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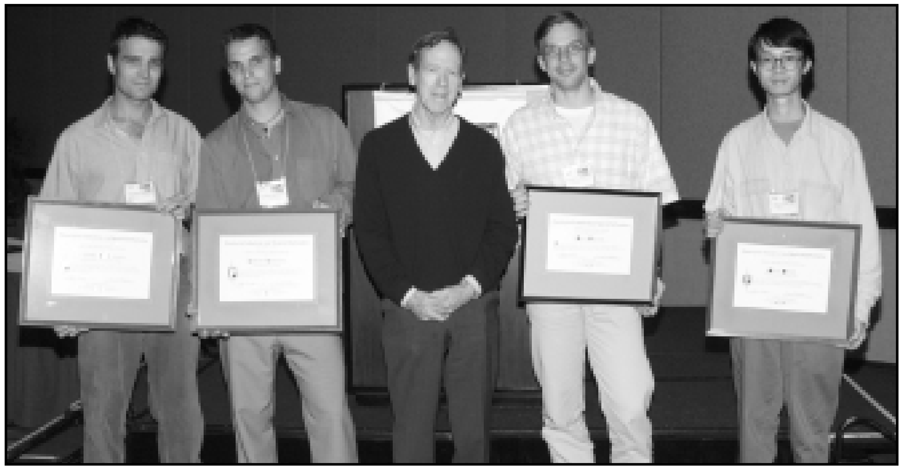
Next-generation Math Scientists Take the Stage In Puerto Rico

By Paul Davis

Rest assured that exposition and mathematics are alive and well in the next generation of applied mathematicians. The proof is in the three SIAM Student Paper Prize presentations given in July at the 2000 SIAM Annual Meeting in Puerto Rico.



Polished presentations by the recipients of the SIAM Student Paper Prize have become a standard feature at SIAM meetings, and this year was no exception. Pictured here in Puerto Rico with SIAM president Gilbert Strang are the three prize recipients for 2000: Raphael Hauser of Cambridge University (left), whose paper was titled "Target Directions for Primal–Dual Interior-point Methods for Self-scaled Conic Programming"; Robert Scheichl of the University of Bath (second from left), whose winning paper was "A Decoupled Iterative Method for Mixed Problems Using Divergence-free Finite Elements"; and Jian Deng of Brown University (far right), who wrote and spoke about weakly reversible chemical reaction networks. Also shown is Axel Facius of the Universität Karlsruhe, who was awarded an honorable mention for his paper "Verified Stopping Criteria for Krylov Type Linear System Solvers." The prize committee awarded a second honorable mention, to Niyazi Sahin of the University of Pittsburgh (not pictured), whose paper considered boundary conditions for large eddies.

Raphael Hauser, currently of the Department of Applied Mathematics and Theoretical Physics at Cambridge University, described the theoretical umbrella he has developed for a large class of path-following, primal–dual interior point algorithms. His work covers linear, semidefinite, and other convex programming problems.

In the simplest case, interior point methods replace a constrained linear program with an unconstrained problem whose objective function includes a barrier function that grows near the constraint boundary. (The classic barrier function is logarithmic in the constraint margin.) Interior point algorithms construct a path from an initial point interior to the feasible region toward the optimal vertex on the constraint boundary. The path is parametrized by the (decreasing) weight given to the barrier term in the objective function.

Primal–dual methods solve primal and dual programs simultaneously (and reasonably cleverly). The duality gap, the difference between the primal and the dual objective functions, is a measure of the accuracy of the current estimate of the optimal value of the objective function.

Nonlinear programs are reduced to a sequence of linear problems, each to be solved approximately, via Newton linearization. The central path of an interior point optimization can be regarded as aimed at a target point that is being pushed closer to the true optimum by the Newton updates.

Hauser's initial goal was the development of a preconditioner to avoid blow-up near the boundary for the key interior point calculation, a Newton update of the form $F''(w)\Delta x + \Delta s = \cdots$, where $F''(w)$ is the Jacobian of the objective function and x and s are the primal and dual variables, respectively. He discovered that he could do much more.

