Solution Methods for Fractional Diffusion Problems and Related Rational Approximations

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Our study is motivated by the recent achievements in fractional calculus and its numerous applications related to anomalous diffusion. Let us consider a fractional power of a self-adjoint elliptic operator introduced through its spectral decomposition, which is self-adjoint but nonlocal. The nonlocal problems are computationally expensive. Several different techniques were recently proposed to localize the nonlocal elliptic operator, thus increasing the space dimension of the original computational domain.

An alternative approach is discussed in this talk. The goal is to reduce the computational complexity. Let A be a properly scaled symmetric and positive definite (SPD) sparse matrix. A method for solving algebraic systems of linear equations involving A^α, $0 < \alpha \leq 1$ is presented. The solver is based on best uniform rational approximations (BURA) of the scalar functions $t^{\beta-\alpha}$, $0 < t \leq 1$, β is a small integer. Although the fractional power of A is a dense matrix, the algorithm has complexity of order $O(N)$, where N is the number of unknowns. Robust error estimates for the BURA based algorithm are obtained. A stable modification of the Remez algorithm is developed to compute BURA for $t^{\beta-\alpha}$.

Two kinds of numerical experiments are presented. The 1D tests illustrate the sharpness of the error estimates, the positivity of the BURA based approximate inverse, as well as the mass conservation properties. The algorithm has optimal computational complexity, assuming that some optimal PCG solver is used to solve the involved auxiliary systems with certain positive diagonal perturbations of the original matrix A. The scalability analysis includes 3D tests with up to 512^3 degrees of freedom. At the end, some promising parallel results on Intel Xeon Phi architecture towards scalability for extreme scale problems with fractional Laplacians are shown.

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