NANOTCAD ViDES
Versatile DEvice Simulator

NANOTCAD ViDES User's Manual

by

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Contents

License term

Chapter 1

Getting started

The provided *NanoTCADViDES.tgz* archive contains the *NanoTCAD ViDES* source code, the User's manual and the post processing utility *fplot*, which allow to elaborate in an user-friendly way the data provided by *NanoTCAD ViDES*.

In order to install the software you have first to accomplish the following software requirements. In particular you need :

- fortran 77 compiler
- C compiler
- make
- gnuplot
- python
- python tcl/tk libraries

To install, simply run the tcsh script *install.sh*, or just go in the ./src directory and type *make*, and then *make install*. Please note that the *Makefile* included in the *./src* directory, and the *install.sh* script are meant to be used on a machine in which g77, gcc compilers are installed. The optimization flag *-O3* has also been set. If you want to use other compilers or different flag options, please make changes in the Makefile in the *./src* directory.
If compilation has been succesfull, you will find in the *./bin* directory the compiled *ViDES* code, the utility *fplot* and its file (*sectionx, sectiony, sectionz*), as well as the file *input.material* and *dimension.max*.
SUCH FILES HAVE TO RESIDE IN THE SAME DIRECTORY YOU LAUNCH THE CODE AS WELL AS THE INPUT DECK. So, if you copy the code into another directory, different from the ./bin directory, take care of copying all the files contained in the ./bin directory.

To run the code, just simply type *./ViDES inputdeck*, where *inputdeck* is the input file in which the nanoscale device has been defined.

Chapter 2

Implemented Physical Models

The implemented code is a three-dimensional Poisson solver, in which different physical models for the simulation of nanoscale devices have been included. In particular, *ViDES* is able to

- compute transport in (n,0) zig-zag carbon nanotubes with general geometries, by means of atomistic p_z tight-binding Hamiltonian, within the real and mode space approximation.
- compute transport in Silicon Nanowire Transistors, within the effective mass approximation.
- solve the 3D Poisson/Laplace equation at the equilibrium, assuming semi-classical models for the electron and hole densities.

In particular, the potential profile in the three-dimensional simulation domain obeys the Poisson equation

$$\begin{aligned}\nabla\left[\epsilon(\vec{r})\nabla\phi(\vec{r})\right] &= -q\left[p(\vec{r})-n(\vec{r})+N_D^+(\vec{r})\right.\\ &\left.\quad -N_A^-(\vec{r})+\rho_{fix}\right], \qquad (2.1)\end{aligned}$$

where $\phi(\vec{r})$ is the electrostatic potential, $\epsilon(\vec{r})$ is the dielectric constant, N_D^+ and N_A^- are the concentration of ionized donors and acceptors, respectively, and ρ_{fix} is the fixed charge. For what concerns the electron and hole concentrations (n and p, respectively) instead, they are computed by means of the different physical models, which will be described in the following sections.

2.1 Transport in zig-zag Carbon Nanotubes Transistors

The simulations are based on the self-consistent solution of the 3D Poisson-Schrödinger equation with open boundary conditions, within the Non-Equilibrium Green's Function formalism, where arbitrary gate geometry and device architecture can be considered [1].

The electron and hole concentrations are computed by solving the Schrödinger equation with open boundary conditions, by means of the NEGF formalism. A tight-binding Hamiltonian with an atomistic (p_z orbitals) basis, has been used both in the real and the mode space approach [2].

The Green's function can be expressed as

$$G(E) = [EI - H - \Sigma_S - \Sigma_D]^{-1} , \tag{2.2}$$

where E is the energy, I the identity matrix, H the Hamiltonian of the CNT, and Σ_S and Σ_D are the self-energies of the source and drain, respectively. As can be seen, transport is here assumed to be completely ballistic. In the released code, **ONLY doped source and drain reservoirs can be considered**. In addition, the considered CNT are **ALL** *(n,0)* **zig-zag nanotube**, where n is the chirality.

Once the length L and the chirality n of the nanotube are defined, the coordinates in the three-dimensional domain of each carbon atom are computed, and the three-dimensional domain is discretized **so that a grid point is defined in correspondence of each atom, while a user specified grid is defined in regions not including the CNT**.

A point charge approximation is assumed, i.e. all the free charge around each carbon atoms is spread with a uniform concentration in the elementary cell including the atom.

Assuming that the chemical potential of the reservoirs are aligned at the equilibrium with the Fermi level of the CNT, and given that there are no fully confined states, the electron concentration is

$$\begin{aligned} n(\vec{r}) &= 2\int_{E_i}^{+\infty} dE\,\left[|\psi_{\mathrm{S}}(\mathrm{E},\tilde{\mathrm{r}})|^2 f(E - E_{F_S})\right. \\ &\quad \left.+|\psi_{\mathrm{D}}(\mathrm{E},\tilde{\mathrm{r}})|^2 f(E - E_{F_D})\right] , \end{aligned} \tag{2.3}$$

while the hole concentration is

$$\begin{aligned} p(\vec{r}) &= 2\int_{-\infty}^{E_i} dE\,\left\{|\psi_{\mathrm{S}}(\mathrm{E},\tilde{\mathrm{r}})|^2 \left[1 - f(E - E_{F_S})\right]\right. \\ &\quad \left.+|\psi_{\mathrm{D}}(\mathrm{E},\tilde{\mathrm{r}})|^2 \left[1 - f(E - E_{F_D})\right]\right\} , \end{aligned} \tag{2.4}$$

where $\vec{r}$ is the coordinate of the carbon site, f is the Fermi-Dirac occupation factor, and $|\psi_S|^2$ ($|\psi_D|^2$) is the probability that states injected by the source (drain) reach the carbon site ($\vec{r}$), and E_{F_S} (E_{F_D}) is the Fermi level of the source (drain).

The current has been computed as

$$I = \frac{2q}{h}\int_{-\infty}^{+\infty} dE\mathcal{T}(E)\left[f(E - E_{F_S}) - f(E - E_{F_D})\right] , \tag{2.5}$$

where q is the electron charge, h is Planck's constant and $\mathcal{T}(E)$ is the transmission coefficient

$$\mathcal{T} = -Tr\left[\left(\Sigma_S - \Sigma_S^\dagger\right) G \left(\Sigma_D - \Sigma_D^\dagger\right) G^\dagger\right] , \tag{2.6}$$

where Tr is the trace operator.

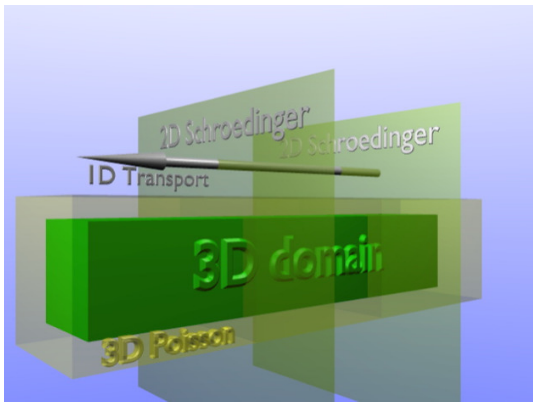


Figure 2.1: In the SNWT model, the 3D Poisson, the 2D Schrödinger and 1D transport equations are solved self-consistently.

2.2 Transport in Silicon Nanowire Transistors

Simulation of Silicon Nanowire Transistors, are based on the self-consistent solution of Poisson, Schrödinger and continuity equations on a generic three-dimensional domain. Hole, acceptor and donor densities are computed in the whole domain with the semiclassical approximation, while the electron concentration in strongly confined regions needs to be computed by solving the Schrödinger equation, within the effective mass approximation. We assume that in the considered devices the confinement is strong in the transversal plane x-y and the potential is much smoother in the longitudinal direction z. As a consequence the Schrödinger equation is adiabatically decoupled in a set of two-dimensional equations with Dirichlet boundary conditions in the x-y plane for each grid-point along z, and in a set of one dimensional equations with open boundary conditions in the longitudinal direction for each 1D subband (Fig. 2.1).

