Abstract Submitted
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New eigensolvers and preconditioners for large scale nanoscience simulations[1] ANDREW CANNING, OSNI MARQUES , LIN-WANG WANG , CHRISTOF VOEMEL, CRD, Lawrence Berkeley National Laboratory, STANIMIRE TOMOV, JULIEN LANGOU, University of Tennessee — First-principles materials science calculations typically involve a self-consistent solution of the Kohn-Sham equations. These types of methods typically scale with the cube of the system size and can only be used to study systems of up to a thousand atoms. To study larger systems we use semi-empirical potentials or approximated ab initio potentials such as those constructed using the charge patching method. Using these types of potentials does not require a selfconsistent solution of our effective single particle equations and we can solve directly for the few states of interest around the gap. This leads to a method that is effectively O(N) if we consider the number of states we require to be fixed as the system size increases. The solution of our single particle equations now becomes an interior eigenvalue problem for a few states around a given energy rather than the self-consistent solution for the lowest n states where n is the number of bands. I will compare different methods (conjugate gradient, Jacobi-Davidson, Lanczos) for this problem with particular emphasis on solving large nanosystems on parallel computers. Work supported by the DOE under the Modeling and Simulation in Nanoscience Initiative.

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