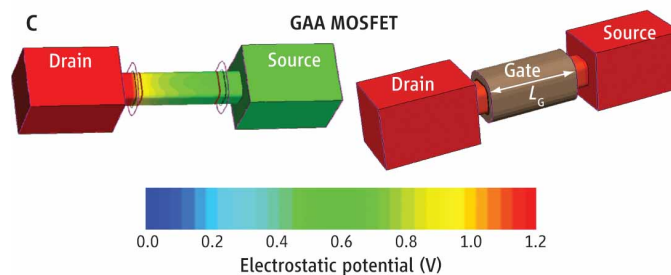


Semester/Master Thesis

Implementation of a FEM Poisson Solver into a Next-Generation Quantum Transport Simulator

Short Description

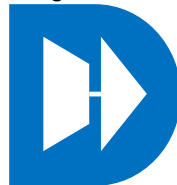
Electrostatics are at the heart of the operating principle of nanoscale devices, like Metal-Oxide-Semiconductor Field-Effect Transistors (MOSFETs). By modulating a gate potential, the channel of the device can be switched between an off- and an on-state. It is therefore critical to accurately describe device electrostatics, governed by Poisson's equation. Due to the irregular geometry of many devices, the finite element method (FEM) is the preferred numerical approach. In our group we are collaboratively developing a next-generation quantum transport (QT) simulator (QuaTrEx) with emphasis on modern high performance computing (HPC) principles. Including a Poisson solver in this novel code will open up many more possibilities for device and material simulation. The development will start with a general approach to set up and solve a system of linear equations. Afterwards, iterative and machine-learning enhanced methods may be investigated.



Electrostatic potential profile of a modern Gate-All-Around (GAA) MOSFET.
Image from *Science*, Vol. 341., pp. 140-141

Opportunity

If you want to be part of the collaborative development of a modern Python computational physics code, this is the project for you! You will be able to familiarize yourself with the physics and the numerical aspects of atomistic quantum transport and electrostatics. You will use modern high-performance Python libraries such as CuPy and mpi4py. The open-source fast parallel programming framework DaCe can also be used for parts of the project.



CuPy

Prerequisites

We are seeking a candidate with a strong interest in numerical algorithms and parallel computing. Interest in material and device simulation is desired. Don't hesitate to contact the supervisors if you want to learn more.

Status: Available

Looking for 1 or more Master/semester student(s)

Interested candidates please contact:

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