In particular, the two-dimensional Schrödinger equation for each cross section along z reads,

$$\begin{aligned} &-\left[\frac{\hbar^2}{2}\frac{\partial}{\partial x}\frac{1}{m_x}\frac{\partial}{\partial x}+\frac{\hbar^2}{2}\frac{\partial}{\partial y}\frac{1}{m_y}\frac{\partial}{\partial y}\right]\chi_{i\nu}(x,y,z) \\ &\qquad +V\chi_{i\nu}(x,y,z)=\varepsilon_{i\nu}(z)\chi_{i\nu}(x,y,z). \end{aligned} \tag{2.7}$$

where i runs over subbands, ν runs over the three pairs of minima of the conduction band, $\chi_{i\nu}$ and $\varepsilon_{i\nu}$ are the 2D eigenfunctions and the corresponding eigenenergies computed in the transversal plane at a given z, while $m_{\nu x}$ and $m_{\nu y}$ are the effective masses along the k_x and k_y axis, respectively, on the conduction band pair of minima ν.

The main assumption, based on the very small nanowire cross section considered, is that an adiabatic approximation can be applied to the Schrödinger equation, so that transport occurs along one-dimensional subbands.

Transport is computed by means of the NEGF formalism in one-dimensional subbands within the mode space approach, taking into account inter and intra subbands scattering, and the one-dimensional electron density $n_{1D_i}(z)$ is therefore obtained.

The three-dimensional electron density n to be inserted into the right hand side of the Poisson equation reads

$$n(x,y,z) = \sum_{i}^{M} |\chi_{i\nu}(x,y,z)|^2 n_{1D_i}(z), \tag{2.8}$$

where the sum runs over the M considered modes. Even in this case a point charge approximation has been assumed.

2.3 Semiclassical Models

No transport is computed within this approximation, while only a simple semiclassical expression is assumed for the hole and electron concentrations. Such a model can be used for example, in order to simulate polysilicon gate when CNT or SNWT transport simulations are performed.

In the non-degenerate statistics we obtain

$$n(\vec{r}) = N_c e^{-\frac{E_C(\vec{r})-E_F}{KT}}, \tag{2.9}$$

where

$$N_c = 2\left(\frac{2\pi KT}{\hbar^2}\right)^{\frac{3}{2}} M_c \tag{2.10}$$

For the holes,

$$p(\vec{r}) = N_V(\vec{r}) e^{-\frac{E_F-E_V(\vec{r})}{KT}} \tag{2.11}$$

where E_V is the valence band and N_V is the equivalent density of states in the valence band.

For the non-completely ionized impurities we have

$$\begin{cases} N_D^+(\vec{r}) = \frac{N_D(\vec{r})}{1+g_D\exp\left(\frac{E_F-E_D(\vec{r})}{KT}\right)}\ ,\ g_D = 2 \\ \\ N_A^-(\vec{r}) = \frac{N_A(\vec{r})}{1+g_A\exp\left[\frac{E_A(\vec{r})-E_F}{KT}\right]}\ ,\ g_A = 4 \end{cases} \tag{2.12}$$

where E_A and E_D are the acceptors and donors level, N_A e N_D are the acceptor and donors concentrations and g_A e g_D are the degeneration factors.

2.4 Numerical Implementation

The Green's function is computed by means of the Recursive Green's Function (RGF) technique [4, 5]. Particular attention must be put in the definition of each self-energy matrix, which can be interpreted as a boundary condition of the Schrödinger equation. In particular, in our simulation we have considered a self-energy for semi-infinite leads as boundary conditions, which enables to consider the CNT as connected to infinitely long CNTs at its ends.

From a numerical point of view, the code is based on the Newton-Raphson (NR) method with a predictor/corrector scheme [3]. In Fig. 2.2 we sketched a flow-chart of the whole code. In particular, the Schrödinger/NEGF equations are solved at the beginning of each NR cycle, starting from an initial potential $\tilde{\Phi}$, and the charge density in the CNT and SNWT is kept constant until the NR cycle converges (i.e. the correction on the potential is smaller than a predetermined value). The algorithm is then repeated cyclically until the norm of the difference between the potential computed at the end of two subsequent NR cycles is smaller than a predetermined value.

Some convergence problems however may be encountered using this iterative scheme. Indeed, since the electron density is independent of the potential within a NR cycle, the Jacobian is null for points of the domain including carbon atoms/SNWT region, losing control over the correction of the potential. We have used a suitable expression for the charge predictor, in order to give an approximate expression for the Jacobian at each step of the NR cycle. To this purpose, we have used an exponential function for the predictor In particular, if n is the electron density as in (2.3), the electron density n_i at the i-th step of the NR cycle can be expressed as

$$n_i = n \exp\left(\frac{\phi_i - \tilde{\phi}}{V_T}\right), \tag{2.13}$$

where $\tilde{\phi}$ and ϕ_i and are the electrostatic potential computed at the first and i-th step of the NR cycle, respectively, and V_T is the thermal voltage. Same considerations follow for the hole concentration. Since the electron density n is extremely sensitive to small changes of the electrostatic potential between two NR cycles, the exponential function acts in the overall procedure as a dumping factor for charge variations. In this way, convergence has been improved in the subthreshold regime and in the strong inversion regime. Convergence is still difficult in regions of the device where the charge is not compensated by fixed charge, where the right-hand term of the Poisson equation is considerably large.

An under-relaxation of the potential and of the charge can also be performed in order to help convergence. In particular, three different under-relaxations can be performed inside *ViDES* :

- relaxation on the potential at each NR cycle ϕ_i

$$\Phi_i^{new} = \Phi_i^{new} + \varepsilon\left(\Phi_i^{old} - \Phi_i^{new}\right) \tag{2.14}$$

- relaxation on the potential at the end of each NR cycle Φ_f

$$\Phi_f = \Phi_f + \varepsilon\left(\tilde{\Phi} - \Phi_f\right) \tag{2.15}$$

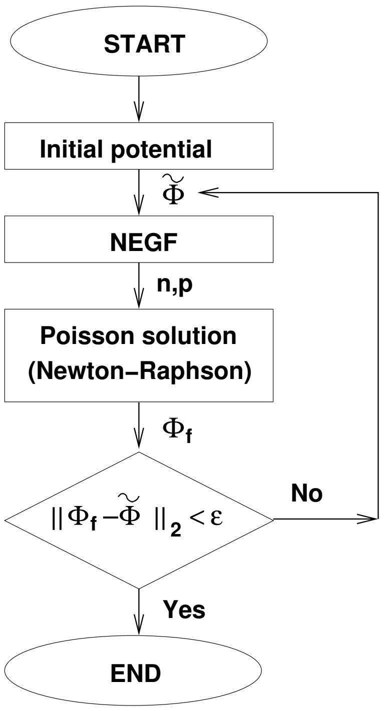

START
Initial potential
$\tilde{\Phi}$
NEGF
n,p
Poisson solution (Newton−Raphson)
Φ_i
Φ_f
$\|\Phi_f - \tilde{\Phi}\|_2 < \varepsilon$
No
Yes
END

Figure 2.2: Flow-chart of the self-consistent 3D Poisson-Schrödinger solver.

