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 has to be solved for a great number of energy points. Especially in our newly developed *ab initio* NEGF+self-consistent GW model, not only a small grid resolution but also using a wide range of energy values is critical. Using a uniform energy grid with the resolution dependent on the critical part of the bandstructure can make calculations extremely expensive. It is therefore desirable to tune a local resolution of the energy grid with an adaptive algorithm, which is equivalent to a one-dimensional mesh refinement problem. Firstly, different adaptive algorithms should be investigated and implemented. An additional challenge is performing a non-uniform Fast-Fourier Transform (NuFFT) as well as redistributing the computational load in a shared- or distributed memory system.

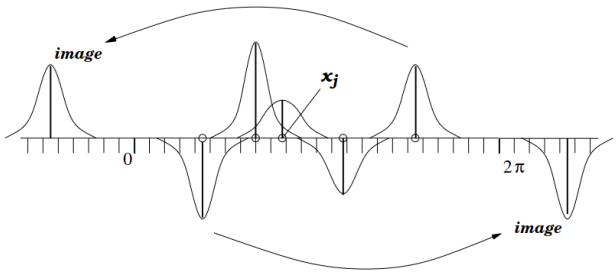

Illustration of the NuFFT algorithm. Image from *SIAM, Review, Vol. 46, pp. 443-454*

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 be able to familiarize yourself with one-dimensional mesh refinement. 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.

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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