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All-electron KKR Calculations for Metallic Systems with Thousands of Atoms Per Cell via Sparse Matrix Iterative Solvers[1] SUFFIAN KHAN, AFTAB ALAM, DUANE JOHNSON, University of Illinois at Urbana Champaign — To perform electronic-structure calculations for inherently large systems, such as a quantum dots or interfaces like domain walls, we must perform the calculations over very large unit cells (10^4 to 10^8 atoms). For the inverse Green's function G^{-1}, KKR methods typically solve for G by direct inversion. Using a screened, k-space hybrid KKR, we solve Dyson's equation for the Green's function using a reference state via $G = G_{ref}\ [\ I - (t - t_{ref})\ G_{ref}]^{-1}$, scattering matrices t and t_{ref} are known and the non-Hermitian tensor G_{ref} is chosen for convenience and sparsity [1]. The approach is O(N) for bandgap materials, whereas it is $O(N^2)$ for metals but with a potentially large prefactor. Based upon Sparse Approximate Inverse (or SPAI) technique [2], we generalize the algorithm for complex, non-Hermitian matrices, then use the method as a preconditioner for the inversion to reduce the iteration counts (hence, reduce the prefactor) of the iterative Krylov-space inverses, such as TFQMR, to address large-scale metallic systems. Parallel iterative and energy contour solves are made also. We explore the numerical efficiency and scaling versus atoms per unit cells.
[1] Smirnov and Johnson, Comp. Phys. Comm. 148, 74-80 (2002).
[2] Grote and Huckle, SIAM J. Sci. Comput. 18, 8

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