Extension of Parallel Schur Reduction algorithm to the computation of lesser Green's function

Short Description

In Quantum Transport (QT) simulations and under the Non-Equilibrium Green's Function (NEGF) formalism, the computational burden comes from 2 sequentially executed process:

1. Computation and application of Open Boundary Conditions (OBC) to the system matrix

2. Selected inversion of the system matrix

The selected inversion of the system matrix is usually computed through a recursive, serial algorithm: *The Recursive Green's function algorithm (RGF)*. Parallel algorithms have been developed for the solution of the selected inversion problem; *The Parallel Schur Reduction (PSR)* algorithm is a multi-sided version of the RGF algorithm. Using the propagation of a Schur-reduction inside several partitions of the system matrix at the same time.

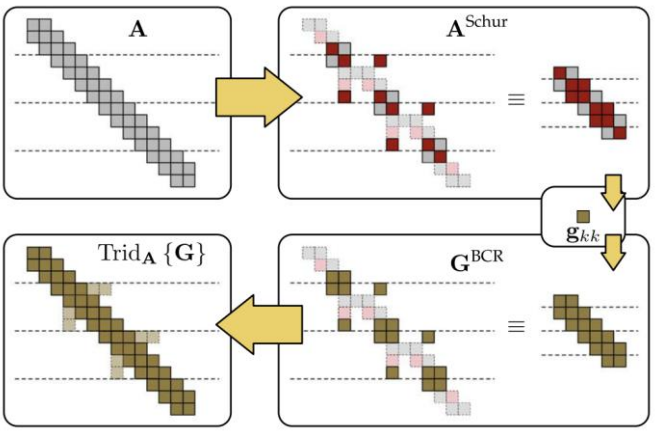

Figure 1- PSR phases, D.E. Petersen et al.

Precedent work on this algorithm have only led to the solution of the retarded Green's function.

$$AG^r = I$$

Using the well-known work on the RGF algorithm, one may extend the PSR algorithm to compute the lesser and greater Green's function, allowing parallel computation capability in the case where scattering self-energies are taken into account.

$$G^l = G^r \Sigma^l G^a$$

$$G^g = G^r \Sigma^g G^a$$

Project Scope

The main scope of this (semester) project is to study and extend the PSR algorithm to the computation of the lesser and greater Green's Function.

The code will be based on actual implementation of the PSR algorithm for the computation of the retarded Green's function.

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. Parallel Schur Reduction

Status: Available

Looking for a 1 semester 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]

Character

Theory (30%), algorithm development (50%), simulation & analysis (20%)

Professor

[Prof. Dr. Mathieu Luisier]