TNL

Particle DeviceSimulator (TNL-PD Simulator) Tutorial

Particle based device simulationSoftware

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TNL

Contents

TNL

1.1 Getting Started

To use the TNL Particle Device (TNL-PDS) simulator user needs to get the official license. Once they get the license for the same, they can verify it by opening the TNL-Framework. At framework user will see a tick mark on the side of the name Particle Device Simulator (2D Poisson Solver) in green color which confirms the license for same as represented in Fig. 1. But if a cross mark in red color is seen then user might not using valid license (in this case user needs to contact Tech Next Lab Pvt. Ltd.). For more information user needs to go through the License Manual.
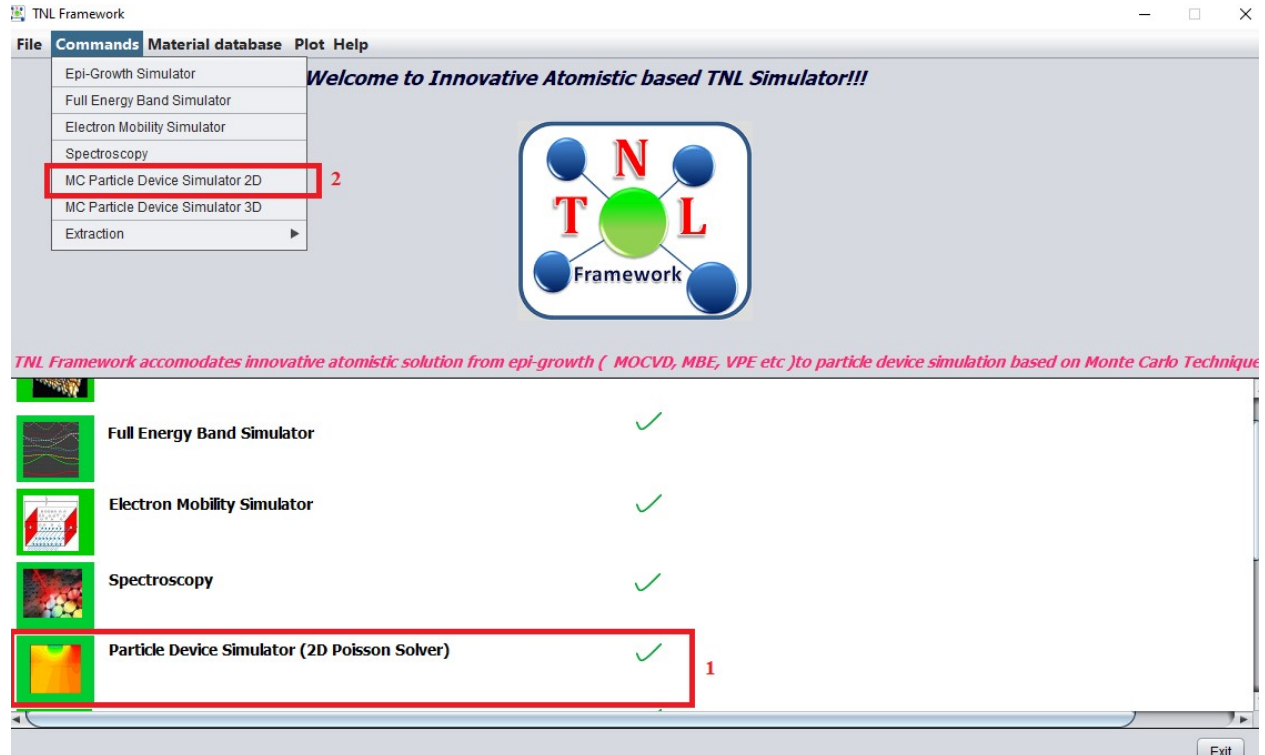

Fig. 1 : TNL-Framework

There are two ways to open the TNL-PD Simulator from the Framework shown in Fig.1. Those ways are shown in red rectangular boxes (box1 and box2).

1. This box1 contains PD Simulator's icon and name. By a single click on icon or name user gets access to use the simulator

2. This box2 contains sub menu named as MC Particle Device Simulator 2D and 3D. By clicking on the menu Command user will get several sub-menus containing the names of all simulators of TNL family. By a single click on name user gets access to use the simulator.

Using any of the above two methods user will be directed to the TNL-PD Simulator window frame PDSimulator as shown in Fig. 2.

