A Block GCROT Method for Multiple Right Hand Sides Applied to Large-Scale Electronic Structure Problems

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Abstract

We present a block version of the GCROT method proposed by Eric de Sturler [SIAM J. Numer. Anal., 36(3), 864–889, 1999] for solving complex, non-Hermitian linear systems with multiple right-hand sides. The method is a nested GMRES-type solver. For the outer iteration we propose a block variant of GCR, while for the inner iteration

we adopt a block GMRES algorithm which is a blended version of the standard block GMRES and Ruhe's variant.

We use this method as a linear system solver for inverting complex, non-Hermitian matrices. Such matrices arise from application of large-scale electronic structure calculations to materials science problems.

The method seems to have very good convergence properties. We present numerical results from this application.