

## **A library for Non Equilibrium Green's Functions**

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The understanding of the electronic properties of complex nanoscaled materials and interfaces requires the use of advanced quantum mechanical approaches. Non-Equilibrium Green's Functions (NEGF) is an elegant formalism to treat quantum transport in nanodevices, encompassing, in principles, all the relevant electronic dynamics such as electron-phonon and electron-electron interactions. Yet the method is computationally very demanding because it is a matrix approach typically scaling as  $O(N^3)$ , where  $N$  is the system dimension. State-of-art NEGF implementations are currently exploiting recursive algorithms, multiple levels of parallelism, mixed precision of calculation/storage and complex data distributions. However, highly specialized implementations are inaccessible to the broad community.

Within the EoCoE II project we are developing a new highly scalable tool (libXGf) based on the libNEGF library with the aim of addressing complex materials for energy harvesting such as Si/a-Si heterostructures and interfaces. libNEGF has been developed from the start as a general purpose library, allowing to perform transport calculations based on different types of Hamiltonians, such as Ab-Initio, Tight-Binding or Finite Elements.

A consequence of this is that the library can be easily interfaced and applicable to a wide range of problems, from materials science to device physics. In this work I will present the advances in the development and various applications, including Si/aSi interfaces.