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Flexible Krylov-type Methods for Electronic Structure Calculations

Agnieszka Międlar[1*], Yousef Saad[2]

[1] University of Kansas, Department of Mathematics, 1460 Jayhawk Blvd., Lawrence, KS 66045-7594, amiedlar@ku.edu, http://www.math.ku.edu/u/amiedlar/

[2] University of Minnesota, Department of Computer Science and Engineering, 200 Union Street SE, Minneapolis, MN 55455, saad@cs.umn.edu, http://www-users.cs.umn.edu/ saad/

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Determing excited states in quantum physics or calculating the number of valence electrons in the Density Functional Theory (DFT) involve solving eigenvalue problems of very large dimensions. Moreover, very often the interesting features of these complex systems go beyond information contained in the extreme eigenpairs. For this reason, it is important to consider iterative solvers developed to compute a large amount of eigenpairs in the middle of the spectrum of large Hermitian and non-Hermitian matrices. In this talk, we present a newly developed Krylov-type method and compare it with the well-established techniques in electronic structure calculations. We demonstrate their efficiency and robustness through various numerical examples.