, TSTT technologies are already being inserted into these applications. By working with a large number of applications we will be able to abstract the user requirements with a greater level of generality, thus improving the likelihood of providing common interfaces that are widely applicable.

Interaction with SciDAC Integrated Software Infrastructure Centers (ISICs)

Because meshing and discretization pervades many aspects of the PDE solution process, the TSTT Center must interact with a broad spectrum of other tool providers to ensure that software and interfaces are both flexible and efficient on terascale computers. Therefore, TSTT is committed to working with the other SciDAC ISICs including the Terascale Optimal PDE Simulations (TOPS) ISIC (PI: David Keyes); the Center for Component Technology for Terascale Simulation Software ISIC (PI: Robert Armstrong); the High-End Computer System Performance: Science and Engineering ISIC (PI: David Bailey); and the Algorithmic and Software Framework for Applied Partial Differential Equations ISIC (PI: Phil Collela).

The TSTT Team

The TSTT team comprises researchers from six DOE national laboratories (ANL, LLNL, BNL, SNL, PNNL, and ORNL) and two universities (Rensselaer Polytechnic Institute and SUNY Stony Brook).

More information about the TSTT Center can be obtained by visiting us at http://tstt-scidac.org

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