- relaxation of the charge density ρ_{NEGF} computed by the NEGF modules

$$\rho_{NEGF}^{new} = \rho_{NEGF}^{new} + \varepsilon \left(\rho_{NEGF}^{old} - \rho_{NEGF}^{new}\right) \tag{2.16}$$

Chapter 3

Definition of the Input Deck

Let's now define the input deck of *ViDES* simulator. *ViDES* has its own language composed by a limited set of commands as well as its own syntax, through which it is possible to define both the grid, the structure of the nanoscale device, and the physical models to be used in the simulations. Along *ViDES* commands are also present some *instances* deliminated by the parenthesis { and }, which have other subset of commands. We refer in particular to *gridx, gridy, gridz, solid, gate, region*, whose meaning will be explained in the following sections.

3.1 Main commands

Let's first focus on the list of main commands.

- *#* : comment command (it has to be followed by a space).
- *prev* : the non linear solver starts from the solution provided in the file **Phi.out**.
- *flat* : the non linear solver starts from the flat band solution (**default**). This work both for the SNWT and CNT simulations. **In the case of CNT, the flat band potential computed in correspondence of the drain, is increased by its electrochemical potential. This can be useful in order to start with a drain-to-source voltage different to zero as suggested in the "golden rule" section.**
- *gridonly* : code generates only the grid and then exit.
- *poiss* : the Poisson equation is solved (**default**).
- *ps* : the self-consistent Poisson/Schrödinger equations in the effective mass approximation are solved. This flag has to be set if SWNT simulations want to be performend. Please refer to the *region* section for more details.
- *CNT* : the open-boundary condition Schrödinger equation within the tight-binding NEGF formalism is solved self-consistently with the Poisson equation in order to compute transport in CNT-FETs. As stated in section 2.1, *ViDES* can simulate (n,0) zig-zag nanotubes. In order to specify the chirality and the length of the nanotube, the command *CNT* has to be followed

by two values, the chirality and the length expressed in nanometer, respectively. For example, if a (13,0) CNT, 15 nm long wants to be defined then you have to specify : *CNT 13 15.* **Pay attention that the CNT axis is along the z-direction and coincides with the rect passing for** *x=0 nm; y=0 nm.* In addition the *source* is supposed to lays on the left of the structure, while the *drain* on the right.

- *real* : a real space basis set is used to compute transport in CNT (only if CNT command is specified).
- *mode* : a mode space approach is used to compute transport in CNT (only if CNT command is specified). It has to be followed by the number of modes to be used (the maximum number of modes is equal to chirality). As shown in [2] however, from a computational point of view, it is nonsense to use a large number of modes, since real space simulation will be more efficient.
- $mu1$: this defines the electrochemical potential for the source. It has to be followed by a value expressed in eV.
- $mu2$: this defines the electrochemical potential for the drain. It has to be followed by a value expressed in eV.
- *underel* : under relaxation coefficient for the potential at each NR cycle (**default : underel=0**). This is ε in eq. 2.14.
- *potsottoril* : under relaxation coefficient for the potential at the end of NR cycle (**default : underel=0**). This is ε in eq. 2.15.
- *carsottoril* : under relaxation coefficient for the charge at the end of NR cycle (**default : underel=0**). This is ε in eq. 2.16.
- *tolldomn* : inner tollerance of the linear solver. (**default : tolldomn=0.1**).
- *poissnorm* : tollerance inside the NR cycle (**default : poissnorm=10^{-3}**)
- *normad* : tollerance of the outer cycle (**default : normad=10^{-3}**). This is the ε in Fig. 2.2.
- *temp* : temperature (K) (**default : temp=300**)
- *complete* : complete ionization of donors and acceptors.
- *incompl* : incomplete ionization of donors and acceptors (**default**). This refers to eq. 2.12.
- *field* : the electric field on the six lateral surface of the simulation domain (V/m). If declared it has to be followed by six number corresponding to the electric field at each surface. By default the electric field is imposed to zero on each surface (Null Neumann Boundary condition).
- *maxwell* : Maxwell-Boltzmann statistic for the semiclassical electron density (**default**).

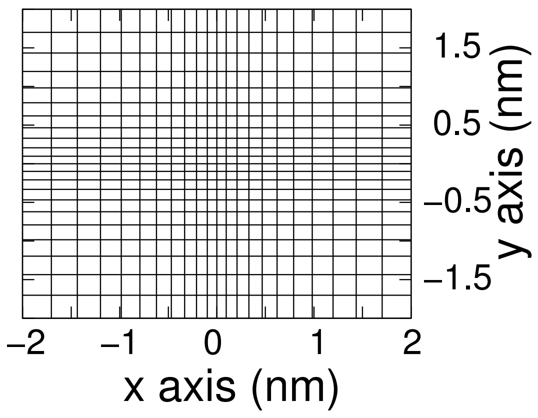


Figure 3.1: Example of generated non-uniform grid along the $x - y$ plane.

3.2 Grid definition

The mesh generator within the *ViDES* simulator defines non-uniform rectangular grids along the three spatial direction. In order to define the grid, the *gridx, gridy, gridz* commands have to be used in the input deck. Let's now focus our attention on the discretization along the x-axis.

The general statement is the following :

```
gridx
{
    mesh x_1 spacing Δ_1
    ..
    mesh x_n  spacing Δ_n
}
```

The *mesh* command followed by a number x_i defines the position in *nm* of the grid point along the x direction, while the number Δ_i after the spacing command, defines the spacing between two user's defined grid points. The same considerations follow for the definition of the grid along the y and z directions, where the *gridx* command has to be replaced by *gridy* and *gridz* commands, respectively.

In Fig. 3.1 is shown an example of generated grid along the $x - y$ plane, when the input file is the following :

```
gridx
{
    mesh -2 spacing 0.3
    mesh 0 spacing 0.1
    mesh 2 spacing 0.3
}


gridy
{
    mesh -2 spacing 0.3
    mesh 0 spacing 0.1
    mesh 2 spacing 0.3
}
```

The grid generator yields as output the files *points.out*, in which the number of points along the *x,y,z* directions are stored, and *gridx.out, gridy.out, gridz.out*, which contain the points of the mesh along *x,y* and *z*, respectively.

NOTE THAT : If a CNT is simulated, the grid along the z-axis is self-computed, so that the *gridz* command has not to be specified.

3.3 Solid definition

The *solid* command defines, in the three-dimensional domain, the regions of different materials that belong to the device to be simulated. As for the the *grid* command, its subset of commands has to be included between parenthesis ({ and }). In particular, within the solid statement we have :

- *rect* : impose the shape of the region to be rectangular (**default**).
- *xmin* : define the minimum coordinate (nm) in the x-direction of the rectangular region. It has to be followed by a number. (**default : xmin=minimum x coordinate of the grid**).
- *xmax* : define the maximum coordinate (nm) in the x-direction of the rectangular region. It has to be followed by a number. (**default : xmax=maximum x coordinate of the grid**).
- *ymin* : define the minimum coordinate (nm) in the y-direction of the rectangular region. It has to be followed by a number. (**default : ymin=minimum y coordinate of the grid**).
- *ymax* : define the maximum coordinate (nm) in the y-direction of the rectangular region. It has to be followed by a number. (**default : ymax=maximum y coordinate of the grid**).
- *zmin* : define the minimum coordinate (nm) in the z-direction of the rectangular region. It has to be followed by a number. (**default : zmin=minimum z coordinate of the grid**).

