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Efficient Calculation of Exact Exchange Within the Quantum Espresso Software Package TAYLOR BARNES, THORSTEN KURTH, Lawrence Berkeley Natl Lab, PIERRE CARRIER, NATHAN WICHMANN, Cray, DAVID PRENDERGAST, Lawrence Berkeley Natl Lab, PAUL KENT, Oak Ridge Natl Lab, JACK DESLIPPE, Lawrence Berkeley Natl Lab — Accurate simulation of condensed matter at the nanoscale requires careful treatment of the exchange interaction between electrons. In the context of plane-wave DFT, these interactions are typically represented through the use of approximate functionals. Greater accuracy can often be obtained through the use of functionals that incorporate some fraction of exact exchange; however, evaluation of the exact exchange potential is often prohibitively expensive. We present an improved algorithm for the parallel computation of exact exchange in Quantum Espresso, an open-source software package for plane-wave DFT simulation. Through the use of aggressive load balancing and on-the-fly transformation of internal data structures, our code exhibits speedups of approximately an order of magnitude for practical calculations. Additional optimizations are presented targeting the many-core Intel Xeon-Phi "Knights Landing" architecture, which largely powers NERSC's new Cori system. We demonstrate the successful application of the code to difficult problems, including simulation of water at a platinum interface and computation of the X-ray absorption spectra of transition metal oxides.

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