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Iterative Eigensolvers for Electronic Structure Calculations in Materials Science and Nanoscience

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Density functional based electronic structure calculations have become the most heavily used approach in materials science to calculate materials properties with the accuracy of a full quantum mechanical treatment of the electrons. This results in an approximate single particle form of the Schrodinger equation which is an eigenfunction problem. In this talk I will present a brief introduction to density functional theory and electronic structure calculations followed by a discussion of the iterative eigensolvers we have developed for these problems. I will discuss and compare the performance of a few different solvers, such as conjugate gradient based methods, on large parallel computers for a variety of physical problems. I will also discuss some of the eigenvalue problems associated with newer electronic structure methods for studying large nanosystems. (This work was supported by the Director, Office of Advanced Scientific Computing Research, Division of Mathematical, Information and Computational Sciences of the U.S. Department of Energy and the Laboratory Directed Research and Development Program of Lawrence Berkeley National Laboratory under contract number DE-AC03-76SF00098)