- *zmax* : define the maximum coordinate (nm) in the z-direction of the rectangular region. It has to be followed by a number. (**default : zmax=maximum z coordinate of the grid**).
- *sphere* : impose the shape of the region to be a spherical shell. It has to be followed by 5 numbers (nm) : the x, y, z coordinates of the center (nm), and the inner and outer radius of the sphere.
- *cylinder* : imposes the shape of the region to be a cylindrical shell. The axis of the cylinder is parallel to the z-axis. Once the *cylinder* commands has been specified, the axis and the radius of the inner and outer cylinder are specified by the following commands:
  - *xcenter* : specify the x-coordinate of the axis.
  - *ycenter* : specify the y-coordinate of the axis.
  - *radius1* : specify the radius of the inner cylinder.
  - *radius2* : specify the radius of the outer cylinder.
- *silicon* : declares that the material of the solid is Silicon.
- *sio2* : declares that the material of the solid is SiO_2.
- *air* : declares that the material of the solid is Air.
- *AlGaAs* : declares that the material of the solid is AlGaAs.
- *Al* : defines the molar fraction of Aluminium in case the AlGaAs material has been defined.
- *nulln* : imposes the semiclassical electron concentration to zero. **Since in general, CNT are embedded in dielectrics, when simulating CNTs and specifing the solid region,** *nulln* **command has to be set.**
- *nullp* : imposes the semiclassical hole concentration to zero. **Since in general, CNT are embedded in dielectrics, when simulating CNTs and specifing the solid region,** *nulln* **command has to be set. In addition, in SNWT simulations, only electron transport is considered. As a consequence, impose** *nullp* **command.**
- *Na* : defines the nominal acceptors concentration (m^{-3}). It has to be followed by a number (**default : Na=0**).
- *Nd* : defines the nominal donors concentration (m^{-3}). It has to be followed by a number (**default : Nd=0**).
- *rho* : fixed charge concentration (m^{-3}). It has to be followed by a number (**default : rho=0**).
- *Ef* : defines the Fermi level of the region (eV). It has to be followed by a number (**default : Ef=0**).

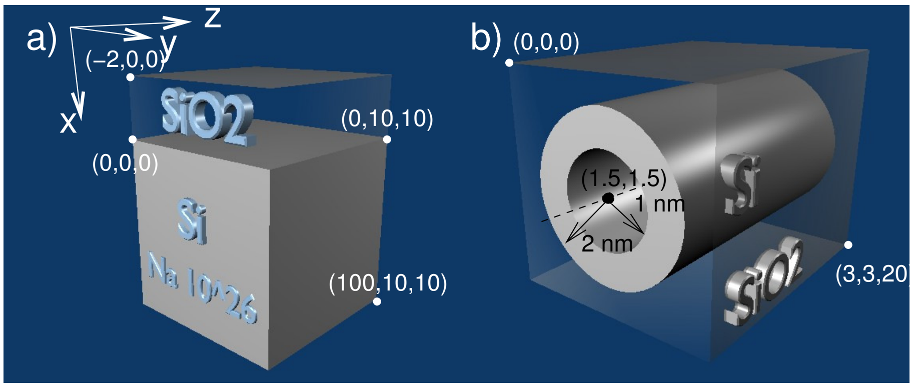


Figure 3.2: Two example of solids : a) MOS structure; b) cylindrical nanowire. The white dots univocally define the rectangular region.

- *fraction* : this command takes effect only if *CNT* command has been specified. In particular, it imposes the doping molar fraction of the nanotube. If a doped nanotube wants to be defined, a solid which contains the part of the nanotube the user wants to dope has to be defined.

NOTE THAT : in case of overlapping solids, the last defined shadows the previous one.

3.3.1 Solid examples

In Figs. 3.2a-b, we show two examples of structures, which can be defined by the *solid* command : a MOS (Fig. 3.2a) and a cylindrical silicon nanowire (Fig. 3.2b). Suppose that you have already defined the grid.

For the MOS case let's assume that *xmin=-2 nm; xmax=2 nm; ymin=zmin=0 nm; and ymax=zmax=10 nm.* The MOS structure can then be defined as :
solid rectangular region which define the SiO2 (I took the whole domain)
{
  SiO2
  nulln nullp

  }

solid rectangular region which define the doped Si (Note the overlap)
{
  Si
  xmin 0

Na 1e26
}

For the cylindrical case let's assume that *xmin=ymin=zmin=0 nm; xmax=ymax=3 nm; zmax=20 nm.* The SNW structure can then be defined as :
solid rectangular region which define the SiO2 (I took the whole domain)
{
SiO2
nulln nullp

}

solid cylindrical nanowire (Note the overlap)
{
Si
xcenter 1.5 ycenter 1.5
radius1 1 radius2 2
}

As you can see, the definition is really straightforward if you take advantage of the default values for the solid coordinates, and the overlap of solids.

3.4 Gate definition

The *gate* command defines the gate region in the three-dimensional domain, i.e. the point in which Dirichlet boundary conditions are imposed. **The first defined gate is the referring gate, whose electrostatic potential is set to zero.** As for the *solid* command, the following ensemble of commands has to be declared and included in brackets { } after the gate statement :

- *xmin* : define the minimum coordinate (nm) in the x-direction of the rectangular region. It has to be followed by a number. (**default : xmin=minimum x coordinate of the grid**).
- *xmax* : define the maximum coordinate (nm) in the x-direction of the rectangular region. It has to be followed by a number. (**default : xmax=maximum x coordinate of the grid**).
- *ymin* : define the minimum coordinate (nm) in the y-direction of the rectangular region. It has to be followed by a number. (**default : ymin=minimum y coordinate of the grid**).
- *ymax* : define the maximum coordinate (nm) in the y-direction of the rectangular region. It has to be followed by a number. (**default : ymax=maximum y coordinate of the grid**).
- *zmin* : define the minimum coordinate (nm) in the z-direction of the rectangular region. It has to be followed by a number. (**default : zmin=minimum z coordinate of the grid**).

- *zmax* : define the maximum coordinate (nm) in the z-direction of the rectangular region. It has to be followed by a number. (**default : zmax=maximum z coordinate of the grid**).
- *Ef* : defines the Fermi energy of the gate (eV) (**default : Ef=0**). **It is equal to the gate voltage changed by sign**.
- *workf* : defines the work function of the gate (eV) (**default : workf=4.1**)
- *cylinder* : imposes the shape of the region to be a cylindrical shell. The axis of the cylinder is parallel to the z-axis. Once the *cylinder* commands has been specified, the axis and the radius of the inner and outer cylinder are specified by the following commands:
  - *xcenter* : specify the x-coordinate of the axis.
  - *ycente* : specify the y-coordinate of the axis.
  - *radius1* : specify the radius of the inner cylinder.
  - *radius2* : specify the radius of the outer cylinder.

3.5 Region command

The *region* command defines where and which kind of quantum analysis has to be performed. The following ensemble of commands has to be declared and included in brackets { } after the region statement :

- *xmin* : define the minimum coordinate (nm) in the x-direction of the rectangular region. It has to be followed by a number. (**default : xmin=minimum x coordinate of the grid**).
- *xmax* : define the maximum coordinate (nm) in the x-direction of the rectangular region. It has to be followed by a number. (**default : xmax=maximum x coordinate of the grid**).
- *ymin* : define the minimum coordinate (nm) in the y-direction of the rectangular region. It has to be followed by a number. (**default : ymin=minimum y coordinate of the grid**).
- *ymax* : define the maximum coordinate (nm) in the y-direction of the rectangular region. It has to be followed by a number. (**default : ymax=maximum y coordinate of the grid**).
- *zmin* : define the minimum coordinate (nm) in the z-direction of the rectangular region. It has to be followed by a number. (**default : zmin=minimum z coordinate of the grid**).
- *zmax* : define the maximum coordinate (nm) in the z-direction of the rectangular region. It has to be followed by a number. (**default : zmax=maximum z coordinate of the grid**).
- *negf2d* : solve the transport along coupled one-dimensional subbands by means of the NEGF formalism and solve the 2D Schrödinger equation in the $x-y$-plane. The physical model is described in section 2.2.