TNL

1.2 TNL-PD SIMULATOR window frame
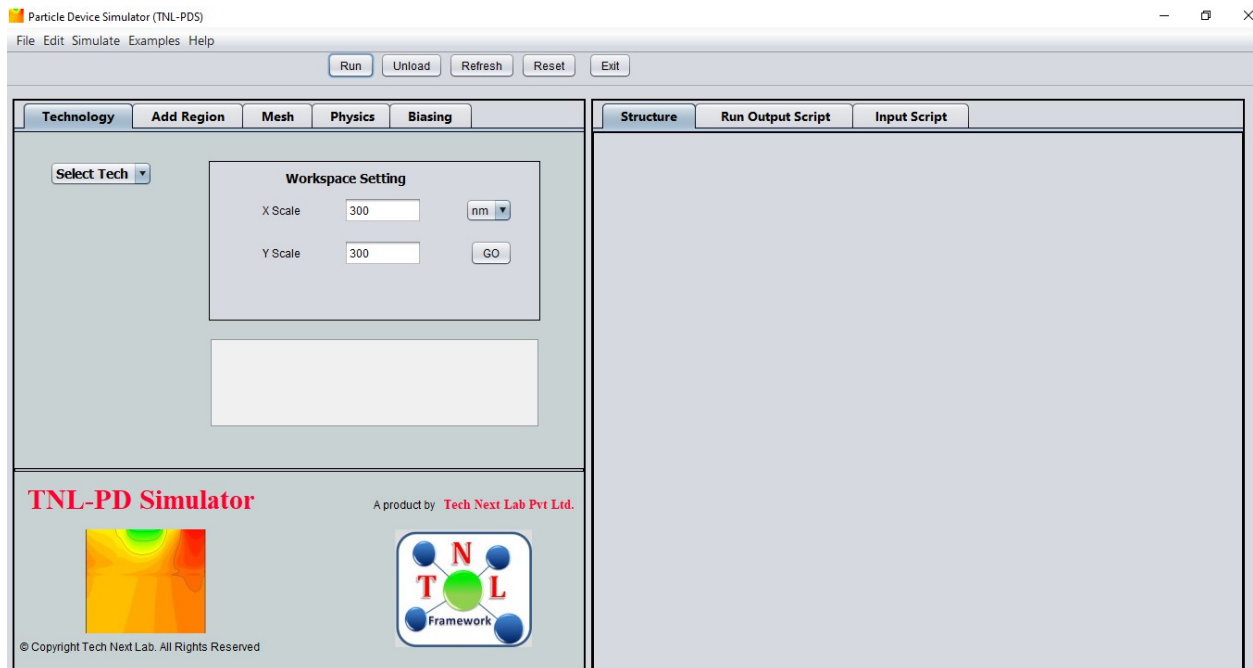
Fig. 2: ParticleDevice Simulator window frame.

TNL-PD Simulator window frame in Fig. 2 divided in two boxes located in left and right of the frame. Each of them consists of several tabs used for dedicated function for different operations.
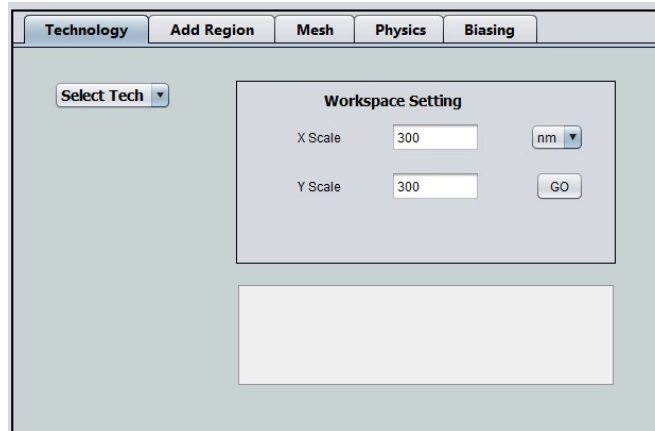
  i.   Technology
 ii.   Add Region
iii.   Mesh
 iv.   Physics
  v.   Biasing
 vi.   Structure
vii.   Run Output Script
viii.   Input Script

The TNL-PD simulator utilizes the essential information needed to define a device structure which flows from selection of technology and work space, designing device structure, choosing appropriate physical models, applied external voltages and running the simulations. Following sections will elaborate about these things.Before starting the simulation,users need to take note of their device type andit's dimensions

1.2.1 Technology tab

This version of the TNL-PD Simulator is structured with the five types of device technology and their related physical models. As shown in Fig. 3 this tab consists of:

    i.   Select Technology
    ii.   Workspace Setting
    iii.   Text field.

Fig. 3: Technology tab.

1.2.1.1 Select Technology

In current version the device technologies included are given below;

    i.   FDSOI (Fully Depleted Silicon on Insulator)
    ii.   MOFET (Metal Oxide Field Effect Transistor)
    iii.   TFET (Tunnel Field Effect Transistor)
    iv.   MESFET (Metal Semiconductor Field Effect Transistor)
    v.   HEMT (High Electron Mobility Transistor)

Depending on the user's requirement to select any of the above technologies specified.

1.2.2.1 Workspace Setting

After selecting the specific device technology, workspace needs to be defined by users for generation of device structure. Workspace is the area within which device dimensions in 'Add Region' tab will be given.

Workspace setting contains X Scale and Y Scale fields, unit of dimension and GO button. X Scale is for setting working Area in towards X Axis & Y Scale is for setting working Area in towards Y Axis. "GO" button is used for set maximum working area as per device structure requirements.

As 'GO' button is clicked the information of the device technology selected and workspace dimensions will get written in the blank text-field present below workspaces setting. TNL-PD simulator allots the selected workspace and device structure environment. Now users can define their required device structure by defining its different regions with suitable materials inbuilt in the simulator or they can accommodate their user define materials. With the addition of

TNL

regions one by one, simulator generates that graphics in right hand of the TNL-PDS frame named under Structure.

1.2.2 Add Region tab

This feature is most useful to select device structure. The structure is created by a set of regions with different coordinates, material and doping. As shown below:

