

A short manual for gDFTB

This program allows one to calculate the transmission coefficients, currents potential and charge distributions and other structural properties of molecules and nanostructures between two semi-infinite contacts under the presence and absence of a voltage bias.

Technical details for performing a job run with gDFTB

1. Create an *xyz* file the system Cartesian coordinates¹ ($^{\circ}A$).
2. Load this file in the gDFTB interface.
3. Go to *compute properties* in the manual.
4. Go to *job control* manual.
5. The calculation *options* available now are
 - *Relaxation (steepest descent)*
 - *Relaxation (conjugated gradient)*
 - *Mulliken analysis + energy calculation + forces*
 - *Like option 5 + current*
6. *max force* – specifies the tolerance for the force (*Hartree/Bohr_radius*): if the total force acting on each atom in the structure is smaller than *max force*, the conjugate gradient or steepest descent routine is converged and the job terminates.
7. *number of movable atoms* – the number of atoms that can move in the geometry relaxation calculation.

For example, if there are 250 atoms in the system and the number of movable atoms is fifty, in a relaxation calculation only the first fifty atoms that were defined in the input file will move in order to calculate the geometry optimization.

¹ The first line of the *.xyz* file is the total number of atoms in the system, the second line is a blank line and in the other lines: the first column - the atom symbol and second, third and fourth columns are its *x*, *y* and *z* coordinates ($^{\circ}A$). You can also use *pdb* format or even use the gDFTB interface to create a *pdb* file from the *xyz* file.

8. *electrons number* – the total number of valence electrons in the system.

The following are some examples of the number of valence electrons of each atom that gDFTB code takes into account:

Au – 11 electrons (only *s*, *p* and *d* orbitals are taking into account, the *f* electrons are not taking into account).

H – 1 electron.

C – 4 electrons.

9. *step size (a. u.)* – the step size of the relaxation in the equation of motion (not relevant for conjugate gradient where it is adjusted automatically).

10. *scalfactor* – We can define a parameter, γ , in the following way:

$$v_{new} = (1 - \gamma)v_{old} + \gamma v_{new}$$

where v_{new} and v_{old} are the new and old electron velocities at each step of the calculation. If, for example, the *scalfactor* is 0.1 the probability that the electron velocity will change in a simulation step to v_{new} is 0.1 ($0 \leq \gamma \leq 1$).

11. *atoms temperature* – In molecular dynamics calculations, one can change the velocity of the atoms according to the atoms temperature ($^{\circ}K$).
12. *electrons temperature* – The electrons temperature ($^{\circ}K$) used for the Fermi distribution function.
13. *max number of steps* – maximum number of steps to perform a relaxation calculation.
14. Go to *contact structure* manual.
15. There are three rows in this section, each row corresponds to one of the following regions: C1 (the first contact), C2 (the second contact) and M (the molecular region, the molecule + two contacts surfaces).
16. *start* – the first atom that belongs to the region (according to the order of atoms in the input file).
17. *end* – the last atom that belongs to the region (according to the order of atoms in the input file).
18. *# electr* – the total number of valence electrons in the region.

19. L_x (*Ang*) – the dimension of the region in the x direction (0A).
20. L_y (*Ang*) – the dimension of the region in the y direction (0A).
21. L_z (*Ang*) – the dimension of the region in the z direction (0A).
22. *Fermi energy* –Fermi’s energy of the metal contacts, C1 and C2 (computed for infinite bulk contacts, ev).
23. If you would like to calculate the transmission coefficient of the system as a function of the energy of an electron injected from the first contact, go to *tunneling options* manual.
24. E_m – the minimum energy of an electron injected from the first contact (ev).
25. E_{max} – the maximum energy of an electron injected from the first contact (ev).
26. *Step* – the step size of the energy in the calculation of the transmission coefficient (as a function of injected electron, ev).
27. If you would like to calculate the current through the molecular region under the presence and absence of an applied bias², go to *current options* manual.
28. V_{min} – the applied voltage bias of the molecular system (*volt*) (the minimum applied bias in an I - V curve, currently not available).
29. V_{max} –the maximum applied voltage bias of a I - V curve (*volt*, currently not available).
30. *# of bias point* – number of bias points in the I - V curve (Currently one can perform a calculation with only one bias point).
31. Go to the *computation options* manual.
32. Go to *Poisson manual* in the *computation manual*.
33. *Min Poisson Grid* – minimal grid spacing for the Poisson solver (0A).
34. *Poisson A* – the accuracy of the Poisson solver (tolerance for multi-grid convergence).
35. L_x – the dimension of the Poisson box in the x direction³ (0A).
36. L_y – the dimension of the Poisson box in the y direction⁴ (0A).

