WHAT IS ANT?

ANT (Atomistic NanoTransport) is a software package to compute the electrical current in atomically defined nanostructures. At present, ANT software package is composed of the independent codes, ANT.G, ANT.1D and ANT.U.

Which are the characteristics of ANT?

ANT combines self-consistent field electronic calculations (typically Density Functional Theory), Landauer transport and the (non-equilibrium) Greens functions formalisms.

ANT.G

Code designed as a generic computational tool with application in nanoelectronics. It provides an excellent compromise between computational cost and electronic structure definition as long as the aim is to compare with experiments where the precise atomic structure of the electrodes is not relevant or defined with precision.

Straightforward use of ANT.G include the computation of the zero-bias conductance (or, alternatively, the electrical current under an applied bias voltage) of a variety of nanoscale systems such as molecular bridges or simply metallic atomic contacts as those created with scanning tunneling microscope or break junction techniques. The use of ANT.G may be naturally extended to the computation of scanning tunnelling spectroscopy and the simulation of scanning tunnelling and electrostatic force microscopy.

The technical specifications are:

- Interface to the quantum chemistry GAUSSIAN03/09 code for practical implementation of the embedded cluster approach, associated with the use of parameterized tight-binding (TB) Bethe lattice model, see Figure 1.
- The electrodes are modelled by parameterized TB Bethe (BL) lattices. The model is generated by connecting a site with N nearest-neighbors in directions that can be those of a particular crystalline lattice.
- The electronic structure of the infinite system is calculated self-consistently only within a finite-size region (the scattering or device region containing the nanoconstriction or molecule) while the electronic structure of the rest of the system (i.e., the two bulk electrodes) is fixed from the very beginning to that of a simplified parameterized BL model.
- ANT.G is written in FORTRAN90 and uses OpenMP directives to take full advantage of multiprocessor nodes.

- It has been thoroughly tested with PGI compilers on various 32- and 64-bit platforms, see Figure 2.

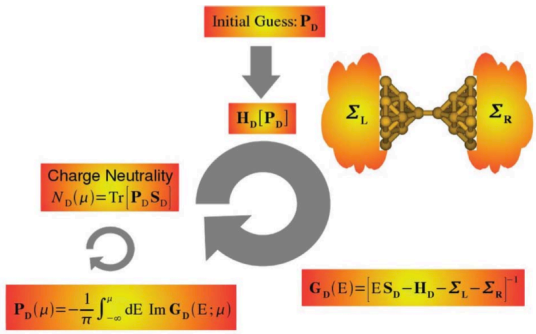

Figure 1. Diagram illustrating the self-consistent procedure for calculating the electronic structure in the embedded cluster approach as implemented in ANT.G. The central aspects of the used approach and of the one-body Green's function and Landauer formalisms are given in D. Jacob and J. J. Palacios, J. Chem. Phys. 134,044118 (2011).

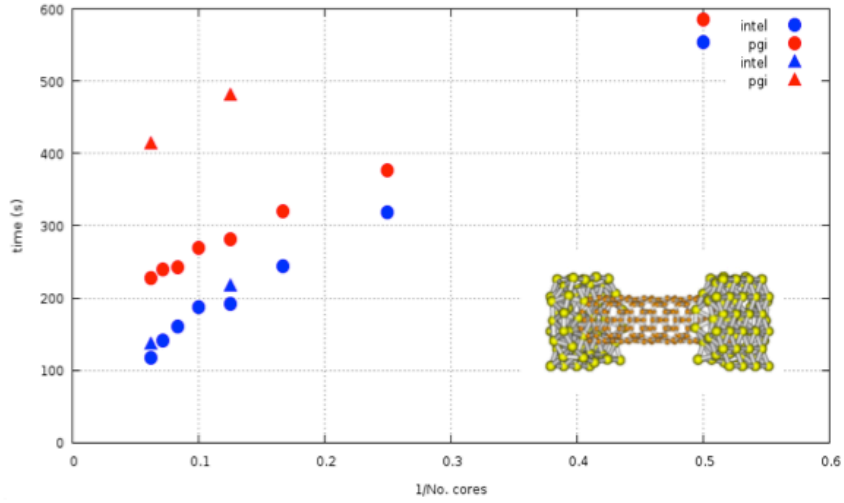

Figure 2. Performance of ANT.G in PGI and Intel compilers at low and high precision calculations

ANT.1D

Software specifically designed for the computation of the conductance at zero bias voltage in quasi-one-dimensional systems such as atomic chains, nanowires, carbon nanotubes, graphene nanoribbons, etc., which may present a disordered central region where scattering takes place. Other systems without an underlying one-dimensional symmetry such as molecular bridges can also be computed with ANT.1D by modeling the electrodes as finite-section quasi-one-dimensional wires.

ANT.1D is more demanding than ANT.G from the computational point of view, but presents the advantage of expanding the range of applicability of transport calculations to situations where the electrodes have a well-defined atomic structure.