Fig. 4: Add Region

This tab provides different material, regions and contact to define the device structure. The semiconducting materials Si, GaAs, AlGaAs, GaN, AlGaN are added to current version of simulator, an oxide region whose dielectric constant can be separately applied, Al and Al-Au alloy can be used as a metal contacts (Ohmic & Schottky), SiO_2 Si_3N_4 as insulator.
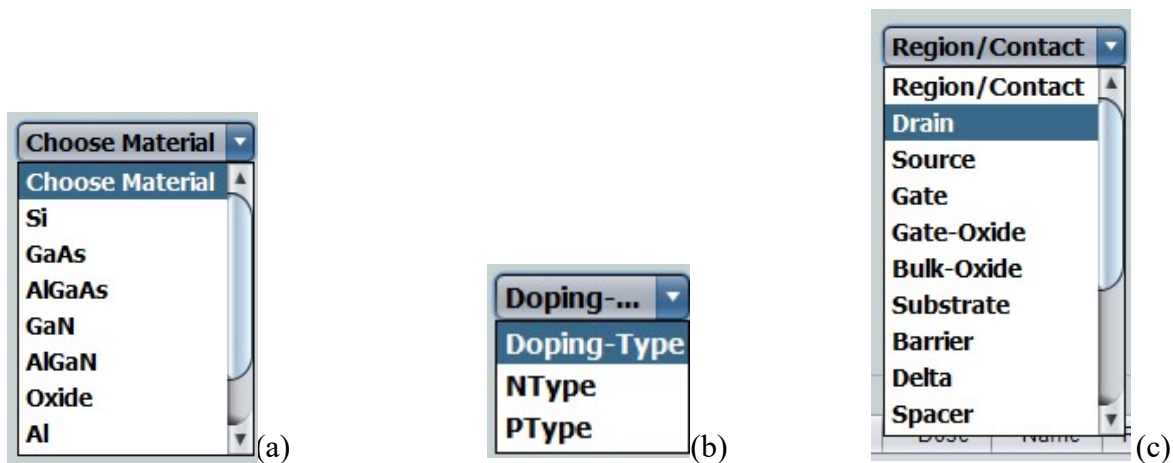
Fig. 5: Feasibility to choose (a) material (b) type of doping and (c) region or contact of device from various options.

(a) Any one from the given options of semiconductor material can be selected for a specific region of the device structure.

(b) From this option acceptor or donor type of doping can be implanted by selecting "P-type" or "N-type" respectively.

(c) The name of the region need to be identified by selecting one of the option like Source, Drain, Gate etc. and Ohmic or Shcottky type contact etc.

Fig. 6: Fields to define the concentration and boundaries of a region

(d) The concentration field shown in Fig. 6 is for the doping density of selected type of the current region you need to define.

(e) The four fields named Xmin, Xmax, Ymin, Ymax are present to give the boundaries in all four directions for a 2D structure.

(f) Oxide dielectric field requires the dielectric constant of the oxide, users need to define it as per device structure requirements. Eg. dielectric constant of SiO_2 is 3.9.

(g) Width field is for defining the width of the device. By-default it 1um, you can edit and can give some other value as per material used, but user need to be careful in choosing the value of dielectric constant, doping concentrations and the mesh sizes (will talk about this later on).


Fig. 7: Add and Delete button. Table for complete data of every single region

(h) Users may choose different regions dimensions with setting minimum and maximum x and y coordinates values after clicking on add button. After adding every region, users need to click refresh button. Every time you click on add button the information of material, xmin, xmax, ymin, ymax, doping type, dose, name of region and region will get print on a new row of the table shown in Fig. 7.

(i) If user finds some wrong information about any region has been chosen, then they can eliminate that particular row by clicking on the Delete button and then click on Refresh button

(j) Every time user have flexibilities to click Add or Delete buttons, the pane in Structure tab present in right column of the simulator main frame to add or delete that respective region.

1.2.3 Mesh tab
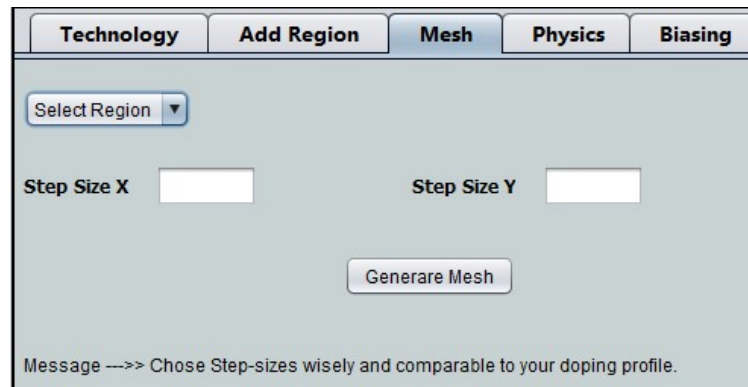
Fig. 8: Mesh tab.

Next tab on main frame is Mesh. Users may choose uniform meshing on the created device geometry. In case of two dimensional (2D) structures, the intersection point of mesh in x and y dimension will be used for charge distribution in form of super particle or charge in cloud (CIC) and calculation of potential by Poisson's equation. Step Size X is for distance between two consecutive mesh lines in X direction and Step Size Y is for distance between two consecutive mesh lines in Y direction. The Step Size X and Y are in the nanometer by default. After inserting suitable values in both of the above fields, click on Generate Mesh button. It will automatically generate mesh on Device Structure pane and also create number of node points in x and y directions which are very important quantity for the simulation.

For more accurate simulation user need to take notice of the following;

i. Try to take square mesh.

ii. Smaller the mesh size, the simulation complexity will be more and thus simulation time will be longer.

iii. There is trade of between doping concentrations and the cell volume in the device.

Cell Volume = step size x * step size y * device depth.

TNL

Doping concentrations of the regions where it should be extrinsically doped needs to be comparable with the cell volume.

Doping concentration * cell volume >= 1.

This version of TNL-PD Simulator, the uniform rectangular meshing can be chosen, in next version of the simulator will be loaded with the capability of non-uniform and triangular meshes.

