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The Solution of the Interior Eigenvalue Problem for Large Scale Nanosystems ANDREW CANNING, LIN-WANG WANG, OSNI MARQUES, Lawrence Berkeley National Laboratory, 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. 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. In this talk 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.

Andrew Canning
Lawrence Berkeley National Lab.

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