The technical specifications are:

- Practical implementation of the super-cell approach, where the electrodes are described by perfect nanowires, to calculate the electronic structure of the device and the leads, see Figure 3.
- In the super-cell approach, the model for the leads consists of semi-infinite nanowires with finite cross-section where the electronic structure is described at the same computational level as that of the device.
- ANT.1D makes use of a pre-computed Hamiltonian for the scattering section and for the disorder-free regions. It can thus be used with tight-binding parameterized models or as a post-processing procedure to a one-dimensional periodic boundary conditions self-consistent electronic structure calculation using, e.g., CRYSTAL or SIESTA codes.
- ANT.1D is completely written in FORTRAN90 and has been parallelized with MPI. It has been tested with the Intel compiler on various 32- and 64-bit platforms with and without MPI. It also been tested with the Portland group compiler, but only without MPI.It is written in Fortran 95 and memory is allocated dynamically. It may be compiled for serial or parallel execution (under MPI).
- The interface with the CRYSTAL03 and CRYSTAL06 code is written in ANSI C++, and has been tested with the gnu C++ compiler on various 32- and 64-bit platforms

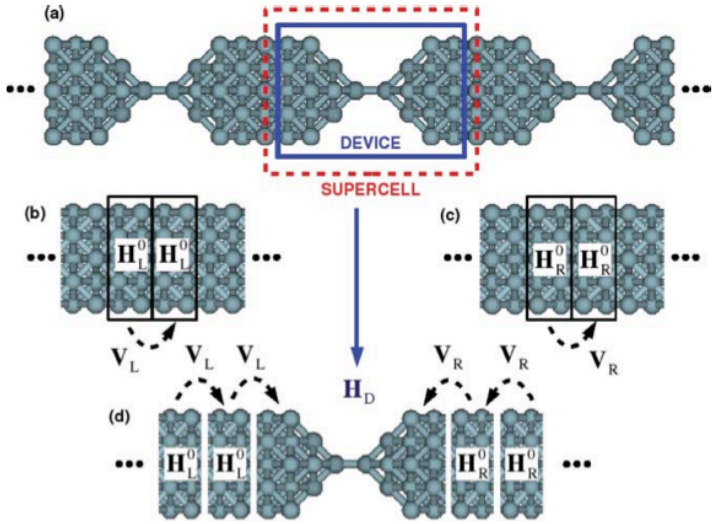

Figure 3. Illustration of the super-cell approach to calculate the electronic structure of the device and of the leads: (a) One-dimensional periodic system to calculate the electronic structure of the device region. (b) and (c): Infinite nanowires to calculate the electronic structure of the left (L) and right (R) semi-

infinite leads. (d) Sketch of the setup of the physical system: The device region (D) is suspended between two semi-infinite leads L and R. Further details of the method are given in D. Jacob and J. J. Palacios, J. Chem. Phys. 134,044118 (2011).

ANT.U

This code is specifically designed for the computation of the conductance at zero bias voltage in, e.g., graphene-based systems using a one-orbital minimal model and on-site interactions (Hubbard model).

ANT.U is an easy-to-use program for the study of spin transport in 1D systems (fundamentally graphene-based systems like nanoribbons and nanotubes) which applies the Landauer formalism to tight-binding Hamiltonians with a local Coulomb interaction (U).

The local Coulomb potential is obtained self-consistently using the mean-field Hubbard model.

What can ANT compute?

ANT can compute the properties and phenomena needed for understanding the charge transport between bulk electrodes when these are connected by an atomic- or a molecular-size region and a bias voltage is applied between them, see Figure 4.

ANT provides;

- Spin-resolved coherent transmission spectrum T(E) → Conductance
- Density of states
- Charge and spin population
- Orbital eigenchannel analysis
- Average electronic potential on atoms

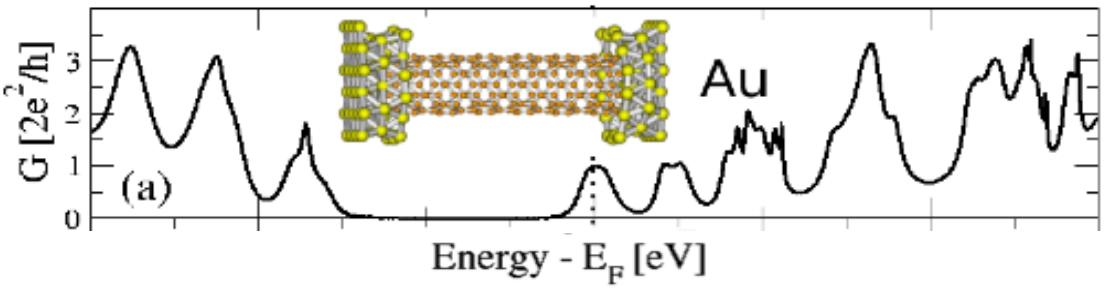

Figure 4. Example of transport calculation performed by ANT.G. The conductance of a six unit-cell (8,0) CNT contacted to Au is computed. Palacios J. J. et. al. Phys. Rev. B. 77, 113403 (2008)

ANT Documentation

- Manuals
- Tutorials
- Publications