1.2.4 Physics tab
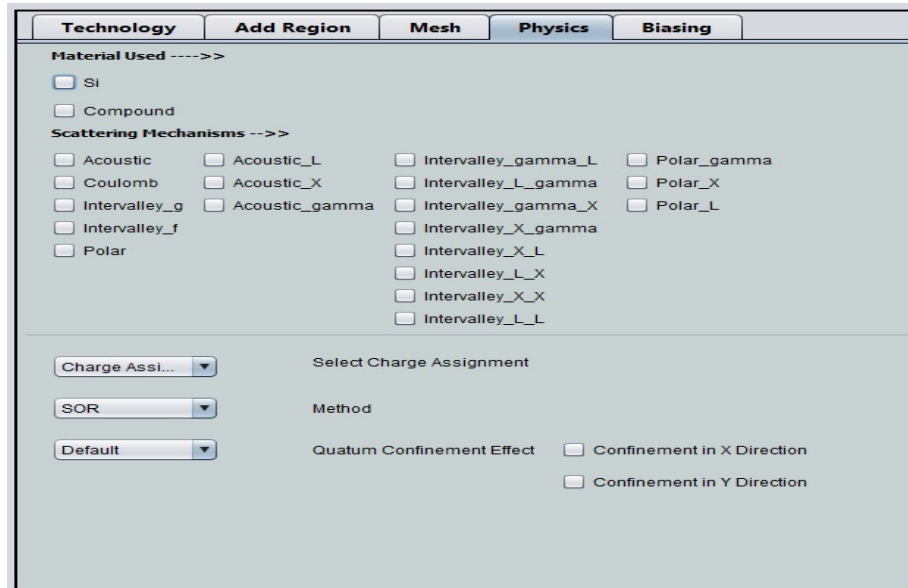
Fig. 9: Physics tab

Under Physics tab users have facility to select scattering mechanism as per their requirements, can choose one of the Charge Assignment Technique i.e. (CIC, NEC, NGP), Numerical Method (SOR) and Quantum Confinement Effect direction.

i. Scattering Mechanism

At least one of the scattering mechanisms is essential requirement to take in consideration for running device simulation. All types of scattering mechanism are given for both single element and compound materials.

There are two ways to select the scattering mechanism. First, if you select Si or Compound semiconductors placed under material used name, all the respective mechanisms will automatically get selected. Second, users can select one by one many of the available mechanism per your requirement.

ii. Select Charge Assignment

Next option is for selection type of charge assignment techniques on the node points of the meshes. Three types of charge assignment techniques have been implemented in the TNL-PD Simulator. All three charge assignment techniques produce similar results.

TNL

(a) Charge in Cloud (CIC)

In the CIC scheme a better approximation can be obtained assigning the charge of a super particle to the two nearest neighbor cell points.

(b) Nearest Element Center (NEC)

The NEC charge assignment force interpolation scheme attempts to reduce the self-forces and increase the spatial accuracy in the presence of non-uniformly spaced tensor-product meshes and/or spatially-dependent permittivity.

(c) Nearest Grid Point (NGP)

In the NGP scheme all the charge from a given particle is assigned to the nearest grid point. The force on the particle is also taken as the one calculated on the nearest grid point.

iii.   **Method**

Next tab is method use for solution of Poisson equation on node points for super particles. The Succession Over Relaxation (SOR) method has been implemented to improve the rate of convergence for solution of Poisson equation. SOR method uses a weighted average of the results of the two most recent estimates to obtain the next best guess of the solution. If the solution is converging, this might help extrapolate to the real solution more quickly.

iv.   **Quantum Confinement Effect**

We have developed a different approach, which introduces an effective potential for consideration of quantum confinement effects in x-, y-, and z- directions separately. Here, the natural non-zero size of an electron wave packet, in the quantized system, is used to introduce a smoothing of the local potential (found from Poisson's equation). This approach naturally incorporates the quantum potentials, which are approximations to the effective potential. The effective potential is related to the self-consistent potential through an integral smoothing relation.

By-default this effect is disabled, if user want to include this effect to their device simulation, they may chose Enable option and also select one check box between confinement in x or confinement in y direction.

1.2.5 Biasing

i.   The biasing tab in main frame is use to provide input voltages at different electrode terminals through "Solve" tab. Four type of terminals are given Source, Drain, Gate and Substrate. Click on insert button number of times as per the electrodes created in the device structure for providing the voltage ramping information.

ii.   User may choose constant or ramping voltage conditions on a particular electrode.

iii.   Give the initial, step and final biasing point. Suppose user gives initial value 0, step value 0.1 and final value 1. Then the simulation will first start at the 0 then it will proceed to 0.1, 0.2, 0.3, …, up to final value 1.

iv.   During the simulation all respective results will be saved at these voltages (we will talk about it later in this tutorial).

v.   Then click on load button on the main frame under solve tab. The given voltage will be added to particular electrode.

vi.   A field named 'Barrier voltage for Schottky contact', if you have added any contact terminal of Schottky type then you need to give the barrier voltage here. Barrier voltage is the difference between the work function of metal and the electron affinity of semiconductor. Unit is in Volt.

$$\varphi_B = \varphi_M - \chi$$

Once all the information has been provided by user, the structure is ready for starting simulation for which there are three ways:

i.   Click on 'RUN' button present above.

ii.   Go to Simulate menu, then click on Run submenu.

iii.   Go with the key combination of Shift+F6.

