# A Coupled Electrostatic - Quantum Transport Framework for Exascale Systems

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Advances in nanoscale sensors using field effect transistors (FETs) have numerous applications in various scientific fields, including astrophysics, biomedicine, and security. These applications require large numbers of FETs to operate together using superior channel materials like carbon nanotubes and silicon nanowires. To study the performance of these FETs, a software framework is needed that can efficiently utilize many-core/GPU architectures and scale effectively on exascale supercomputers.

This work presents our efforts to develop a self-consistently coupled electrostatic-quantum transport framework for exascale systems (see Fig. 1), and its demonstration in modeling multiple carbon nanotube FETs (CNTFETs) functionalized with quantum dots for a novel photodetector [1]. The framework includes an open-source, 3-D exascale electrostatic solver, eXstatic [2], which uilizes the GPU-enabled AMReX library [3] for calculating electrostatic potential. AMReX provides necessary functionalities for writing massively parallel, block-structured adaptive mesh refinement (AMR) applications. The eXstatic solver offers support for specifyings intricate contact types through embedded boundaries as well as various domain boundaries (Dirichlet, Neumann, Robin, periodic) with an option to specify time-varying inputs. The solver provides routines for specifying atom locations of materials, gathering fields at these locations, and depositing charges onto the grid. The multigrid finite-volume approach used by eXstatic, in contrast to the commonly used fast Fourier transform based approach, enables the modeling of large-scale aperiodic array and stacks of FETs.

The framework has been extended to include a quantum transport module using the Nonequilibrium Green's Function (NEGF) method, which will support GPU-enabled matrix operations. The module models contacts as semi-infinite leads and the electronic properties of carbon nanotubes are described through the tight-binding approximation. The framework will be demostrated for its weak-scaling and its application in obtaining current-voltage characteristics of multiple CNTFETs functionalized with quantum dots. In the future, the NEGF module will be extended to include phonon scattering and time-dependent equations based on two-time Green's functions to model the dynamic conductance caused by the presence of point charges.

## SUMMARY

A self-consistently coupled electrostatic-quantum transport framework is being developed that efficiently leverages many-core/GPU architectures and scales well on exascale systems.

## ACKNOWLEDGMENT

This work is supported by the US Department of Energy, Office of Science, Office of Basic Energy Sciences, the Microelectronics Co-Design Research Program, under contract no. DE-AC02-05-CH11231.

## REFERENCES

[1] S. M. Young, M. Sarovar, and F. Léonard, "Nanoscale architecture for frequency-resolving single-photon detectors," 2022, submitted for publication, arXiv No: quant-ph/2205.05817, https://arxiv.org/abs/2205.05817.
[2] *eXstatic*, https://github.com/AMReX-Microelectronics/eXstatic.
[3] W. Zhang, A. Myers, K. Gott, A. Almgren, and J. Bell, "AMReX: Block-structured adaptive mesh refinement for multiphysics applications," *The International Journal of High Performance Computing Applications*, vol. 35, no. 6, pp. 508–526, 2021.

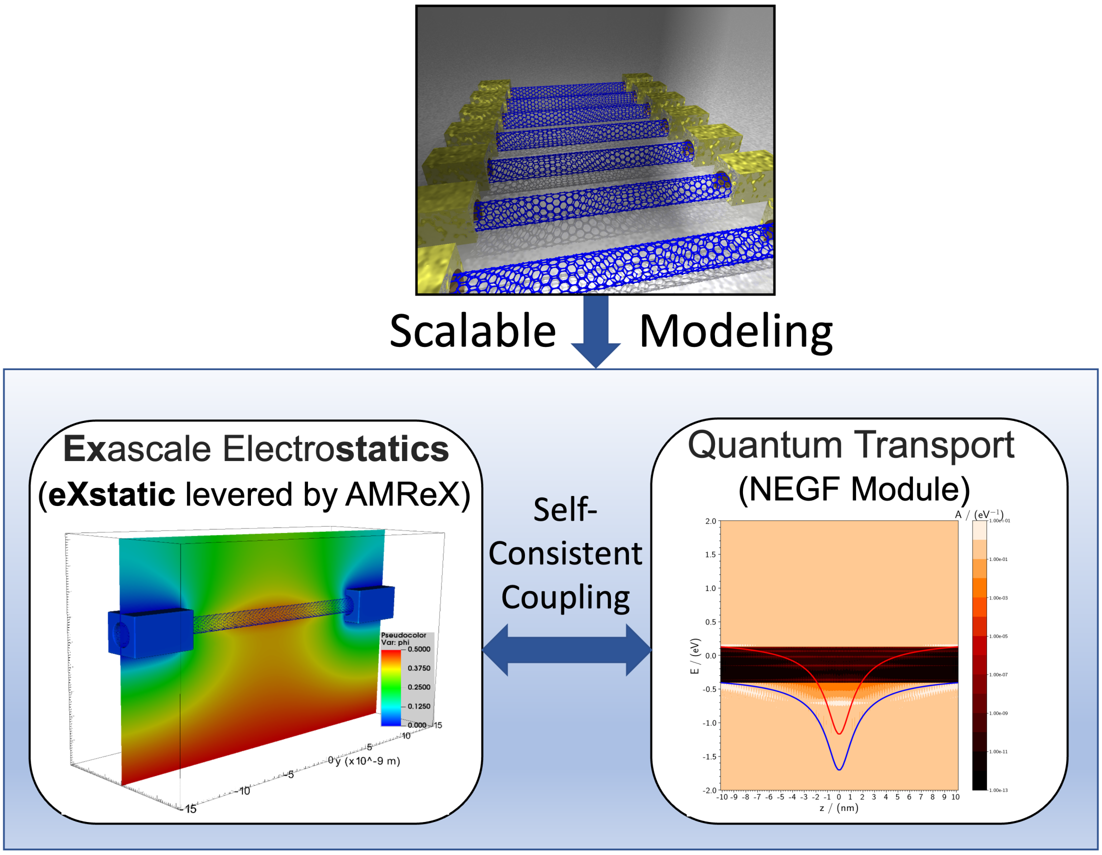


Fig. 1. A scalable approach to modeling multiple CNTFETs using the 3-D, open-source exascale electrostatic solver (eXstatic) and the self-consistently coupled quantum transport module based on the NEGF method.