Nominally, the Newton update equation is derived from the first-order necessary conditions for an optimum. Other researchers had recognized that it could also be derived from a relation involving what Hauser calls the target map, $(x_1 s_1, \ldots, x_n x_n)^T$. The target map rectifies the central path by mapping it onto the ray $\mu\,(1, \ldots, 1)^T$. The primal and dual components of this map are essentially square roots of the inverse of the Jacobian F''.

Prior attempts to extend these ideas to build a unifying interior point framework had been stymied by the assumption that each of these components depends only on the associated primal or dual variable that it maps. Hauser showed that the necessary properties for a generalized target map cannot be attained under this restrictive assumption. He then derived the appropriate operator extensions, indicated how the analysis of computational complexity can be unified, and demonstrated that the relevant geometry generalizes beautifully.

Jian Deng of the Division of Applied Mathematics at Brown University tackled a problem of a completely different type, the existence of nontrivial steady states in mass-action chemical reaction networks. He studied so-called weakly reversible reactions, in which each reaction is part of a loop of reactions, even if each individual reaction is not reversible. The notion of "weakly reversible" defines a graphical structure for the "reacts to" relation among the compounds or chemical complexes involved in the reaction network.

Deng also observed an algebraic structure. The chemical complexes are linear combinations of the species involved and can be represented as vectors in the space of participating chemical species. So-called stoichiometric subspaces are invariant subspaces spanned by the reaction vectors for the reversible reactions. Parallel to these subspaces are invariant linear manifolds, which Deng has proved to contain the nontrivial steady states he was seeking, independent of the values of individual rate constants.

The key argument in this mathematical validation of chemists' intuition involved showing that a certain free energy expression is "almost" decreasing in time. Deng is continuing to study the asymptotic behavior of such systems, the geometric character of their attrac-tors, and variants of these mass-action, weakly reversible systems.

The third of the prize-winning papers describes a decoupled iterative method for mixed three-dimensional elliptic boundary-value problems that uses specially chosen finite elements. The author, Robert Scheichl of the Department of Mathematical Sciences at the University of Bath, considers problems that might arise, for example, in a three-dimensional groundwater flow problem, in which a divergence-free velocity field is driven by the gradient of pressure or other sources like gravity. Mixed boundary conditions on the polyhedral region either prescribe pressure or prohibit flux.

This system is discretized with mixed finite elements that enforce conservation of mass on each of the tetrahedral elements. The resulting indefinite system of linear equations in velocity and pressure is of saddle point form (2×2 block symmetric in velocity and pressure with a block of zeros in the (2, 2) position); the constraint equation has the form $B^T\mathbf{u} = 0$, where $\mathbf{u}$ is velocity.

Scheichl accomplishes the critical step of decoupling the velocity and pressure equations by constructing a basis for the null space of B^T in order to eliminate pressure from the velocity–pressure part of the approximating linear system. The result is a symmetric, positive-definite system for velocity, which could be the only unknown of interest in some groundwater flow problems. A key result in Scheichl's paper is the proof (using ideas from graph theory and algebraic topology) that this basis can be constructed from an appropriately chosen set of piecewise linear functions defined on the edges of the tetrahedral mesh elements, which span the divergence-free part of the velocity space.

To recover the pressure, Scheichl very cleverly constructs a basis for the orthogonal complement of the null space of B^T to form a triangular system that can be solved by simple back-substitution.

In numerical tests with uniform and nonuniform meshes, Scheichl's decoupled method was compared with a preconditioned minimum residual method applied to the full indefinite system. His method was eight to nearly ten times faster.

This year's prize committee members were Terry Herdman, SIAM's vice president for education (chair), Clyde Monma of Telcordia Technologies, Zuhair Nashed of the University of Delaware, and Janet Peterson of Iowa State University. Papers in applied and computational mathematics are eligible for the competition if they were written by a single author who was a student in good standing and had not yet received a PhD when the paper was nominated; the papers must not have been published previously. Three prizes are awarded each year; the recipients present their papers at the SIAM annual meeting. Submissions for the 2001 prize are due in the SIAM office by February 16, 2001 (see www.siam.org for details).

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