

Abstract Submitted
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GPAW on Blue Gene/P¹ NICHOLS ROMERO, Argonne National Laboratory, JUSSI ENKOVAARA, CSC - IT Center for Science Ltd., MARCIN DULAK, CHRISTIAN GLINSVAD, ASK LARSEN, JENS MORTENSEN, Technical University of Denmark, SAMEER SHENDE, University of Oregon, VITALI MOROZOV, JEFFREY GREELEY, Argonne National Laboratory — Density function theory (DFT) is the most widely employed electronic structure method due to its favorable scaling with system size and accuracy for a broad range of molecular and condensed-phase systems. The advent of massively parallel supercomputers have enhanced the scientific community's ability to study larger system sizes. Ground state DFT calculations of systems with $O(10^3)$ valence electrons can be routinely performed on present-day supercomputers. The performance of these massively parallel DFT codes at the scale of 1 - 10K execution threads are not well understood; even experienced DFT users are unaware of Amdahl's Law and the non-trivial scaling bottlenecks that are present in standard $O(N^3)$ DFT algorithms. The GPAW code was ported and optimized for the Blue Gene/P. We present our algorithmic parallelization strategy and interpret the results for a number of benchmark test cases. Lastly, I will describe opportunities for computer allocations at the Argonne Leadership Computing Facility.

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