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Scalable real space pseudopotential density functional codes for materials in the exascale regime[1] CHARLES LENA, JAMES CHELIKOWSKY, GRADY SCHOFIELD, University of Texas at Austin, ARIEL BILLER, LEEOR KRONIK, Weizmann Institute of Science, YOUSEF SAAD, University of Minnesota, JACK DESLIPPE, National Energy Research Scientific Computing Center — 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 using this approach have been routinely obtained for systems with thousands of atoms. Yet, there are many systems of notable larger sizes where quantum mechanical accuracy is desired, but scalability proves to be a hindrance. Such systems include large biological molecules, complex nanostructures, or mismatched interfaces. We will present an overview of our new massively parallel algorithms, which offer improved scalability in preparation for exascale supercomputing. We will illustrate these algorithms by considering the electronic structure of a Si nanocrystal exceeding 10^4 atoms.

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