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New Iterative Eigensolvers and Preconditioners for Electronic Structure Calculations in Nano and Materials Science

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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 approach results in a single particle form of the Schrodinger equation which is a non-linear eigenfunction problem. The standard selfconsistent solution of this problem involves solving for the lowest eigenpairs corresponding to the electrons in the system. In non-selfconsistent formulations the problem becomes one of determining the interior eigenpairs corresponding to the electrons of interest which are typically around the gap in the eigenvalue spectrum for non-metallic systems. In this talk I will present results for new iterative eigensolvers based on conjugate gradients (the LOBPCG method) in the context of plane wave electronic structure calculations. This new method gives significant speedup over existing conjugate gradient methods used in electronic structure calculations. I will also present results for a new preconditioner based on first solving the bulk structure corresponding to a given nanosystem and then using that as a preconditioner to solve the nanosystem. This new preconditioner gives significant speedup compared to previously used preconditioners based on the diagonal of the matrix. These new methods will be demonstrated for CdSe quantum dots as well as quantum wires constructed from layers of InP and InAs. (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)