Conference on Multiscale Optimization Methods and Applications
Gainesville, Florida, February 26–28, 2004
Views on State of the Art

The theme of the conference was the development of new solution methodologies, including general multilevel solution techniques, for tackling difficult large-scale optimization problems that arise in science and industry. Applied problems that were presented at the conference included:

(a) the circuit placement problem in VLSI design
(b) the protein folding problem, and drug design
(c) a wireless sensor location problem
(d) internet optimization
(e) the siting of substations in an electrical network
(f) optimal dosages in the treatment of cancer by radiation therapy
(g) facility location
(h) shape and topology optimization

All of these problems are challenging. They are intriguing in that the problem is often easy to state but difficult to solve. In protein folding, we are given a sequence of amino acids that form a protein, and we seek the structure of the protein. When two amino acids bind together, there is a finite collection of possible bond angles. The orientation of each protein and the bond angles must be chosen so as to satisfy constraints imposed by the geometry, while minimizing a potential energy function. Fast and effective solution techniques must exist, since nature quickly solves the protein folding problem, finding the global minimum. Computational techniques for solving the problem are beginning to emerge. Amino acid zippers are a possible mechanism for incorporating macrostructure within microstructure. Important areas for research include conformational searching for protein folding and clique methods for drug design.

With any of these problems, the complexity is due to geometry: components must be placed so as to satisfy geometric constraints, while optimizing a cost function. The geometric constraints lead to an exponentially large solution space. The development of efficient techniques to probe this huge solution space is an ongoing effort that can have an enormous economic impact. In each application area, the development of techniques that exploit problem structure seem to be a key to success.

In solving difficult problems, it is important to have a quantitative way to compare the effectiveness of different approaches. For the circuit placement problem, benchmarks have been developed with known optimal solutions. When state-of-the-art algorithms for the circuit placement problem were applied to these benchmarks, researchers were startled to see the large gap between the best algorithms and the actual optimum (a factor of two difference between the best approximation and the optimum).

The idea of generating test problems with known optimal solutions seems to be one research direction of importance in the coming years. For certain classes of problems, such as the quadratic assignment problems, best-known solutions as well as lower bounds on the cost are published. Although bounds and estimates are certainly useful, test problems with known optimal solutions represent an extremely useful benchmark for comparing the advantages and disadvantages of algorithms for challenging problems in science and industry. The Netlib LP test set catalyzed the development of linear programming algorithms during the past decade, while the circuit placement benchmarks appear to be having a similar impact in VLSI design. The continued development of such benchmarks should be encouraged.

In the area of VLSI design, a multilevel approach has proved to be an effective way to cope with the huge solution space. This approach, closely connected with ideas developed for multigrid techniques in partial differential equations, uses a series of scaled approximations to the original problem. The coarsest approximation is easiest to solve and coarse information passed on to the next finer level gives a good starting point for a more difficult problem. Research is progressing towards systematic ways of moving back and forth between problem scales in an increasing number of application areas.

In large-scale discrete optimization, another paradigm of interest is that of transforming the problem into a continuous optimization problem. This is being done in many different ways. Semidefinite programming is used to obtain approximations to partitioning problems with a guaranteed error bound. Continuous quadratic programs are used in reformulations of both graph partitioning and maximum clique problems. A parameterized exponential transformation is used in the siting substation problem in order to obtain a feasible point. In the coming years, ways to transform back and forth between continuous and discrete formulations should continue to expand.

Interest in interior point methods remains strong; it is the basis of some powerful optimization packages. On the other hand, recent success was reported with an exterior approach based on a primal-dual nonlinear rescaling

method. This approach was particularly effective in a neighborhood of an optimum where numerical errors and stability issues impede convergence of interior point methods. The understanding of stability and sensitivity in optimization is an area of active research.

In the area of continuous, smooth optimization, the "Newton Liberation Front" (NLF) received strong endorsement. That is, in the past, researchers placed a lot of emphasis on ensuring global convergence of algorithms. This led to rather stringent criteria for the acceptance of a Newton step. A new class of acceptance criteria is emerging today, the so-called filter methods. And a new variation of this criterion, that essentially provides a less stringent acceptance criterion, yielded superior performance on a large set of test problems. Further progress on relaxing the acceptance criteria while ensuring convergence is expected in the coming decade.

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