1.2.6 Structure Tab
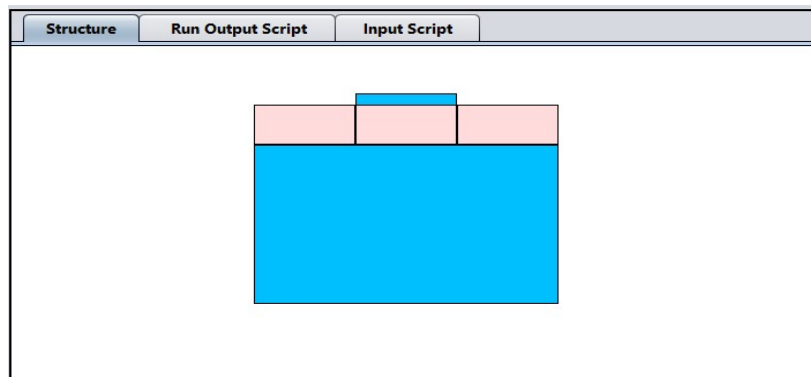
Fig. 10: Structure tab showing graphics of device

This tab shows the graphics of the device structure with all the regions added in the Add Region section. Users may select X-Scale and Y-Scale values in work space setting, the blank space in Structure tab shown in Fig 10. Initializing the working device geometry ranges in it and becomes ready to draw the 2D or 3D structure graphics of the desired structure. When users give dimensions and other data of a region and click on ADD button, then that area will be shown with particular material's convetional color in the workspace. If users found that there is some wrong information has been entered, then you can delete that easily. Users need to select that

TNL

row from the table present in Add Region tab and then click on 'Delete' button. To see that change in graphics users need to click on the 'Refresh' button.

TNL-PD simulator's GUI capabilities provide feasibility to view and verify device structure from table which contains the database of the designed structure or through the structure graphics. Through this it can be easily checked that at the time of input whether there is some unnecessary void or overlapping have been made or not and can be removed easily.

1.2.7 Run Output Script

This column will show the simulation points and few parameters value at each bias point. It will show simulation date and time. When simulation starts it will show the directory where all the simulation results will be saved with the line named working directory. After this some value of each bias point will be shown with the line named Calculation starts at Drain voltage = x and Gate voltage = y. At the end of last bias point it will write a line Simulation Completed which will notify user the successful completion of whole simulation after that he can see the results going to the working directory of respective simulation.

Fig. 11: (a) Output script tab   (b) Input Script tab

1.2.8 Input Script

This tab consists of information about all the input information provided to initiate simulation from all tabs on the left column of the main frame in script form. Users have flexibility to load an example (.txt) file, then that whole script will get printed here.

1.2.9 Menu

i.   File

When users click on File menu option, Open sub-menu will open. Click on Open, a pop-up window will float on user's screen. From this users will go to specific directory and then to that folder in which your script for the device input is present. Select that .txt file and click on open button below of the pop-up window. (See Section 1.3)

TNL

   ii.   Simulate

          This menu contains Run option, click on this users may click to start the simulation after giving the path to save your simulation.

  iii.   Example

          Here five device technology names have been given. Simulator is loaded with an example script of each device technology. User can select any of this and try for simulation. (See Section 1.3)

   iv.   Help

          Here three options named About, TNL-PDS Manual and TNL-PDS Tutorial are provided.

          Clicking on about or by giving shortcut-key combination of Ctrl+H will transfer you the [TechNext Lab Pvt. Ltd.](https://www.technextlab.com) official website https://www.technextlab.com. Clicking on above options TNL-PDS Manual and TNL-PDS Tutorial manual and tutorial file will get open.

1.2.10 Other

    i.   Run Button: This button use to start the simulation.
    ii.   Unload Button: This button use to unload or delete all the input information given previously. This button is necessary when you need to input your data from the script file.
  iii.   Refresh Button: This button is to refresh the graphics of device when there is some edit needed to be performed.
   iv.   Reset Button: This button delete each and every thing and brings it to null value.
    v.   Exit Button: This button closes the simulator GUI window.

1.3 Simulation of Examples (Script)

          Simulator provides flexibility to do device simulation through the script file as by using the ways told in section 1.2.9. To start using Example simulation, go through following steps:

1) Click on Unload button
2) Click on the Example menu and then select any of on technology name.
3) Now go to the Technology tab. Select technology name same as user have selected in step2.
4) Give the workspace (X and Y scale) comparable to the device dimension written in the Example script file. User can see this in the Input Script tab.
5) Click on Refresh button. User's device structure in script file will be loaded on GUI frame.
6) Click on Run button and select any directory or folder or path and give the name of your simulation file, then click on save button, thus simulation will be started of examples.
7) After some time scroll the Run Output Script pane and see the progress of your simulation. At the time of completion 'Simulation Completed Successfully' message will be shown in Run Output Window.

TNL

8) See your results by going to the directory as selected in Step6.

Same steps will be taken if you select a script file from Open option of File menu.

2. Hands-On Tutorial

For new user to get familiar with MC Particle device simulator, user may follow step by step the given tutorial. In current tutorial the Simulation of 20 nm channel length SOI MOSFET is described exploiting the Monte Carlo Particle Device Simulator.

2.1 Technology and Workspace setting

- Set Technology to FDSOI.

- Set workspace as per requirement.

- In present case our device dimension is in nanometer (nm)

- Set X Scale 100nm.

- Set Y Scale 100nm.

- By-default all scale in nm

- Click "GO" button.

- Information about all the above things will get displayed on below blank text area.

