Abstract Submitted
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Scalable real space pseudopotential-density functional codes for materials applications[1] JAMES R. CHELIKOWSKY, CHARLES LENA, GRADY SCHOFIELD, University of Texas at Austin, YOUSEF SAAD, University of Minnesota, JACK DESLIPPE, National Energy Research Scientific Computing Center, CHAO YANG, Lawrence Berkeley National Laboratory — Real-space pseudopotential density functional theory has proven to be an efficient method 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 new algorithms, which offer improved scalability by implementing another layer of parallelism, and by optimizing communication and memory management.

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