- *nauto* : specifies the maximum number of eigenvalues (i.e. the number of one-dimensional subbands) computed by the 2D Schrödinger equation.

3.6 Output files

ViDES produces the following output files :

- "solido.out" : the defined solids along the structure. It can be usesful in order to understand if the defined structure is the one expected. In particular, solids are numbered with an increasing number as they appear in the input deck.
- "tipopunto.out" : specify the type of points along the defined 3D domain. Even in this case, post-processing of this file can reveal to be usesful in order to understand if the defined structure is the one expected.

  In particular, it specifies which kind of boundary conditions have to be applied in each point of the domain.

  If `tipopunto` is smaller than 100, it specifies that the considered point is a point belonging to a gate, and it returns the gate number.

  If `tipopunto`=101, `l` belongs to the surface with $x = x_{min}$, where x_{min} is the least abscissa along x, and where Neumann boundary conditions are imposed (the derivative of the electric field is equal to `E[0]`).

  If `tipopunto`=102, `l` belongs to the surface with $x = x_{max}$, where x_{max} is the largest abscissa along x, and where Neumann boundary conditions are imposed (the derivative of the electric field is equal to `E[1]`).

  If `tipopunto`=103, `l` belongs to the surface with $y = y_{min}$, where y_{min} is the least abscissa along y, and where Neumann boundary conditions are imposed (the derivative of the electric field is equal to `E[2]`).

  If `tipopunto`=104, `l` belongs to the surface with $y = y_{max}$, where y_{max} is the largest abscissa along y, and where Neumann boundary conditions are imposed (the derivative of the electric field is equal to `E[3]`).

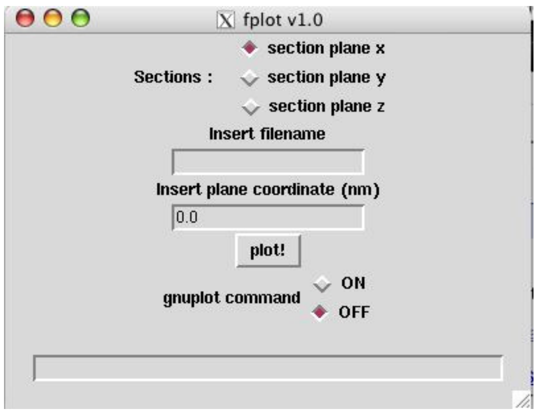
  If `tipopunto`=105, `l` belongs to the surface with $z = z_{min}$, where z_{min} is the least abscissa along z, and where Neumann boundary conditions are imposed (the derivative of the electric field is equal to `E[4]`).

  If `tipopunto`=106, `l` belongs to the surface with $z = z_{max}$, where z_{max} is the largest abscissa along z, and where Neumann boundary conditions are imposed (the derivative of the electric field is equal to `E[5]`).
- "tipopuntos.out" : if a point is in correspondence of a C atom or in correspondence of the nanowire, then *tipopuntos* is equal to 777.
- "Phi.temp" : Temporary electrostatic potential.at each NR step (Φ_i).
- "Phi.out" : Electrostatic potential.
- "Ec.out" : Conduction Band.
- "ncar.out" : electron density. In the case of CNT *ncar* gives the sum of holes and electrons. So positives values are for electrons, negative for holes.

- "pcar.out" : hole density.
- "Nam.out" : Ionized acceptors concentration.
- "Ndp.out" : Ionized donors concentration.
- "jayn.out" : the current obtained in CNT simulations.
- "bandcnt" : the mean intrinsic Fermi level along the nanotube ring, as a function of the z coordinate, along the nanotube. This applies only when *CNT* command is specified.
- "coordcnt.gnu" : coordinates of the atoms of the CNT. Atom positions can be plotted by means of newplot with the command *splot 'coordcnt.gnu' w p*.
- "coordcnt.jmol" : coordinates of the atoms of the CNT. Atom positions can be visualized by means of the jmol code available at *http://jmol.sourceforge.net/download/*.
- "Tn" : transmission coefficient in CNT simulations.
- "jay.out" : the current obtained in SNWT simulations.
- "T1" : transmission coefficient in SWNT simulations for the first couple of minima.
- "T2" : transmission coefficient in SWNT simulations for the first couple of minima.
- "T3" : transmission coefficient in SWNT simulations for the first couple of minima

3.7 "Golden rules" for the simulation

1. When defining a grid, pay attention in imposing fine enough grid in correspondence of interface (e.g. Si/SiO_2 interface). A spacing equal to 0.05 nm should be fine enough.
2. Every time you create a new grid, which means that you do not have a previous initial potential from which to start, you have to impose the flat band solution (*flat* command). In this way, the initial solution is internally generated, starting from the assumption of flat band in the whole semiconductor.
3. When computing transfer characteristic for drain-to-souce voltages (V_{DS}) different to zero, first find a solution for $V_{DS} = 0$ and then, starting from this solution (*prev* command) increase V_{DS} up to the desired value. Experience have tought that step voltage larger than 0.05 V are not extremely good.
4. In CNT simulations, the following parameter has most of the time resulted to be usefull in order to achieve better convergence : *poissnorm 1e-1, normad 5e-2*. Anyway, in order to achieve better accuracy, try to use a *normad* as small as possible.



fplot v1.0

Sections : [✓ section plane x] section plane y section plane z

Insert filename

Insert plane coordinate (nm): 0.0

plot!

gnuplot command: ON [✓ OFF]

Figure 3.3: Picture of fplot as it appears once called.

5. When solving the Schrödinger equation, choose a region which include the Si/SiO_2 interface or other heterostructure interfaces.

6. When simulating SNWT use complete ionization, in order to avoid problems with acceptor/donors level occupations.

3.8 fplot

fplot is a python script which makes use of python tcl/tk libraries. Since output files are concerned with quantities defined in the three-dimensional domain, it is useful to cut such data in slices along the three different axis, in order to be visualized. *fplot* does exactly this, or better, given the input file, the plane through which the cut has to be done, and the coordinate of the plane, it produces an output file which is read and visualized by *gnuplot*.

In Fig. 3.3 it is shown the GUI as it appears once *fplot* is called. The cut plane is specified by means of the radio buttom, while the coordinate and the file name of the *ViDES* output file are specified in the input box.

To plot, just push the *plot!* button, and a window like the one show in Fig. 3.4 will be displayed.

Imagine can also be rotated. If this not happens, add the following line to the .gnuplot file in the user's home :

set mouse on

As can be noted, there is also another input field which appears in the GUI. In such a field gnuplot commands can be specified, and take effect only when the ON radio button on the right is setup. If for example a colormap of the plot wants to be displayed, the following commands have to be written :

set pm3d map; unset surf; rep

The colormap will be shown after pressing the *plot!* button.

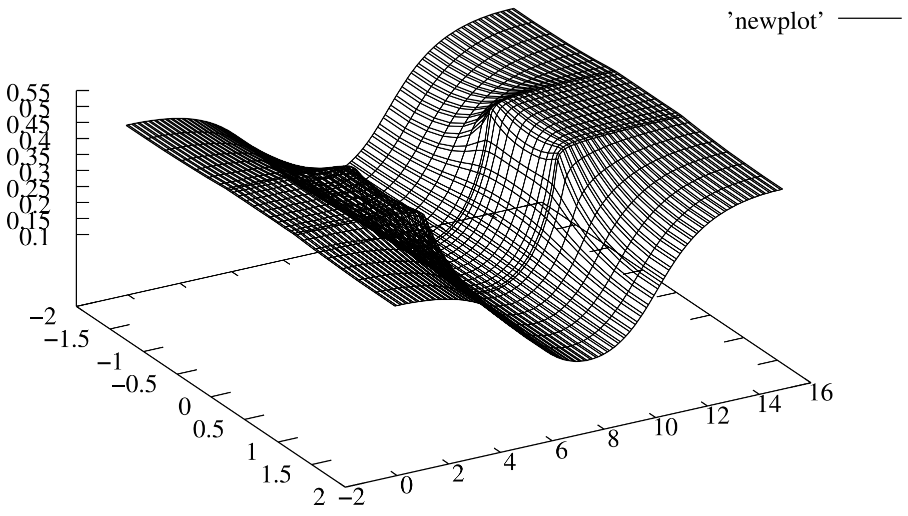


Figure 3.4: Example of the fplot displayed output : the electrostatic potential in a CNT is shown.