2.2 Add Region

Adding Source Region:
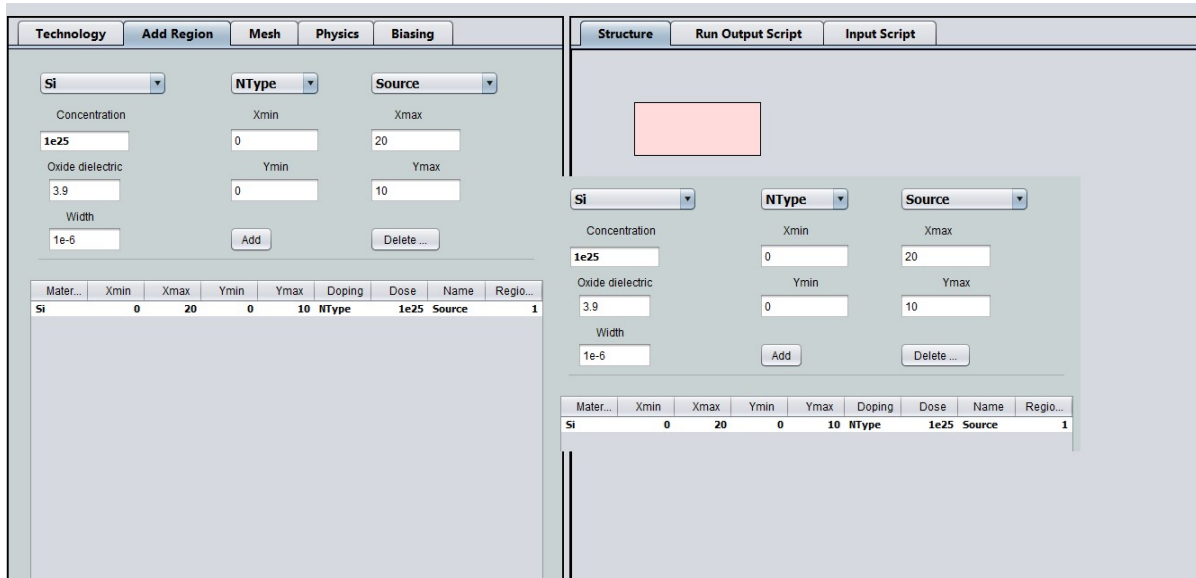
- Choose Source as a First region. For source region choose material Si (Silicon) using mouse orup/down key in keyboard.

- Doping type, N Type, Dose 1E25.

- Select region Source.

- Set X and Y Dimensions as

TNL

X Min: 0, X Max: 20nm.Y Min: 0, Y Max: 10nm.

- Click Add Button.

Adding Drain Region:

- For Drain Region choose material Si (Silicon) using.

- Doping type N Type, Dose 1E25.

- Select region Drain.

- Set X and Y Dimensions as

  X Min: 40, X Max: 60nm.Y Min: 0, Y Max: 10nm.
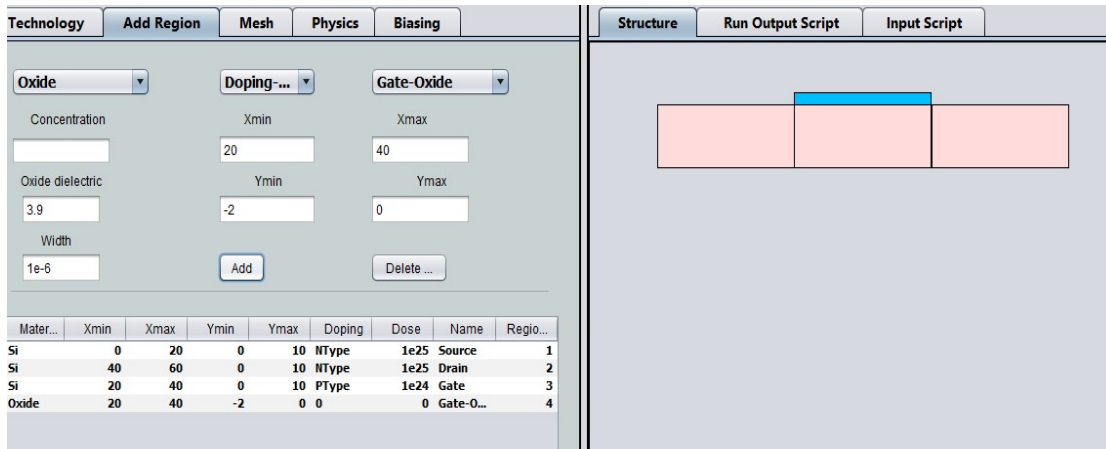
- Click Add Button.

Adding Gate Region:

- For Gate Region choose material Si (Silicon).

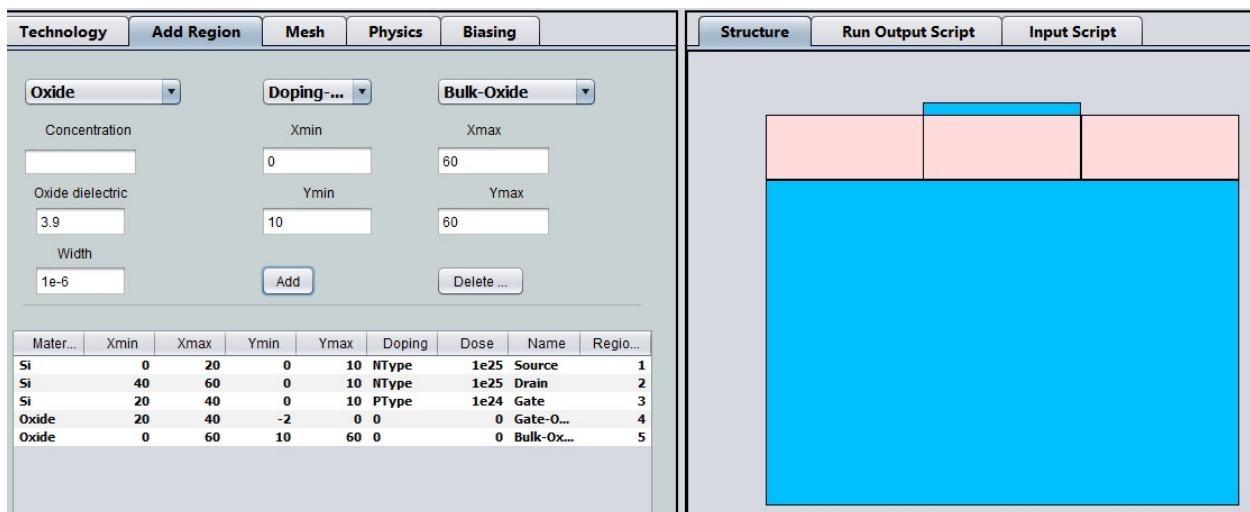- Doping type P Type, Dose 1E24.