² When an external voltage bias is applied on the molecular systems, the code shifts the energy levels of the second contact and computes the energy shifts for the molecule’s atoms solving the self-consistent Hartree potential of the system.

³ Assuming that the bias is applied along the x direction, the code itself actually calculates L_x . However, it does not calculate L_y and L_z .

37. L_z – the dimension of the Poisson box in the z direction (0A).
38. *compute bulk potential* – reconstruct the Hartree potential generated by the charge transfer of an 3D infinite (bulk) contact and use it as boundary conditions on the contacts to solve the Poisson equation. This option is useful only if there is some charge transfer in your "bulk" contacts (for example, if the contact is a polar semiconductor).
39. You can save the calculated potential on the full volume of Poisson box, by pressing on the *save potential on full volume* button.
40. You can also save the potential on a plane of Poisson box, by pressing on *save potential on plane* button. You can decide on what plane to save it by pressing the *direction x, y* or *z* buttons and you can also choose where to cut Poisson's box.
41. Go to *SCC-Cycle manual* in the *computation manual*. In this section you can choose the parameters for the self-consistent charge calculation.

42. *Broyden Mix* – One can look in the following equation

$$q_{new} = \alpha q_{new} + (1 - \alpha) q_{old}$$

where q_{new} , q_{old} are the charges that were calculated in the present and in the last SCC cycle, respectively and α is the *Broyden Mix* ($0 \leq \alpha \leq 1$).

43. *Max SCC iter* – the maximum number of self-consistent iterations.
44. *SCC toleran* – specifies the tolerance of the SCC calculations. The difference between the total charge of the system of two following iterations (e).
45. *scc off/on* – one can switch the self-consistent charge mode on and off.
46. *read charge off/on* – gDFTB can save the calculated charge of the last iteration in the output file *CHR.DAT*; enabling *read charge* you can perform a new simulation using the saved charges as starting point for the SCC cycle.
47. Go to *Integration Path manual* in the *computation manual*. In this section we define the parameters for the integration of Green's function in order to get the electron density of the system.

⁴ Poisson box dimensions in the y and z directions should be larger than the dimension of the system + $4.5 \text{ } ^0A$ at each direction. However, if the Poisson box that you define is too small, the gDFTB will automatically extend it to the minimum dimension needed to get valid results.

