Component-Based Mesh and Geometry Services for Accelerator Modeling

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Summary

Software components for geometry and mesh have been used to construct a CAD-based shape optimization library and adaptive mesh refinement service. Shape optimization and adaptive mesh refinement are crucial to improving the performance of existing accelerators like PEP-II and to design new accelerators like the ILC and RIA.

The Terascale Simulation Tools & Technologies (TSTT) SciDAC project is developing common interfaces for geometry, mesh, field, and relations data. The interfaces are designed to minimize dependencies, simplifying the use of one without the others, while also allowing relations between geometry, mesh, and field data using a higher-level "relations" interface (see Figure 1). Geometry and mesh services such as CAD geometry construction, adaptive mesh refinement, and mesh smoothing/improvement have been implemented through these interfaces. Several important applications developed using these services are described below, and show the benefits of interoperability.

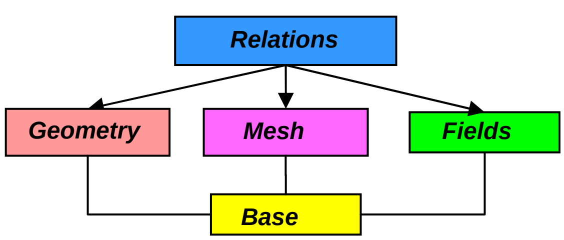

Figure 1: Structure of TSTT interfaces; Base interface defines sets & tags used by others; Relations interface relates data between geometry, mesh, fields interfaces.

Particle accelerators are the focus of seven of the twenty facilities in the Office of Science 20-year plan, and include the International Linear Collider, the Rare Isotope Accelerator, and the CEBAF upgrade. High-resolution modeling and end-to-end simulation are crucial to designing these devices, and can also be used to improve existing accelerators like the PEP-II at Stanford Linear Accelerator Center. For new accelerator designs, shape optimization is being developed to tune the exact geometric shape parameters of an accelerator cavity, both to maximize the acceleration and minimize disruptive electro-magnetic wake-fields of the accelerated particles. The DDRIV library, based on TSTT interfaces and tools, provides geometry and mesh support for shape optimization,

Several distinct geometry and mesh capabilities are used in the shape optimization process. First, a set of design parameters *p* is used to generate a geometric model *G(p)* of an accelerator cavity (see Figure 2). Parametric construction of new models can be added to DDRIV in the form

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of a function, which is used to support the remaining shape optimization functions.

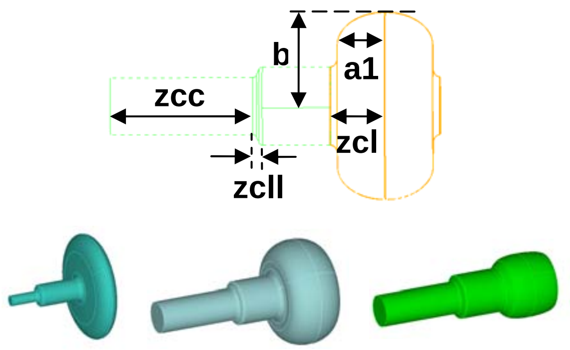

Figure 2. A parametric depiction of the ILC cavity, and models based on several parameter sets.

The geometric model is discretized with a finite element mesh, which is the basis for an electro-magnetic simulation. Solution gradients provided by that simulation are combined with mesh sensitivities to compute new design parameters *p'* for the next iteration of the process. Derivatives of mesh position with respect to design parameters are computed in DDRIV, by generating geometric models from small variations of each parameter and projecting the mesh onto those modes. Mesh projection to new geometric models is performed using the Mesquite mesh improvement tool [3].

Particle accelerator cavities are particularly sensitive to geometric shape; simulations of cavity performance must accurately resolve fine details in order to achieve the required accuracy. However, a coarser mesh resolution is sufficient in many other parts of the cavity. To make optimal use of computational resources, an adaptive procedure has been developed to concentrate mesh close to geometric details [2]. This service, also written based on the TSTT interfaces, has been used to model cavities for the Rare Isotope Accelerator (RIA) (see Figure 3). These models achieved up to an order of magnitude increase in accuracy for a fraction of the computational cost.

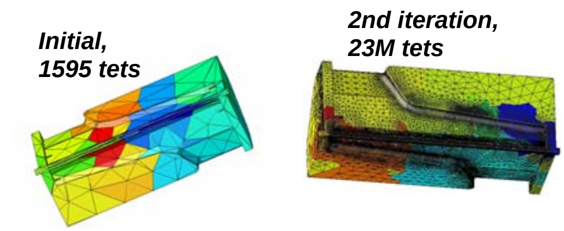

Figure 3: Parallel adaptive mesh refinement, applied to cavity of Rare Isotope Accelerator.

Ongoing work developing interoperable mesh and geometry technologies, and their deployment into a number of different applications through common interfaces, is a continued focus of work in TSTT. Near term development will include a stronger emphasis on services needed for effective petascale computing such as parallel mesh generation and mesh to mesh transfer, mesh partitioning, and efficient parallel adaptive loops.

[1] Chand, K.K. et al, "Toward interoperable mesh, geometry and field components for PDE Simulation Development", to appear Eng. with Comp, 2006.

[2] Alauzet, F. et al, Parallel Anisotropic 3D Mesh Adaptation by Mesh Modification, to appear Eng with Comp, 2006.

[3] M. Brewer, L. Diachin, P. Knupp, T. Leurent, and D. Melander, "The Mesquite Mesh Quality Improvement Toolkit," p239-250, Proceedings of the 12th Int Meshing Roundtable, Santa Fe NM, 2003.

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