- Select region Gate.

- Set X and Y Dimensions as

  X Min: 20, X Max: 40nm.Y Min: 0, Y Max: 10nm.

- Click Add Button.

Adding Gate Oxide Region:

- For Gate Oxide Region choose material Oxide.

- Set Doping type as Doping type, Dose 0.

- Select region Gate-Oxide.

- Set X and Y Dimensions as

  X Min: 20, X Max: 40nm.Y Min: -2, Y Max: 0nm.

- Click Add Button.

Adding Bulk Oxide Region:

- For Bulk Oxide Region choose material Oxide.

- Set Doping type as Doping type, Dose 0.

- Select region Bulk-Oxide.

- Set X and Y Dimensions as

  X Min: 0, X Max: 60nm.Y Min: 10, Y Max: 60nm.

- Click Add Button.

Adding Contact1 (Ohmic):

- Ohmic contact over **Gate** region.

- For Contacts choose material Al (Aluminium).

- Set Doping type as Doping type, Dose 0.

- Select region Ohmic.

- Set X and Y Dimensions as

  X Min: 20, X Max: 40nm.   Y Min: -2, Y Max: -2nm.

- Click Add Button.

Adding Contact2 (Ohmic):

- Ohmic contact under **Source** region.

- For Contacts choose material Al (Aluminium).

- Set Doping type as Doping type, Dose 0.

- Select region Ohmic.

- Set X and Y Dimensions as

  X Min: 0, X Max: 20nm.Y Min: 0, Y Max: 0nm.

- Click Add Button.

Adding Contact3 (Ohmic):

- Ohmic contact under **Drain** region.

- For Contacts choose material Al (Aluminium).

- Set Doping type as Doping type, Dose 0.

- Select region Ohmic.

- Set X and Y Dimensions as

  X Min: 40, X Max: 60nm.   Y Min: 0, Y Max: 0nm.

- Click Add Button.

TNL

Adding Contact4(Ohmic):

- Ohmic contact under **Substrate** region.

- For Contacts choose material Al (Aluminium).

- Set Doping type as Doping type, Dose 0.

- Select region Ohmic.

- Set X and Y Dimensions as

  X Min: 0, X Max: 60nm.Y Min: 60, Y Max: 60nm.

- Click Add Button.

2.3 Mesh

- Select Mesh tab
- In Step-size X write 1.
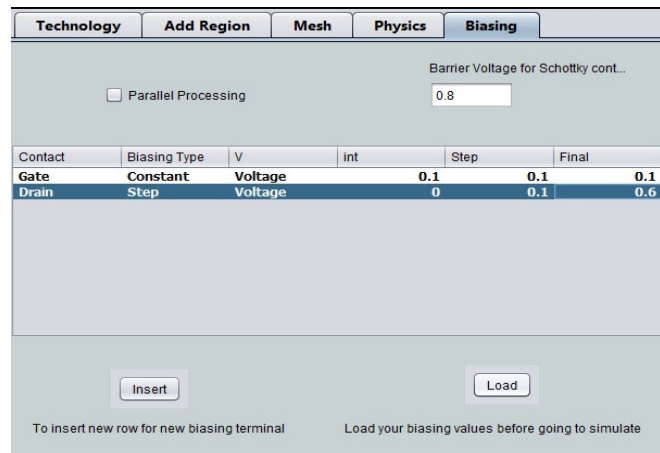- In Step-size Y write 1. It means you are working on 1nm X 1nm mesh.

- Click on Generate Mesh
- Mesh graphics will be seen in Structure tab.