48. A schematic representation of the integration path can be the following:

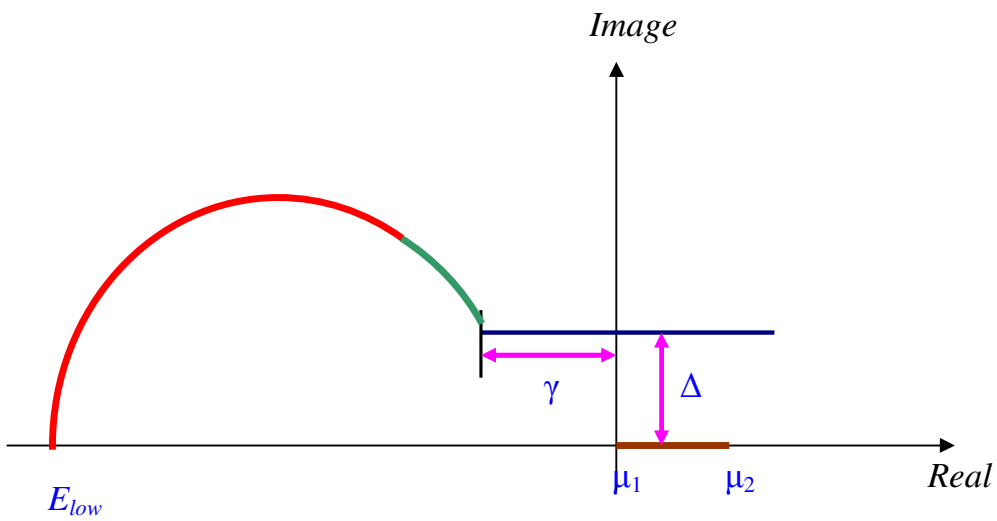


Figure 1

where μ_1 and μ_2 are the chemical potentials of the first and second contacts, Δ is the distance of the segment part of the integration contour from the real axis⁵ (this distance is different from zero just in the case of finite temperature calculations, when the contour must include the Fermi function poles positioned along the vertical axis passing from μ_1). n the integer number of $K_B T$, used to calculate $\gamma = nK_B T$

⁵ See figure 1.

49. T – the temperature ($^{\circ}K$).
50. E_{low} – the lowest energy for integration (ev).
51. N_1 – the number of integration points in the first part of the integration, further from the imaginary axis (the red part of the contour).
52. N_2 – the number of integration points in the second part of the integration, closer to the imaginary axis⁶ (the green part of the contour).
53. N_3 – the number of integration points in the third part of the integration (the brown part of the counter).
54. δ - the infinitesimal imaginary part of the energy of Green's function (ev).
55. One can perform a calculation that reads the old surface Green functions by pressing the *read old sgf*.

The output files of gDFTB

After saving the input file⁷ (*SAVE PRO*) and performing the calculation (*DO COMPUTATI*), the following output files are obtained

1. *jobs* directory – some technical details of the jobs: the job number, the user name, the working directory, the date and the time of the job submission etc.
2. *xyztopdb.log* – in this file there are possible errors of the pdb-xyz structure files conversion.
3. *pdb* file – the system in *pdb* format ($^{\circ}A$).
4. *tabella_sk* file– information about the available elements for calculation with the gDFTB code and the available interactions between them.
5. *gen* file – the system in *general* format ($^{\circ}A$).
6. *dftb.in* file – some input details of the job.
7. *PAR.IN* file – some input parameters.
8. *basis_0n.dat* file – periodic cell grid dimension of contact n ($^{\circ}A$).
9. *GDFTB_ser* file – a java interface file for job control.

⁶ We usually use N_2 that is larger than N_1 .

⁷ It is most recommended to save each input file in a separate directory in order to prevent confusion.

10. *jobinfo* file – information about the type of calculation and about the job number.
 11. *user_nameGDFTB.ojob_number* file- a java interface file for job control.
 12. *user_nameGDFTB.ejob_number* file – the calculation errors.
 13. *outfileGDFTB.log* file – some details on the input and the output of the job performed.
 14. *current.dat* file – the calculated current through the system at each bias point (*Amp*).
 15. *ENERGY.TMP* file – this file contains some details about the calculated energy of the valence electrons of the system: number of cycles, number of iterations until the convergence of the total charge, the energy of the valence electrons of the device (*Hartree*), the maximum displacement of atomic position during relaxation and the maximum atomic force reached.
 16. *fort.79* & *fort.1* files are files generated by the compiler.
 17. *scfsum* file – first column – the iteration number, second column – the energy of the valence electrons of the device (*Hartree*), third column – the total number of electrons in the system in the current iteration and the fourth column is the maximum difference between the atomic charges on the atoms at the present iteration and the last iteration (*e*).
 18. *eshiftn.dat* file – first column – the atom number, the second and third columns are shifts that are added to the Hamiltonian matrix elements at the *n*th iteration of the self-consistent-charge computation (*Hartree*); in the second column the shifts of the contacts atoms are put to zero, while in the third one they are the only non-null values.
 19. *partial.dat* file – a file generated just for checking purposes; it contains some partial results, of charge and energy⁸.
- CHR.DAT* file – first column – the atom number, the second column – the atomic total charge (just for valence electrons) that is computed during the self-consistent computation and gives information about charge transfer among atoms. The other columns are the contribution of the single electronic

⁸ This file will be removed.

orbitals to the total atomic charge, and their number varies according to the number of valence orbitals of each particular atom (e).

