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Hybrid OpenMP/MPI Conjugate Gradient Iterative Eigensolver for First-principles Plane Wave Electronic Structure Codes on Many-core Architectures

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Density Functional Theory (DFT) based First-principles materials science codes using plane waves (PW Fourier basis) have become the largest user, by method, of computer cycles at scientific computer centers around the world. At NERSC (National Energy Research Scientific Computing Center) an estimated 17cycles are used by DFT-PW codes such as VASP, Quantum Espresso, Abinit, PEtot, PARATEC etc. These codes commonly use conjugate gradient based iterative eigensolvers to solve the density functional theory based approximation to the many-body Schrodinger Equation (usually the Kohn-Sham form). In this approach 3D FFTs are used to move between real and Fourier space to construct the matrix-vector product such that the different parts of the Hamiltonian matrix are calculated in the space where they are sparse. The parallel scaling of the 3D FFTs in the conjugate gradient solver is particularly challenging as rather than one large grid, as is the case in other scientific applications using spectral methods, we have many medium sized grids (one for each electronic state) which can limit scaling. We therefore developed a specialized hybrid OpenMP/MPI version of the 3D FFT to scale efficiently on modern many-core platforms.

Overall the conjugate gradient solver uses a two level parallelization scheme where the high level parallelization divides the eigenvectors (electronic states) among groups of nodes and then within a group each eigenvector is divided among the nodes. OpenMP and threading is then used to parallelize the solver on the node while MPI is used for the communications between the nodes. Details of how OpenMP and threading is used to parallelize the 3D FFT and other parts of the solver will be given in the talk. We will present results for the complete code as well as separately for the 3D FFT on the many-core architecture Intel MIC Xeon NERSC computers Edison (Cray XC30 with 12 core Intel Ivy Bridge Xeon) and Cori phase one (Cray with 16 core Intel Haswell Xeon). By sending fewer larger messages the hybrid OpenMP/MPI version of the 3D FFT significantly outperforms the pure MPI version on large core count many-core architectures allowing the solver to scale efficiently to 10,000s of cores. This work was done in collaboration with L-W Wang, J. Shalf, N.J.