Abstract Submitted
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**Massively Parallel Spectrum Slicing Eigensolver for Ab Initio Calculations**[1] MURAT KECELI, HONG ZHANG, Argonne National Laboratory, USA, FABIANO CORSETTI, Imperial College, UK, CARMEN CAMPOS, JOSE ROMAN, Universitat Politecnica de Valencia, Spain, ALVARO VAZQUEZ-MAYAGOITIA, PETER ZAPOL, ALBERT WAGNER, Argonne National Laboratory, USA — Hartree-Fock or density functional theory (DFT) based methods require the self-consistent solutions of the generalized eigenvalue problem, which means solving a similar problem many times until a convergence criteria is met. Computation of the eigensolutions (matrix diagonalization) becomes the bottleneck when the number of basis functions reaches thousands. We developed and benchmarked a PETSc and SLEPc based sparse eigensolver suitable for such applications. The eigensolver makes use of shift-and-invert parallel spectral transformations and we integrated this eigensolver into Siesta ab initio molecular dynamics package. By performing DFT energy and gradient calculations for water clusters, Boron nitride films, and polyethylene; we demonstrated up to seven-fold speed-up and better strong scaling efficiency compared to default eigensolver in Siesta. There are three main advantages of our solver compared to dense solvers: 1) reduced memory footprint, and computational complexity (exploits sparsity) 2) less global communications (does not require fast interconnects) 3) job balance and performance improvement at subsequent iterations. Moreover, in contrast to diagonalization free methods, it provides eigensolutions and it is applicable for both metals and insulators.

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