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Plane Wave First-principles Materials Science Codes on Multicore Supercomputer Architectures[1] ANDREW CANNING, Computational Research Division, Lawrence Berkeley National Laboratory, JACK DESLIPPE, National Energy Research Scientific Computing Center, Lawrence Berkeley National Laboratory, STEVEN.G. LOUIE, Dept. of Physics, University of California, Berkeley and Materials Science Division, Lawrence Berkeley National Laboratory, SCIDAC TEAM — Plane wave first-principles codes based on 3D FFTs are one of the largest users of supercomputer cycles in the world. Modern supercomputer architectures are constructed from chips having many CPU cores with nodes containing multiple chips. Designs for future supercomputers are projected to have even more cores per chip. I will present new developments for hybrid MPI/OpenMP PW codes focusing on a specialized 3D FFTs that gives greatly improved scaling over a pure MPI version on multicore machines. Scaling results will be presented for the full electronic structure codes PARATEC and BerkeleyGW. using the new hybrid 3D FFTs, threaded libraries and OpenMP to gain greatly improved scaling to very large core count on Cray and IBM machines.

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