RESEARCH STATEMENT
JAMES RATH

My expertise lies in numerical analysis and scientific computing, specifically numerical linear algebra. I have varied interests, but most of my work has centered on modeling subsurface flow and transport problems.

Thesis work

My thesis was about a novel iterative solver for symmetric, positive-definite, linear systems. Put simply, solving a linear system is a nonlinear process: it requires division. At first blush, one might expect that iterative algorithms for solving linear systems can achieve superlinear convergence since Newton's method does for nonlinear ones. However, only a handful of algorithms for linear problems have this property.

My algorithm can be described in a purely algebraic fashion and can be applied to any symmetric positive definite linear system. However, it is easier to describe in the context of discretizations of second order elliptic partial differential equations. Indeed, the original motivating problem was solving Darcy flow problems; in the problems we consider there are two challenges — high resolution and heterogeneous data — that make the use of conventional solvers impractical. That is, the linear systems that result from discretizing the flow equations are very poorly conditioned (and not just poorly scaled).

Simple coarsening of the problem gives a faster approximation of the flow but sometimes loses essential details. The algorithm obtains the fully resolved approximation but only iterates on a sequence of coarsened problems. The sequence is chosen by optimizing the shapes of the coarse finite element basis functions. Since we optimize the basis (and not the solution directly), we trade solving a linear system for solving a nonlinear optimization problem. Intuition tells us that a nonlinear problem is more difficult to solve. However, we do this because we trade a large linear system for a small nonlinear one, and this nonlinear problem has a special structure we can further exploit.

As a stand-alone method, the algorithm converges globally and monotonically with a quadratic asymptotic rate. Per-iteration costs are cheap: a coarse-scale solve and a fine-scale residual calculation. However, it is assumed that an externally provided error estimate is available at each step. The algorithm could be effective as an accelerator: an inner iteration of another iterative method would provide an error estimate after which an outer iteration of the new method would act on that estimate. I hope to investigate this further.

More excitingly, some computational experience has shown the number of iterations needed is independent of the resolution and heterogeneity of the medium (the condition number of the problem). A proof of this insensitivity is a target of future research. Also, I know how to adapt my techniques to solving equilibrium systems; however, I have yet to write a proof of convergence for the new technique.

Other multiscale finite element research

Along with the research I have done for my thesis, I have worked extensively with my advisor on issues in using multiscale finite elements. For instance, we recently came to the realization that several multiscale finite element schemes do not converge under refinement. The coarse basis shapes in these schemes are chosen during a simulation in an attempt to match the shape of the solution (features of the flow field). This is a desirable aim; it tends to improve accuracy. However, the resulting shapes are not interpolatory; this accounts for the lack of convergence under refinement. This non-convergence is not just of theoretical interest; it is an issue of some practical importance because the threshold where errors stop decreasing is near the size of typical industrial simulations.

We have also recently developed a homogenization-inspired family of multiscale macro-elements for Darcy flow problems. One issue that we wanted to address is variational multiscale elements do not allow for (or, rather, do not give a means for systematically deriving) variation along coarse element boundaries. As mentioned above, various fixes have been proposed but can result either in non-conforming methods, non-convergence, or both. A fix comes from homogenization theory: there is an operator that tells us how to modify coarse shapes over their whole support (as compared to variational multiscale theory which just tells us to modify them on the interior of coarse elements).

Part of the motivation was to obtain interelement fluxes that, in the limit, are interpolatory and so avoid the problem mentioned above. Another motivation is a result from homogenization theory that the coarse-scale part of the solution is smoother than the fine-scale part; this also jibes with physical intuition. One trouble is increased continuity requirements for the coarse part, but we hope that increased accuracy compensates for the greater number of degrees of freedom needed. That is, we expect it to be more regular hence it would benefit from an element that reflects that higher degree of regularity. There are certainly many experiments and much research we would like to try in this direction.

Other potential research

I am interested in expanding my knowledge of applications of multiscale finite elements and variational multiscale methods in other fields. In particular, I am currently learning about the use of multiscale for stabilization in computational fluid dynamics and global climate models, and about the use of multiscale for incorporating subscale physical models.

More tangentially related to my current research, I was recently introduced to the problem of stitching together images to form a panorama. Usually the original image edges result in noticeable transitions in the panorama (even if there is good registration of features between the images). A popular idea is to use the inverse Laplacian to smooth the gradients of the images together; it is a open research question on how best to compute this smoothing (or an approximation thereto).

I have also done a little research on the worm blanket problem: find the smallest blanket that can cover a (vanishingly thin) worm if the worm is allowed to take up any position in the plane. With the assumption that any placement of a worm configuration under the blanket can be continuously (smoothly) deformed into any other configuration, one can pose this as a variational minimization problem. It can be approximated using segmented wriggling worms, and minimal blankets constructed using ODE solvers. Aside from keeping worms warm through the winter, this problem has applications in physics, chemistry, and biology. For instance, in a three-dimensional version, one might ask the question: what is the smallest nucleus that can accommodate a given length of DNA if the DNA strand is allowed to take on any configuration? Or: what is the smallest working volume needed to assemble a protein of a given length of peptides if the ultimate shape of the protein is not known in advance?