20. *BROYD* files – information about the mixing of the present calculated charge and the charge calculated in the last iteration.
21. *box3d.dat* file – the number of points at each direction in Poisson box.
22. *Kvector.dat* file – the points along the K axis of Poisson box (0A), where $K = x, y$ and z .
23. *potential.dat* file – the calculated potential of the last iteration saved over all the 3D Poisson box (*volts*). For each fixed value of x (according to the *Xvector.dat* file), y takes all its values (according to the *Yvector.dat* file) and, in the same way, for each fixed value of y , z takes all its values (according to the *Zvector.dat* file).
24. *charge_density.dat* file – the 3D electron charge density according to the following calculation. For each atom i , the difference of the electron charge is calculated as

$$\Delta q_i = q_i^{last_cycle} - q_i^0$$

where $q_i^{last_cycle}$ is the electron charge associated with the i atom that was calculated in the last iteration cycle and q_i^0 is the electron charge associated with the neutral atom i . For each point on space $\vec{r}_j = (x_j, y_j, z_j)$, we get

$$u(\vec{r}_j) = \sum_i \sum_{v \in i} \Delta q_i \varphi_v(\vec{r}_j)$$

where φ_v the atomic orbital and $u(\vec{r}_j)$ is the charge density at \vec{r}_j . Thus the dimension of the charge density is $e / (^0A)^3$. The *charge_density.dat* file contains this electron charge density in the same order as the *potential.dat* file.

25. *pot2D.dat* file – the calculated 2D potential saved on a surface specified in the input file (*volt*). One can plot this file using the HyperPlotter of ICODE.
26. *charge2D.dat* file – the calculated 2D charge density saved on the surface specified in the input file. One can plot this file using the HyperPlotter of ICODE.

27. *surfden0n_0001.dat* file – the density of states of the n surface as a function of the energy of an electron injected from the contact.
28. *tunneling_0001.dat* file – the transmission coefficient as a function of the energy of an electron injected from the contact.
29. *EqDOS_0001.dat* file - the equilibrium density of states of the molecule as a function of the energy of an electron injected from the contact.
30. *FRC.DAT* file – the forces on each atom in the device region (*Hartree/Angstrom*).
31. *MAS.DAT* file – the atomic mass of each atom in the device region (the first line is the number of atoms in the device region (*gr/mole*)).
32. *out0001* file – the geometry optimization⁹ of the device region ($^{\circ}A$).

33. Go to *GS* directory.
34. *GS0n_m.dat* file –Green surface on contact n in the m integration point. The total number of integration points is $N_1 + N_2 + N_3$ that are defined in the *Integration Path* section of the input file.
35. Get out from the *GS* directory
36. Go to *contacts* directory.
37. *cont0n.in* file – some input details on the n contact.
38. *cont0n.out0001* file – the relaxation positions of the atoms of the n contact ($^{\circ}A$).
39. *cont0n.gen* file – the position of the atoms of the n contact written in a *gen* format.
40. *H_0n.dat* file – the Hamiltonian matrix of the n contact.
41. *S_0n.dat* file – the overlap matrix of the n contact.
42. *CHR_0n.dat* file – some details about the charge distribution of the contacts.
43. *CHS_0n.dat* file – the tight-binding expansion coefficients of the electronic states of the n contact.

⁹ The geometry relaxation is currently unavailable.

44. *SPE_On.dat* file – the first line is Fermi's level of the contact n . In the other lines, the first column is the energy of the molecular orbital and the second column is the occupation number (*Hartree*).
45. *basis_On.dat* file – the vector of the periodic cell of the n contact.