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Phanish Suryanarayana, Phanisri P. Pratapa, John E. Pask



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Alternating Anderson-Richardson method: An efficient alternative to preconditioned Krylov methods for large, sparse linear systems

Phanish Suryanarayana*,a, Phanisri P. Pratapaa, John E. Paskb

^aCollege of Engineering, Georgia Institute of Technology, Atlanta, GA 30332, USA ^bPhysics Division, Lawrence Livermore National Laboratory, Livermore, CA 94550, USA

Abstract

We present the Alternating Anderson-Richardson (AAR) method: an efficient and scalable alternative to preconditioned Krylov solvers for the solution of large, sparse linear systems on high performance computing platforms. Specifically, we generalize the recently proposed Alternating Anderson-Jacobi (AAJ) method (Pratapa et al., *J. Comput. Phys.* (2016), 306, 43–54) to include preconditioning, discuss efficient parallel implementation, and provide serial MATLAB and parallel C/C++ implementations. In serial applications to nonsymmetric systems, we find that AAR is comparably robust to GMRES, using the same preconditioning, while often outperforming it in time to solution; and find AAR to be more robust than Bi-CGSTAB for the problems considered. In parallel applications to the Helmholtz and Poisson equations, we find that AAR shows superior strong and weak scaling to GMRES, Bi-CGSTAB, and Conjugate Gradient (CG) methods, using the same preconditioning, with consistently shorter times to solution at larger processor counts. Finally, in massively parallel applications to the Poisson equation, on up to 110,592 processors, we find that AAR shows superior strong and weak scaling to CG, with shorter minimum time to solution. We thus find that AAR offers a robust and efficient alternative to current state-of-the-art solvers, with increasing advantages as the number of processors grows.

Key words: Linear systems of equations, Parallel computing, Anderson extrapolation, Richardson iteration, Electronic structure calculations

PROGRAM SUMMARY

Program Title: AAR
Program Title: AAR
Program Files doi: http://dx.doi.org/10.17632/669xrdcwry.1
Licensing provisions: GNU General Public License 3 (GPL)
Programming language: MATLAB for the MATLAB version. C/C++ for the PETSc version. C/C++ for
the standalone version.
External routines/libraries: MATLAB 2014a or later for the MATLAB version.
PETSc 3.5.3 (http://www.mcs.anl.gov/petsc) or later and
MVAPICH2 2.1 (http://mvapich.cse.ohio-state.edu/) or later for the PETSc version.
MVAPICH2 2.1 or later for the standalone version.

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^{*}Corresponding Author (*phanish.suryanarayana@ce.gatech.edu*)

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