Advanced Scientific Computing Research
Computer Science
FY 2006 Accomplishment

“R-adaptive Mesh Quality Improvement using the Target-Matrix Paradigm”

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Summary

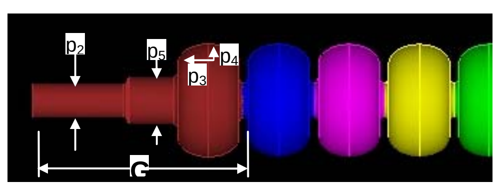
The goal of this project is to provide basic mathematical research on mesh optimization methods for improvement of simulation accuracy, efficiency, and stability. A new paradigm for mesh optimization has been developed which, for the first time, encompasses the many varieties of mesh optimization goals within a single theoretical framework. The framework provides fresh insight into mesh improvement algorithms and their theoretical foundation. The paradigm employs advanced metrics and target-matrices to provide a crisp conceptual mapping between application goals and mesh optimization algorithms. Portions of the new paradigm are implemented in the Mesquite code and have been successfully applied to deforming mesh problems at SLAC, SNL, and CSAR.

Suitable computational meshes can favorably impact simulation accuracy, efficiency, and stability. Suitable meshes can be obtained in a variety of ways, including mesh smoothing and optimization. Optimization provides a rigorous mathematical framework for the improvement of meshes that is lacking in other approaches.

We are developing a ‘target-matrix’ paradigm of mesh optimization that naturally addresses many application goals of optimization including deforming meshes, ALE rezoning, r-type adaptivity, mesh fix-up, and anisotropic mesh improvement. Considerable elaboration and development of the paradigm will be required in the coming years to fully demonstrate and realize its potential. In the short-term, however, successful applications of the paradigm have already occurred via their implementation in the Mesquite (Mesh Quality Improvement Toolkit) software library. Successful applications include (i) incorporation of the deforming mesh algorithm within the accelerator shape optimization capability under development at SLAC (figure 1), (ii) incorporation of the Mesquite rezone algorithm into the Alegra code at SNL, and (iii) use of the deforming mesh algorithm at the UIUC CSAR Rocket Center for propellant burn (figure 2).

The deforming mesh algorithm in Mesquite is used to provide gradual mesh movement for updating the mesh to changes in the accelerator cavity design parameters. The algorithm makes extensive use of target matrices to ensure the resulting mesh is valid (i.e., untangled) and bears a close resemblance to the initial good-quality mesh on the un-deformed geometry. This constitutes an advance over the commonly used elastic-springs model of mesh deformation. The method is also helping CSAR analysts to maintain good quality mesh during propellant burn while preserving mesh topology. By preserving topology, simpler algorithms can be used by the analysis code.

Fig. 1. Shape Optimization (ILC)



FY06 Accomplishments:

Accomplishments in FY06 for this project were (1) completion of Part 1 of the mathematical analysis of the Target-Matrix paradigm, (2) mathematical proofs of convexity of certain mesh quality metrics and objective functions, (3)

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a draft write-up on a thorough literature survey on impact of mesh on solution accuracy & efficiency, and (4) a mathematical derivation of a new a priori, anisotropic error bound for finite element meshes.

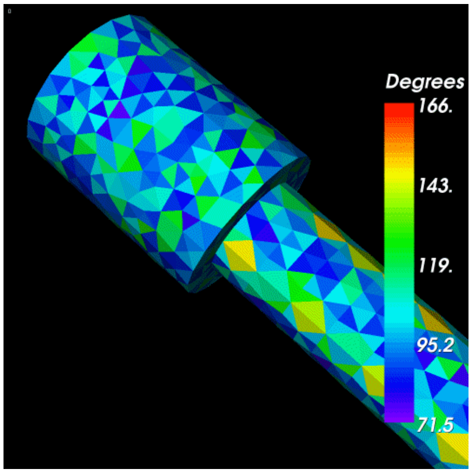

Fig. 2. Rocket Propellant Burn Simulation (CSAR)

The first part of the Target-Matrix paradigm (TMP) was investigated this year and a paper entitled "Formulation of the Target-Matrix paradigm for mesh optimization" is ready to be submitted for publication. The paper describes a high-level view of the paradigm in terms of its fundamental mathematical objects. The fundamental objects are matrices, local mesh metrics, non-local mesh metrics, and objective functions. The matrices represent the Jacobian of the mapping from the master element to physical element (the active matrix) and to the ideal element (resulting in the target-matrix). Precise definitions of these terms are given, along with analysis of such topics as invertibility-barriers, the power-mean, hierarchical mesh metrics & objective functions. Numerical results are given that illustrate how the various objects fit together and can be used to control the mesh quality. The theory is unique in that it is the most sophisticated attempt to date to formulate mesh optimization techniques for unstructured and/or hybrid meshes. The goal, of course, is to implement the TMP within the Mesquite code in order to deliver the latest techniques to applications.

Ideally, the objective functions in the TMP are convex and possess a unique minimum. A careful study of convexity within the TMP was performed, resulting in a paper submitted for publication that shows the TMP objective functions are convex provided the local mesh metric is convex. In addition, proofs of convexity of some important local mesh metrics are given. Of course, not everything is convex and some important local mesh metrics are non-convex.

A major theme in the mesh optimization work is to better understand the impact of mesh quality on simulation solution accuracy and efficiency. If this can be accomplished, then one should be able to construct better meshes via mesh optimization. As an initial step, we performed a thorough literature survey, in which over 100 papers on the topic were identified. The main results of these papers were summarized in a draft document which we intend to publish as a survey paper next year. The survey makes it clear that this is a difficult topic and that important gaps in understanding remain, particularly with regard to non-simplicial mesh elements and impact of mesh on solution efficiency. We organized & held a SIAM minisymposium for the annual meeting in Boston on this topic and were pleasantly surprised at the considerable degree of interest within the broader community.

One result of the literature survey was a realization that the commonly known a priori error bounds for finite element meshes were incomplete, particularly with regard to mesh anisotropy. As part of this project, we wrote a paper giving a new a priori bound for fully anisotropic meshes that is sharp, coordinate-free, and is more general than the previous bounds. The paper will be submitted shortly. In addition, we intend to use the new bound in developing a new r-adaptive method of mesh improvement.

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