Numerical methods in Quantum Transport Ballistic solvers

Short Description

Ballistic quantum transport is the most-widely used type of transport simulation. It allows us to study current flowing through nano-devices and quantum effects such as electron tunnelling. Simulation is done under the wave-function formalism and require on the side of the numerical methods two main building blocks:

- An *eigenvalue solver* that compute the boundary conditions and the injections terms in the system

- A *block tridiagonal linear system solver* that solves the system matrix [LHS] for the injections vectors [RHS].

$$A \cdot x = b$$

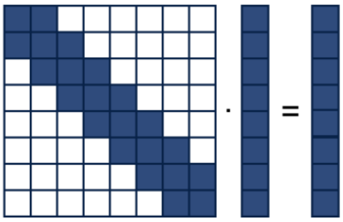

Figure 1 Block tridiagonal linear system solver.

Tools that perform such ballistic simulation have been developed for years *[OMEN]* but containing old legacy code and often with a deep entanglement between the high-performance computing layer and the numerical algorithms, these solvers aren't suited to tackle modern supercomputer architectures (Large distributed systems + GPUs).

A recent dynamic of writing such solver in an high level language such as Python coupled with some performances frameworks *(DaCe, cuPY..)* have emerged. By doing so one may, on the way, investigate all the new algorithmic developments that occurred to not only write a clean, portable and modular code. But also, an innovative one on the algorithmic side.

Project Scope

The main scope of this project is to implement a quantum transport ballistic solver. The student will have to tackle both algorithmic blocks:

- Eigenvalue solver

- Block tridiagonal linear system solver

Freedom will be given in the choice of the numerical methods used for each of these algorithmic blocks.

The code will be developed in Python, using good computer science practices aiming to develop an efficient but *portable and modular code*. Some backbone implementations will be provided, and you'll get all the support needed on the CS side.

We are looking for an *independent* and *highly motivated* student to tackle this project.

Looking forward to hear what you can bring to us?!

References:

1. RGF algorithm
2. Beyn
3. OBC

Status: Available

Looking for 1 master's student.

Interested candidates please contact: vmaillou@iis.ee.ethz.ch

Prerequisites

- Sufficient knowledge of Python.

- Interest in quantum transport theory and nano-device modeling [227-0159-00L]

- Independent and motivated student, eager to learn.

Character

Algorithms development (40%), Code implementation (40%), Testing and profiling (20%)

Professor

[Prof. Dr. Mathieu Luisier]