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Deflated GMRES and BiCGStab for Multiply Shifted Systems in QCD

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Large systems of linear equations with complex coefficients must be solved in QCD (quantum chromodynamics) physics. In some cases these systems not only have multiple right-hand sides, but also several shifts $A - \sigma_i I$ for each right-hand side. We will discuss version of GMRES and BiCGStab for solving such problems.

For systems with multiple right-hand sides, it is important to share information. Block methods are one possibility. We will look first at another approach of computing eigenvectors during the solution of the first right-hand side with deflated GMRES. These eigenvectors are used to aid GMRES or BiCGStab in the solution of the other right-hand sides. This approach can also be combined with block methods.

For multiply shifted systems, it is important to solve all of them in about the same cost as for only one system. We give a version of GMRES-DR (a deflated GMRES method) that works for multiple shifts with the first right-hand side. For the other right-hand sides, it is difficult to deflate eigenvalues and still solve multiple shifts unless the eigenvectors have been determined exactly. However, we show a way to get mostly around this difficulty using an Arnoldi recurrence for the approximate eigenvectors generated by GMRES-DR.