2.4 Physics
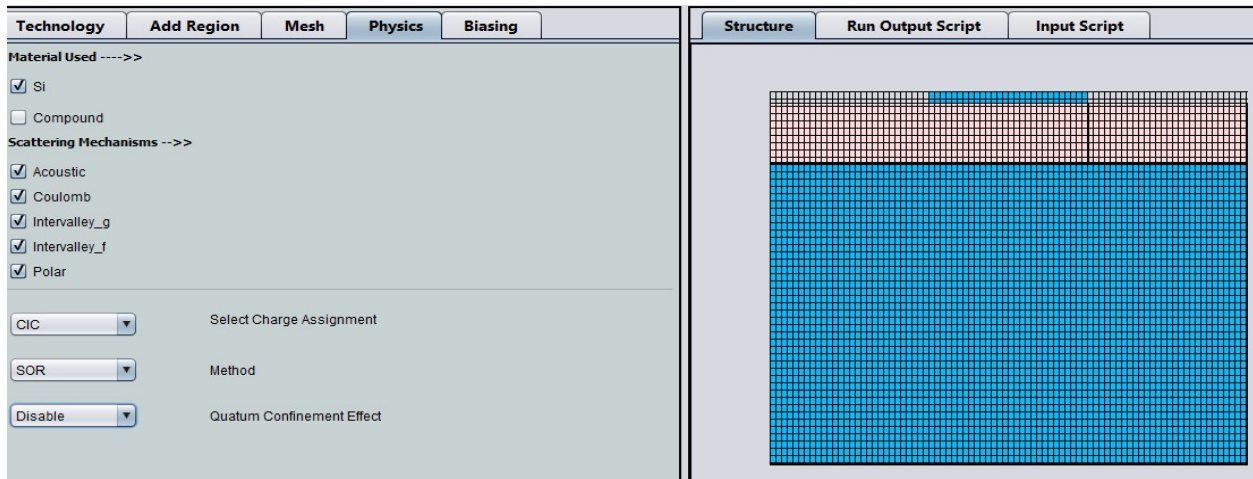
- Select Si check-box in Material Used options
- In Scattering Mechanism all five mechanism are auto-selected
- In Select Charge Assignment select option CIC.
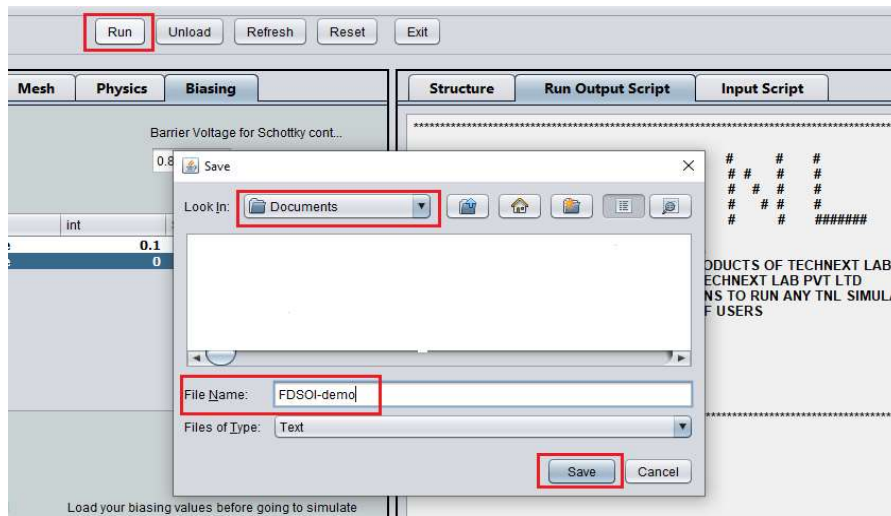- In Quantum Confinement Effect choose Disable option.

2.5 Biasing

- For biasing click below Contact in the table,

- Choose Gate, chose Constant bias, Voltage in next field.

- Gate initial voltage 0.1, step size 0.1, final 0.1 V.

- Click insert choose Drain as contact,

- Chose step bias, provide initial voltage 0.0, step size 0.1, final 0.6 V.

- Click Load Button.

2.6 Start Simulation

- Click on Run button, a Save pop-up window opened as shown in above figure.
- In save window default directory is 'Documents'. Go to field named File name and write name of your file name (FDSOI-demo for this example) to create a folder in the 'Documents' path of your system.
- Now click Save button. With this step your FDSOI device simulation starts and you can see the information about this in Run Output Script.
- Output script column shows the working directory "C:\Users\...\Documents\FDSOI-demo\FDSOI-demo\...". It also shows calculation points, no. of particle initialized at a bias point and no. of particles used in every steps.
- When simulation gets completed 'Simulation Successful message will be displayed

2.7 Output Files

- After the completion of simulation, go to the directory you selected there is a folder named FDSOI-demo.
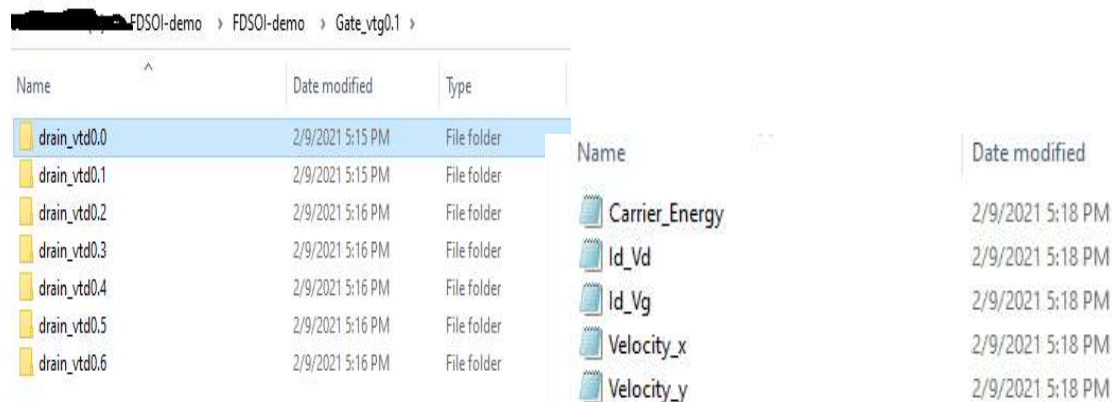
- Open this folder, you get several folder and text file like FDSOI-demo, plot and FDSOI-demo.txt
- FDSOI-demo folder will contain data folder for drain voltage steps at every gate voltage steps. (drain_vtd_y within Gate_vtg_x). Open these folders which contains various file related to the simulation.
- Plot folder contains i-v curves data, velocity-energy-average and carrier energy data files.
- The text file contains all the input information of the device given to simulator.
- User can plot this data on TNL-PLOT by importing the data file.

TNL