Chapter 4

Examples

Here we give two examples of input files for two different nanoscale devices : a CNT-FET and a SNWT device.

4.1 Carbon Nanotube Field Effect Transistors

To run the example, in the *bin* directory type the command *./ViDES inputdeckCNT*. The simulated device is a double gate CNT-FET shown in Fig. 4.1. The CNT is a (13,0) zig-zag and 15 nm long. The channel is 5 nm, and the doped source and drain extension are each 5 nm. Their molar fraction is equal to 5×10^{-3}. The nanotube diameter is 1 nm, and the oxide thickness is 1,5 nm. The lateral spacing is equal to 1.5 nm. The whole nanotube is embedded in SiO_2 dielectric. A mode space approach is followed and 2 modes are considered.

Here follows the input file (inputdeckCNT).

```
gridx
{
   mesh -2 spacing 0.3
   mesh 0 spacing 0.1
   mesh 2 spacing 0.3
}

gridy
{
   mesh -2 spacing 0.3
   mesh 0 spacing 0.1
   mesh 2 spacing 0.3
}

gridz
{ mesh -0.1 spacing 0.1
   mesh 0 spacing 0.1
   mesh 10.05 spacing 0.1
   mesh 10.2 spacing 0.1
}
```

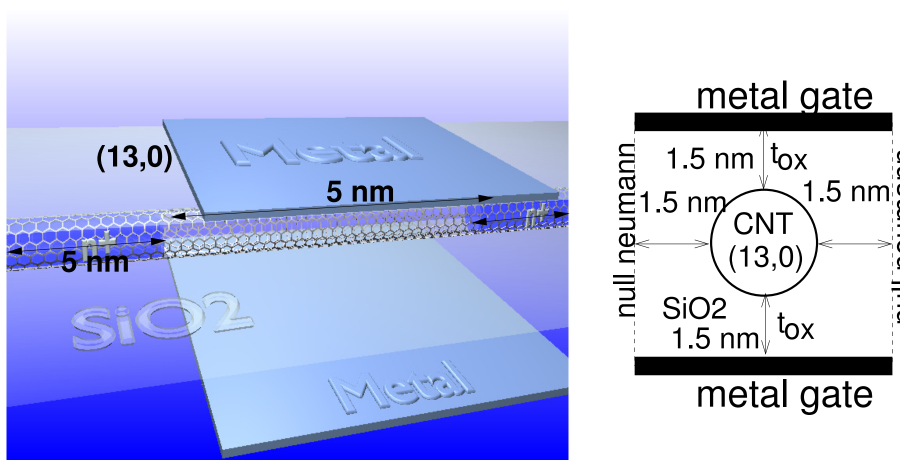


Figure 4.1: Example of the defined CNT-FET in the inputdeckCNT file.

```
CNT 13 15

# Here it starts the definition of the structure

tolldomn 1e-1
normad 5e-2
poissnorm 1e-1
mu1 0 mu2 -0.1
mode 2
flat
potsottoril 0.2
solid field oxide
{
    sio2
    nulln nullp
}

solid source
{
    sio2
    nulln nullp
    zmax 5
    fraction 5e-3
}

solid drain
{
    sio2
    nulln nullp
    zmin 10
    fraction 5e-3
```

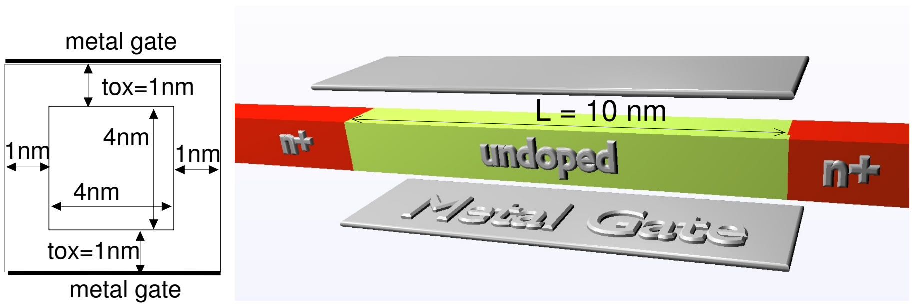


Figure 4.2: Example of the defined SNW-FET in the inputdeckSNWT file.

```
}

gate out
{
    xmin 190
    xmax 200
}

gate bottom
{
    xmax -1.7
    zmin 5 zmax 10
    Ef 0.0
}

gate top
{
    xmin 1.7
    zmin 5 zmax 10
    Ef -0.1
}
```

4.2 Silicon Nanowire Transistors

To run the example, in the *bin* directory type the command *./ViDES inputdeck-SNWT*. The simulated device is a double gate SNWT-FET shown in Fig. 4.2. The device cross-section is rectangular (4x4 nm^2), the channel length is 10 nm, and the source and drain reservoirs are 10 nm long. The oxide thickness is equal to 1 nm. 4 modes have been taken into account.

Here follows the structure definition :

```
gridx
{
    mesh -3 spacing 0.1
    mesh -2 spacing 0.05
    mesh 0 spacing 0.2
    mesh 2 spacing 0.05
    mesh 3 spacing 0.1
}

gridy
{
    mesh -3 spacing 0.1
    mesh -2 spacing 0.05
    mesh 0 spacing 0.2
    mesh 2 spacing 0.05
    mesh 3 spacing 0.1
}

gridz
{
    mesh -0.1 spacing 0.1
    mesh 0 spacing 0.2
    mesh 29.9 spacing 0.2
    mesh 30.0 spacing 0.1
}

tolldomn 1e-1
normad 1e-2
poissnorm 1e-1
mu1 0.0 mu2 -0.5
flat
ps
prev
potsottoril 0.2
complete
solid field oxide
{
    sio2
    nulln nullp
}

solid field oxide
{
    silicon
    nullp
    xmin -2 xmax 2
    ymin -2 ymax 2
}

solid field source
{
    silicon
    nullp
    xmin -2 xmax 2
    ymin -2 ymax 2
    zmax 10
    Nd 1e26
}

solid field drain
{
    silicon
    nullp
    xmin -2 xmax 2
    ymin -2 ymax 2
    zmin 20
    Nd 1e26
}

gate out
{
    xmin 190
    xmax 200
}

gate top
{
    xmin 3
    zmin 10 zmax 20
    Ef -0.5
    workf 4.1
}

gate bottom
{
    xmax -3
    zmin 10 zmax 20
    Ef -0.5
    workf 4.1
}

region
{
    negf2d
    xmin -2.5 xmax 2.5
    ymin -2.5 ymax 2.5
    nauto 4
}
```

Chapter 5

Inside the code

The following notes are a brief summary of what is inside the *ViDES* code. Hopefully a more detailed Developer's guide will follow.

In the first section we will discuss how equations are discretized in the three-dimensional domain, while in the following sections we will take a look to the data structures as well as to the two subroutines which constitutes the main body (*struttura* and *solvesystem*).

5.1 Discretization of the three-dimensional domain

The discretization method used in ViDES is the so-called "box-integration" method. Let us suppose to discretize a 2D dimensional problem, which is simpler to be handled as compared to a 3D problem, and from which general considerations valid also for a 3D system of equations can be easily derived.

