High-Performance NEGF: A Low-Rank Approximation Approach

Min-Ji Seo [1]

1) *School of Mathematics and Computing, Yonsei University, Seoul 03722, KOREA*

Corresponding Author : Eun-jung Lee, eunjunglee@yonsei.ac.kr

ABSTRACT

Unlike classical mechanics, modeling nanoscale devices must capture quantum effects. Among quantum transport formalisms, the Non-Equilibrium Green's function (NEGF) method is a powerful and widely used. However, computing the electron density with NEGF is computationally expensive because it requires large sparse matrix inversion for every energy levels. To alleviate this computational burden, we apply low-rank approximation (LRA) based on eigendecomposition following a matrix decomposition step, and we establish theoretical convergence guarantees. This new approach dramatically reduces the cost of computational time, while maintaining acceptable accuracy.

PROBLEM SETUP AND METHODOLOGY

Our governing equations are the stationary single-electron Schrödinger equation coupled to the Poisson equation. Due to these two equations are dependent, we solve them using a self-consistent field (SCF) method. For spatial discretization, we employ finite element method (FEM) with tetrahedral elements and piecewise linear nodal basis functions. In the Non-Equilibrium Green's function (NEGF) framework, computing the electron density requires the retarded Green's functions, which involves large sparse matrix inversion [1]. To reduce computational cost, we decompose the inverse of retarded Green's function into 2 by 2 block matrices and apply a low-rank approximation (LRA) [2] to the most time consuming part in the computation of the decomposed block matrix. Our analysis shows that when the truncated eigenvalues are sufficiently far from the energy level E used in the electron density computation, the approximation converges. In a homogeneous model, applying LRA method achieved up to 88.23 speed up using only 10% of the rank, while relative difference of 3.01×10^{-2} (electron density) and 4.83×10^{-3} (electrostatic potential).

REFERENCES

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