Electronic Transactions on Numerical Analysis.
Volume 31, pp. 126-140, 2008.

ISSN 1068-9613.

ETNA
Kent State University
http://etna.math.kent.edu

ON A WEIGHTED QUASI-RESIDUAL MINIMIZATION STRATEGY FOR SOLVING COMPLEX SYMMETRIC SHIFTED LINEAR SYSTEMS*

T. SOGABE†, T. HOSHI‡, S.-L. ZHANG†, AND T. FUJIWARA§

Abstract. We consider the solution of complex symmetric shifted linear systems. Such systems arise in large-scale electronic structure simulations, and there is a strong need of algorithms for their fast solution. With the aim of solving the systems efficiently, we consider a special case of the QMR method for non-Hermitian shifted linear systems and propose its weighted quasi-minimal residual approach. A numerical algorithm, referred to as shifted QMR_SYM(B), is obtained by the choice of a weight which is particularly cost-effective. Numerical examples are presented to show the performance of the shifted QMR_SYM(B) method.

Key words. Complex symmetric matrices, shifted linear systems, Krylov methods, COCG, QMR_SYM.

AMS subject classifications. 65F10.

* Received November 30, 2007. Accepted August 17, 2008. Published online on January 22, 2008. Recommended by Martin H. Gutknecht. This work was partially supported by KAKENHI (Grant No. 18760063, 19560065).

† Department of Computational Science and Engineering, Nagoya University, Furo-cho, Chikusa-ku, Nagoya 464-8603, Japan ({sogabe,zhang}@na.cse.nagoya-u.ac.jp).

‡ Department of Applied Mathematics and Physics, Tottori University, Japan, and Core Research for Evolutional Science and Technology, Japan Science and Technology Agency (CREST-JST), 4-1-8 Honcho, Kawaguchi-shi, Saitama 332-0012, Japan (hoshi@damp.tottori-u.ac.jp).

§ Center for Research and Development of Higher Education, The University of Tokyo, Hongo, 7-3-1, Bunkyo-ku, Tokyo 113-8656, Japan, and Core Research for Evolutional Science and Technology, Japan Science and Technology Agency (CREST-JST), 4-1-8 Honcho, Kawaguchi-shi, Saitama 332-0012, Japan (fujiwara@coral.t.u-tokyo.ac.jp).