Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Planning the next generation of density functional codes[1] GRADY SCHOFIELD, JAMES R. CHELIKOWSKY, University of Texas at Austin, YOUSEF SAAD, University of Minnesota — Real-space pseudopotential density functional theory has proven to be an efficient avenue for computing the properties of matter in many different states and geometries, including liquids, wires, slabs and clusters with and without spin polarization. Fully self-consistent solutions have been routinely obtained for systems with thousands of atoms. However, there are still systems where quantum mechanical accuracy is desired, but scalability proves to be a hindrance, such as large biological molecules or complex interfaces. We will present an overview of our work on algorithms for this problem, which has taken the route of improved scalability by spectrum slicing in the eigensolver, *i.e.*, the construction of a "parallel" eigensolver. We will also discuss how accurate forces can be obtained for "coarse grids."

[1]We acknowledge support provided by DOE SciDAC program funded by ASCR and BES under award DE-SC0008877. Computational resources were provided by the National Energy Research Scientific Computing Center (NERSC), and the Texas Advanced Computing Center (TAC

James Chelikowsky
University of Texas at Austin

Date submitted: 14 Nov 2013 Electronic form version 1.4