Parallelized electronic transport calculations in real space
BARUCH FELDMAN, Weizmann Institute of Science, Israel, ODED HOD, Tel Aviv University, Israel, TAMAR SEIDEMAN, Northwestern University, LEEOR KRONIK, Weizmann Institute of Science, Israel — We present a real-space method for first-principles nano-scale electronic transport calculations, using the non-equilibrium Green’s function (NEGF) method and complex absorbing potentials (CAPs) to represent the effects of the semi-infinite leads. In real space, the electronic Hamiltonian from Density Functional Theory (DFT) is very sparse. As a result, the transport problem parallelizes naturally and can scale favorably with system size. We illustrate our method with calculations on several realistic test systems and find good agreement with a reference calculation.