"Mesh Quality Improvement & Optimization"

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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 'Target-matrix' 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.

During this fiscal year we pursued two topics within mesh optimization. The first topic centered on the development of the theoretical framework mentioned above. Local quality metrics for two-dimensional triangle, quadrilateral, or hybrid meshes were devised for paradigm consistency. The metrics were required to satisfy a number of important mathematical properties including (1) continuity and differentiability, (2) semi-infinite range, wherein the ideal is attained only at the finite endpoint of the range, and (3) the set of stationary points of the metric coincides with the set of global minimizers (a pseudo-convexity property). Additionally, the metrics' ideals consist of four canonical types to control various combinations of element shape, size, and orientation. Both barrier and non-barrier forms of the metrics were devised in order that both initially untangled and initially tangled meshes can be optimized.

A highlight was the discovery of a new metric which can be used to control both element shape and element size within a single metric, instead of using a blended metric as has been done in the past. A paper has been submitted to SIAM describing these new metrics, along with numerical examples.

The second topic that was focused on this fiscal year was the development of mesh optimization techniques for solution-adaptive meshing. There are basically three approaches to adaptive meshing, typically referred to as "h", "p", and "r" adaptivity. Mesh optimization techniques fall naturally under the category of r-adaptivity, in which mesh vertices are moved to new locations in response to the developing solution to the governing partial differential equations. A considerable number of r-adaptive schemes have been proposed in the past, but most of them are lacking in one way or another. We

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developed an r-adaptive scheme based on the a priori bounds on interpolation error of Ciarlet. An advantage of this approach is that one does not need a lot of *a priori* knowledge about the governing PDE nor about the type of mesh element involved. We focused on the upper bound to the H1 norm of the error (this is based on the Hessian of the solution). Two fundamental challenges arise when attempting to develop r-adaptive schemes based on this bound: (1) ensuring that the optimal adapted mesh consists of non-inverted elements only, and (2) dealing with special cases in which the Hessian is either degenerate or not positive definite. The difficulty is that the theoretical bounds can be applied when the mesh is inverted or when the Hessian is degenerate; regularization techniques are necessary to ensure the desired properties. A very important additional requirement is that the error in the solution is guaranteed to decrease as a result of applying the optimization-based r-adaptive scheme. This requirement is highly significant since a majority of the papers published in this area fail to verify that a reduction in the error occurs as a result of applying their adaptive scheme.

The result of our work on this topic this fiscal year is that we now have an optimization-based r-adaptive scheme that appears to satisfy all these requirements. The two figures below show an example, wherein the function to which the mesh is adapted is given in the first and the adapted mesh is shown in the second figure. We are very excited by this development since the next step will be to implement the metric (and supporting infrastructure) within the Mesquite mesh optimization code which we are developing under SciDAC funding. With this capability in place we will be able to combine our r-adaptive scheme with other ITAPS mesh adaptive schemes and apply them toward problems of interest to the SciDAC applications. A paper describing the new approach will be submitted by the end of the fiscal year.

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