Let us consider Fig. 5.1, which shows the Voronoi cell around $\mathbf{r_l}$, the position of the l-th point of the mesh. We want to discretize around point l a generic equation

$$\nabla \cdot \vec{f} = g, \tag{5.1}$$

on a Delauney mesh using box integration.

If we integrate (5.1) on the surface Ω_l, we obtain

$$\int_{\Omega_l} \nabla \cdot \vec{f} dr^2 = \int_{\Omega_l} g dr^2 \tag{5.2}$$

and applying the Gauss-Green theorem on the left hand side,

$$\int_{\sigma_l} \vec{f} \cdot dr = g_l \Omega_l \tag{5.3}$$

where the surface integral becomes a flux integral over the boundary of the Voronoi cell σ_l, while the right hand term has been simplified, bringing out of the integral the argument, since Ω_l is small and the argument can be considered constant.

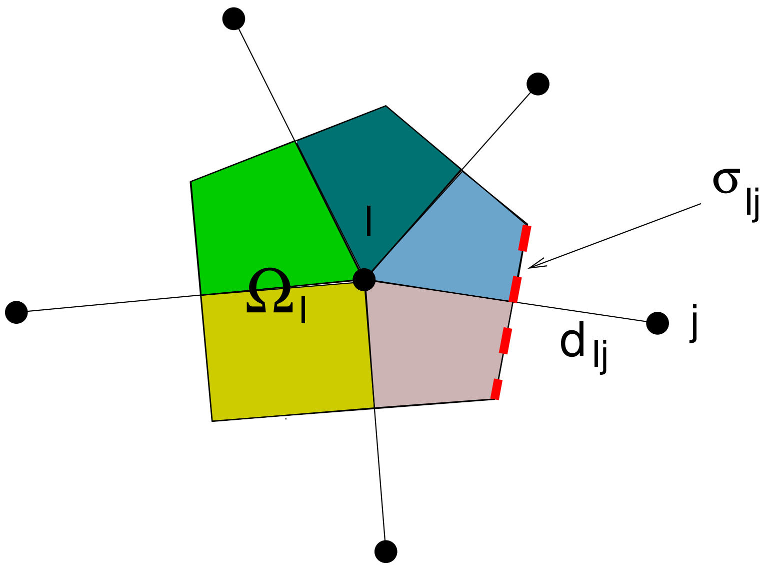


Figure 5.1: Voronoi cell associated to the l-th point of the mesh, at position $\mathbf{r}_l$.

The discretized equation can then be written as

$$\sum_j \frac{\sigma_{lj}(f_j - f_l)}{d_{lj}} = g_l\Omega_l, \tag{5.4}$$

where the sum is performed all over the nearest neighbor j, d_{lj} is the distance between j and l, and σ_{lj} is the boundary of the Voronoi cell, which cuts the d_{lj} segment.

In three dimensions, Ω_l is the volume of the Voronoi cell, d_{lj} is still the distance between l and its nearest neighbors j, while σ_{lj} is the surface of the Voronoi cell cut by the segment d_{lj}. Since it is easier to work with vectors rather than with matrices, the discretized quantities function of the point are mapped in ViDES as in Fig. 5.2 : points are ordered first along x, then along y and z. This means that in the 3D domain, if the generic point $\mathbf{r_l}$ has index i, j and k along the three axis, its index l in the mapped vector is

$$l = i + j \cdot nx + k \cdot nx \cdot ny \tag{5.5}$$

with

$$i = 0..n_x - 1 \tag{5.6}$$
$$j = 0..n_y - 1 \tag{5.7}$$
$$k = 0..n_z - 1 \tag{5.8}$$
$$\tag{5.9}$$

The grid used in ViDES is a non-uniform rectangular grid, so the Voronoi cell is a parallelepiped. Fig. 5.2, which does not represent the Voronoi cell, shows 8 different parallepipeds : each parallelepiped is the element associated with each grid point. This distinction is necessary because, as we will see later, each element can be associated to different a material.

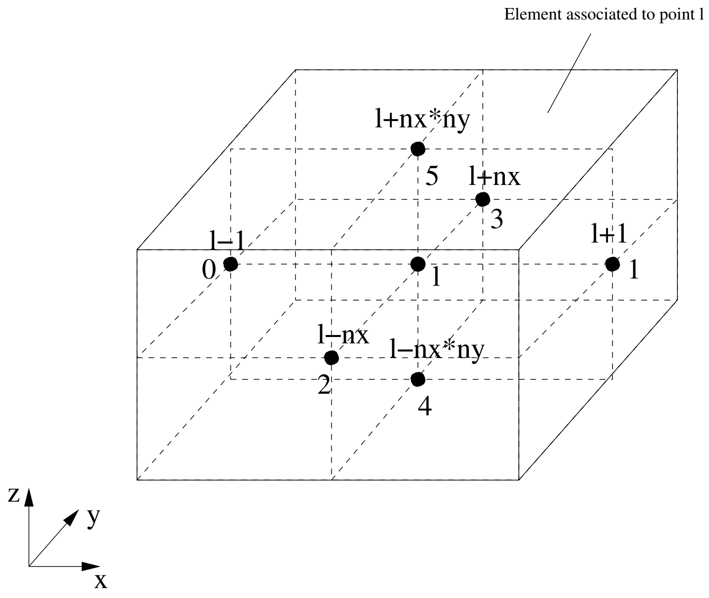


Figure 5.2: Three-dimensional grid : index of the nearest neighbors.

5.2 The main body

ViDES is a three-dimensional Poisson solver, so (5.1) becomes

$$\nabla\left[\epsilon(\vec{r})\nabla\phi(\vec{r})\right] = -q\left[p(\vec{r}) - n(\vec{r}) + N_D^+(\vec{r}) - N_A^-(\vec{r})\right] + \rho_{fix}, \tag{5.10}$$

where ϕ is the electrostatic potential, ϵ is the dielectric constant, q is the elementary charge, p and n are the hole and electron densities, respectively, N_D^+ is the concentration of ionized donors and N_A^- is the concentration of ionized acceptors, while ρ_{fix} is the fixed charge.

The main body of the code is constituted by two subroutine : *struttura*, which takes care of all the quantities needed to define the discretized Poisson equation, like the volume and the surface of the Voronoi cell, as well as all the distances between the neighbors, while *solvesystem* implements the 3D Poisson solver.

All the physics instead is included in separate modules, which can be developed and passed to *solvesystem* as functions, as we will see in the next sessions.

Before focusing our attention on the main subroutines, we have to spend some comments on the data structures which are defined inside *ViDES*, and which are the arguments of the subroutines of the code. Passing all the data through structures has the benefits of leaving unchanged the header of the subroutines as changes to the code are concerned.

5.2.1 physical_quantities.h

This structure which contains all vectors associated with physical quantities, which are generally function of the point, i.e. vectors which depends only on the index l of the discretized domain.

Here is the listing of the data structure :

```
typedef struct {
      double *Phi;
      double *Na;
      double *Nd;
      double *Ef;
      double *rhof;
      double *phim1;
      double *ef1;
      double *vt;
      char *flagmbfd;
      char *flagion;
      double *pot;
      double *E;
    } physical_quantities;
```

- `Phi` : vector associated with the electrostatic potential defined in the three-dimensional domain.
- `Na` : vector associated with the acceptor concentration.
- `Nd` : vector associated with the donor concentration.
- `Ef` : the Fermi level defined in the considered domain.
- `rhof` : the fixed charge concentration.
- `phim1` and `ef1` : they are the workfunction and the Fermi level, respectively, of the first defined gate in the *str3d.in* file, which is the referring gate for the potential.
- `vt` : the thermal energy expressed in eV defined as K_BT/q, where K_B is the Boltzmann constant, and T the temperature.
- `flagmbfd` : a flag which specify if a Maxwell-Boltzmann or a Fermi-Dirac statistic has to be used for the semiclassical expression of the electron and hole densities.
- `flagion` : a flag which specify if a complete or incomplete ionization for the acceptor and donor concentrations has to be considered.
- `pot` : it is the vector function of the gate index, which specifies the electrostatic potential l at the gate (Dirichlet boundary conditions).
- `E` : it is the electric field imposed on the six lateral surface of the three-dimensional domain (Neumann boundary conditions).

