TranSiesta Tutorial

The TRANSIESTA method is a procedure to solve the electronic structure of an open system formed by a finite structure sandwiched between two semi-infinite metallic leads. A finite bias can be applied between both leads, to drive a finite current. The method is described in detail in Phys. Rev. B **65**, 165401 (2002). In practical terms, calculations using TRANSIESTA involve the solution of the electronic density from the DFT Hamiltonian using Green's functions techniques, instead of the usual diagonalization procedure. Therefore, TRANSIESTA calculations involve a SIESTA run, in which a set of routines are invoked to solve the Green's functions and the charge density for the open system.

Please read the transiesta section in the manual (see below) before you start with the tutorial.

http://departments.icmab.es/leem/siesta/Documentation/Manuals/siesta-3.1-manual/node94.html

or

/group/allatom/siesta/transiesta-trunk-458/Docs/siesta.pdf

Your transiesta install is ***/group/allatom/siesta/transiesta-trunk-458/Obj/transiesta***

Now copy and unzip the Fast.tgz file to your home folder.

Electrode run

TranSIESTA calculations will always involve doing electrode calculations. Go inside the "Fast" directory and

```
$ cd Elec
$ /type-full-path/transiesta < elec.fast.fdf > elec.fast.out
```

1.What are the (TranSIESTA specific) files generated after an electrode run?
2.For an electrode run, what are the important TranSIESTA fdf flags?

TranSIESTA run

Now we'll do the scattering region calculation. We will also call this kind of calculations *TranSIESTA calculations*.

```
$cd ../TS_run
$cp ../Elec/elec.fast.TSHS
$ /type-full-path/transiesta < scat.fast.fdf > scat.fast.out
```

1.What **fdf flag** differentiates an electrode run from a TranSIESTA run (one that uses the TranSIESTA method)?
2.What are the essential files needed for a TranSIESTA run (apart from the files usually needed by SIESTA)?
3.How many types of self consistent cycles (not iterations !) are there when performing a TranSIESTA calculation from scratch (no atomic relaxations)?

TSHS and TSDE files

Now we want to discuss two important files created/used by TranSIESTA: the <SystemLabel>.TSHS and <SystemLabel>.TSDE files.

1.What do you think is the main information stored in a .TSHS file?
2.One of the output files of a TranSIESTA run is the <SystemLabel>.TSDE file. What is stored there?
3.If the .TSDE file is found by TranSIESTA, what happens?
4.If you erase the .TSDE file, what happens?
5.From what you have seen so far, what is the main thing that TranSIESTA does?

TBTrans and the transmission function

In the previous section we wanted to emphasize that what TranSIESTA does is essentially to find the density matrix of a *contact* region connected to two (metallic) electrodes. Once it has converged to a self consistent solution, it writes the corresponding Hamiltonian to the <SystemLanel>.TSHS file. Electronic transport properties are computed with a post-processing code named **TBTrans**.

```
$cd ../TBT_run
$cp ../Elec/elec.fast.TSHS .
$cp ../TS_run/scat.fast.TSHS .
```

```
$  /group/allatom/siesta/transiesta-trunk-458/Util/TBTrans/tbtrans < scat.fast.fdf > tbt.out
```

1.From what you have just seen, which files are needed for a TBTrans calculation (apart from the input file)?
2.Where is the transmission function stored ?
3.How does it look like (use xmgrace, or gnuplot, etc ... to visualize it)?
4.Can you give examples of things that can, and things that can't be controlled by (fdf) input options for tbtrans?

Extras

1.Why is it that there is only one iteration at the TranSIESTA SCF loop?
2.If you have some familiarity with the SIESTA structure and methods, at which part of the code would you expect a *transiesta* subroutine to be found ?
3.What is the electronic current in this example ? Why ?