Semester/Master Thesis

Adaptive Energy Grid Algorithm for a Next-Generation Quantum Transport Simulator

Short Description

In a typical quantum transport simulation, a large system of linear equations is solved for a great number of electron energies. In our newly developed *ab initio* NEGF+self-consistent GW model, numerical energy integrals have to be performed over very densely sampled and large energy ranges. Using a uniform sampling of the energies makes calculations extremely expensive. Therefore, it is desirable to use non-uniform energy grids with fewer energy points, but that have the same accuracy as the uniform grid. These non-uniform grids are usually found with adaptive algorithms. In this project, different adaptive algorithms will be investigated. Normally, the energy integrals are convolutions that can be efficiently calculated with Fast Fourier Transforms (FFT). However, the FFT necessitates a uniform grid, so different non-uniform Fast-Fourier Transforms (NuFFT) will also be studied in the project. Ultimately, the best approach will be implemented in our parallel quantum transport simulation code.
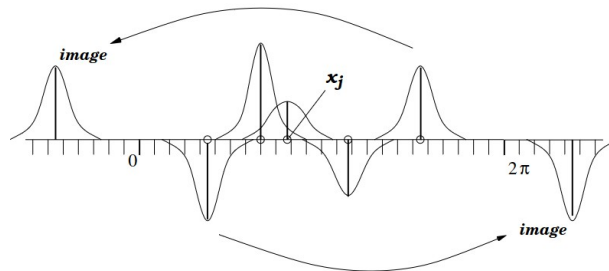

Illustration of the NuFFT algorithm. Image from *SIAM, Review, Vol. 46, pp. 443-454*

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 familiarize yourself with one-dimensional mesh refinement, non-uniform Fast-Fourier transforms, and quantum transport. Additionally, given the interest of the applicant, you will use modern high-performance Python libraries such as cupy and mpi4py.

Prerequisites

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

Status: Available

Looking for 1 or more Master/semester student(s)
Interested candidates please contact: Anders Winka awinka@iis.ee.ethz.ch
ETH Professor: Prof. Mathieu Luisier mluisier@iis.ee.ethz.ch

Integrated Systems Laboratory (IIS)