5.2.2 device_mapping.h

Let us consider the other data structure *device_mapping.h*, which instead passes to the subroutine all the quantities related to the grid.

```
typedef struct {
  int nx;
  int ny;
  int nz;
  int *solido;
  int *ele;
  double **dist;
  double **surf;
  double **dVe;
  int **corrSP;
  int **corrPS;
  int *tipopunto;
  int *tipopuntos;
} device_mapping;
```

- `nx` : number of points along the x axis.
- `ny` : number of points along the y axis.
- `nz` : number of points along the z axis.
- `solido` : it is a vector function of element : given the element to which the generic l point belongs, `solido` returns the solid number to which the element belongs. The solid is defined in *str3d.in* file by means of the *solid* command.
- `ele` : vector which returns the elements to which the generic points l belongs.
- `dist` : the matrix which implements d_{lj}, i.e. the distances between the l and j points, as explained in the first section of the manual. In particular, working with rectangular grid, the generic point l has six prime neighbors : the first index runs over the points of the grid, while the second index over the six prime neighbors. As in Fig. 5.2, index 0 refers to $l-1$ point, index 1 to $l+1$, index 2 to $l-n_x$, index 3 to $l+n_x$, index 4 to $l-n_xn_y$, and index 5 to $l+n_xn_y$.
- `surf` : is a matrix which implements the surfaces σ_{lj} of the Voronoi volume multiplied by the dielectric constant, as explained in the first section of the manual. Its indexes are ordered in the way as the `dist` matrix.
- `dVe` : is a matrix which implements the Ω_l volume of the Voronoi cell. While the first index runs over the points of the grid as in `dist` and in `surf`, the second index runs over the eight sub-volumes belonging to the Voronoi elements.
- `corrSP` : as explained in the *ViDES User Manual*, user can specify regions belonging to the three-dimensional domain, in which quantum analysis are performed. It can be useful to reorder points belonging to these regions identifying them with a relative index r. It is however necessary to define also a correspondence between the relative index r and the absolute index l. This is accomplished by means of the matrix `corrSP[r][region]`, which returns the absolute index l, given the relative index `r` and the `region`, to which r belongs.

- `corrPS` : `corrPS[l][region]` returns instead the relative index r of the absolute index `l`, which belongs to the region `region`.
- `tipopunto` : it is a vector function of l, which specifies which kind of boundary conditions have to be applied in the point l.

  If `tipopunto[l]` is smaller than 100, it specifies that the considered point is a point belonging to a gate, and it returns the gate number.

  If `tipopunto[l]`=101, `l` belongs to the surface with $x = x_{min}$, where x_{min} is the least abscissa along x, and where Neumann boundary conditions are imposed (the derivative of the electric field is equal to `E[0]`).

  If `tipopunto[l]`=102, `l` belongs to the surface with $x = x_{max}$, where x_{max} is the largest abscissa along x, and where Neumann boundary conditions are imposed (the derivative of the electric field is equal to `E[1]`).

  If `tipopunto[l]`=103, `l` belongs to the surface with $y = y_{min}$, where y_{min} is the least abscissa along y, and where Neumann boundary conditions are imposed (the derivative of the electric field is equal to `E[2]`).

  If `tipopunto[l]`=104, `l` belongs to the surface with $y = y_{max}$, where y_{max} is the largest abscissa along y, and where Neumann boundary conditions are imposed (the derivative of the electric field is equal to `E[3]`).

  If `tipopunto[l]`=105, `l` belongs to the surface with $z = z_{min}$, where z_{min} is the least abscissa along z, and where Neumann boundary conditions are imposed (the derivative of the electric field is equal to `E[4]`).

  If `tipopunto[l]`=106, `l` belongs to the surface with $z = z_{max}$, where z_{max} is the largest abscissa along z, and where Neumann boundary conditions are imposed (the derivative of the electric field is equal to `E[5]`).
- `tipopuntos` : is a vector function of l, which specify if a point belongs to a region in which quantum analysis has to be performed.

5.2.3 soliduzzo.h

This structure contains all the quantities which are related to the material, like the effective mass, the energy gap, the dielectric constant etc., and which are function of the solid. Here we will explain some quantities included in soliduzzo :

```
typedef struct {
  double eps;
  double chi;
  double Egap;
  double me1;
  double me2;
  double me3;
  double Nc;
  double Nv;
} soliduzzo;
```

- `eps` : dielectric constant.
- `chi` : electron affinity.

- `eps` : energy gap.
- `me1` : effective mass along the k_x direction.
- `me2` : effective mass along the k_y direction.
- `me3` : effective mass along the k_z direction.
- `Nc` : equivalent density of states in the conduction band.
- `Nv` : equivalent density of states in the valence band.

If for example we want the value of the dielectric constant of the material in correspondence of l-th point, we have to define a structure `soliduzzo mat`, and write in the code `mat[d.solido[d.ele[l]]].eps`, where `d` is a *device_mapping* structure.

5.2.4 struttura.c

This subroutine implements the parser, which reads the input deck *str3d.in* and returns all the quantities associated to the grid like, for example, the `dist`, the `surf` and the `dVe` matrices, and properly fills the structures explained above.

5.2.5 solvesystem.c

This subroutine implements the three-dimensional non-linear Poisson solver, by means of the Newton-Raphson algorithm.

```
void solvesystem(physical_quantities p,device_mapping d,
                 int *IERR,double tolldomn,
                 int neq,soliduzzo *mat,double normapoisson,
                 double sottoril,dfunpoint *nf,dfunpoint *pf,
                 dfunpoint *accf,dfunpoint *donf,
                 dfunpoint *dnf,dfunpoint *dpf,
                 dfunpoint *daccf,dfunpoint *ddonf);
```

Apart from the structures already explained, vectors of pointer to function are passed as argument of *solvesystem*, which represents the terms belonging to the right hand term of (5.10) and their derivatives with respect to the electrostatic potential ϕ. Having defined vectors of pointer to function, has the advantage of separating the physics from the numerics. In this way indeed, all the numerics concerned with the solution of the Poisson equation is included in *solvesystem*, while all the physics is defined specifying for each point l, which function (i.e. which physical model) has to be solved in that point.

In particular the structure `dfunpoint` is defined as :

```
 typedef double(*dfunpoint)(int i,physical_quantities p,
                            device_mapping d,soliduzzo *mat);
```

and

- `nf` : vector of pointer to functions associated to the electron charge density.

- `pf` : vector of pointer to functions associated to the hole charge density.
- `accf` : vector of pointer to functions associated to ionized acceptors density.
- `donf` : vector of pointer to functions associated to ionized donors density.
- `dnf` : vector of pointer to functions associated to the derivative of the electron charge density, with respect to the electrostatic potential.
- `dpf` : vector of pointer to functions associated to the derivative of the hole charge density, with respect to the electrostatic potential.
- `daccf` : vector of pointer to functions associated to the derivative of the ionized acceptors density, with respect to the electrostatic potential.
- `ddonf` : vector of pointer to functions associated to the derivative of the ionized donors density, with respect to the electrostatic potential.

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