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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, DUANE JOHNSON, University of Illinois at Urbana-Champaign — To perform electronic-structure calculations for inherently large systems, such as a quantum dots with heterogeneous interfaces, we must perform the calculations over very large unit cells (10^4 to 10^8 atoms). KKR methods typically solve for G by direct inversion G^{-1}, with known analytic form. 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. We use Krylov-space solvers to reduce storage and exploit known symmetries. 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! [1]Phys. Comm. 148, 74-80 (2002).

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