nanoFET: Upgrading to NEMO5

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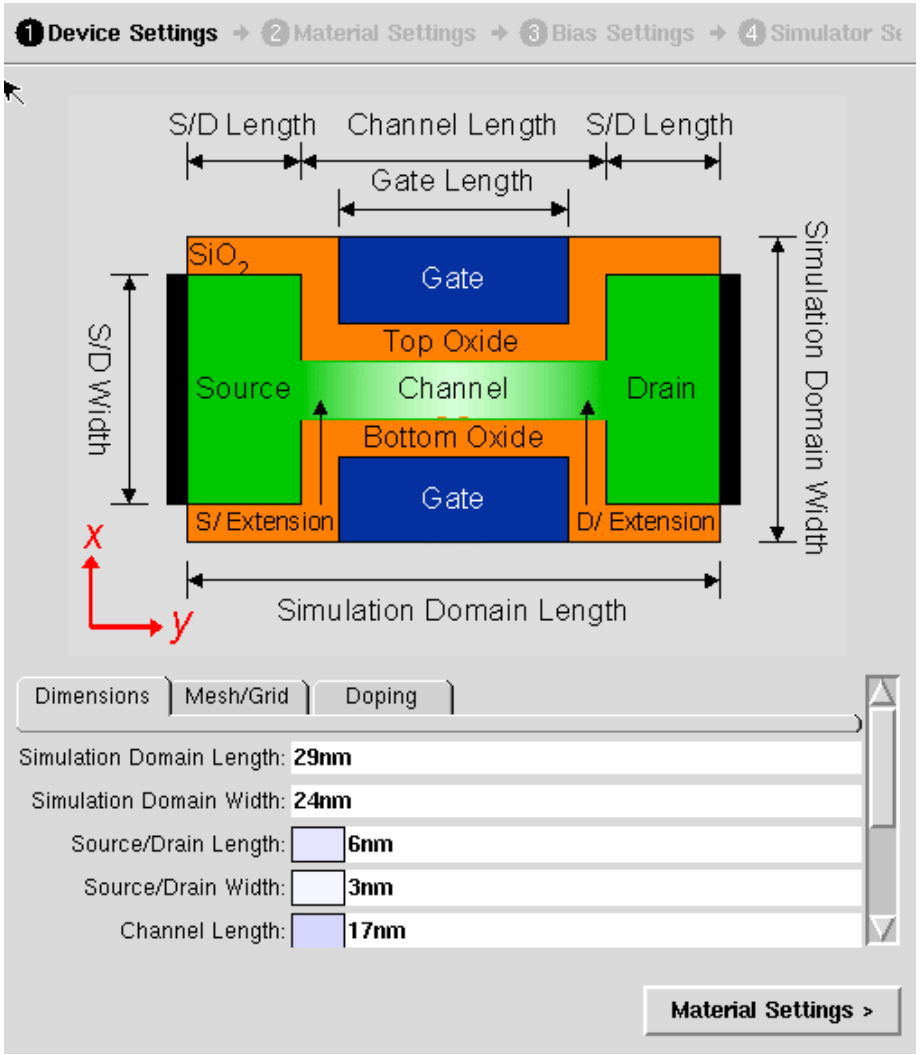
Outline

- Introducing nanoFET
- Software & Simulations
- Working with Inputs
- Current Status
- Future Work
- Questions

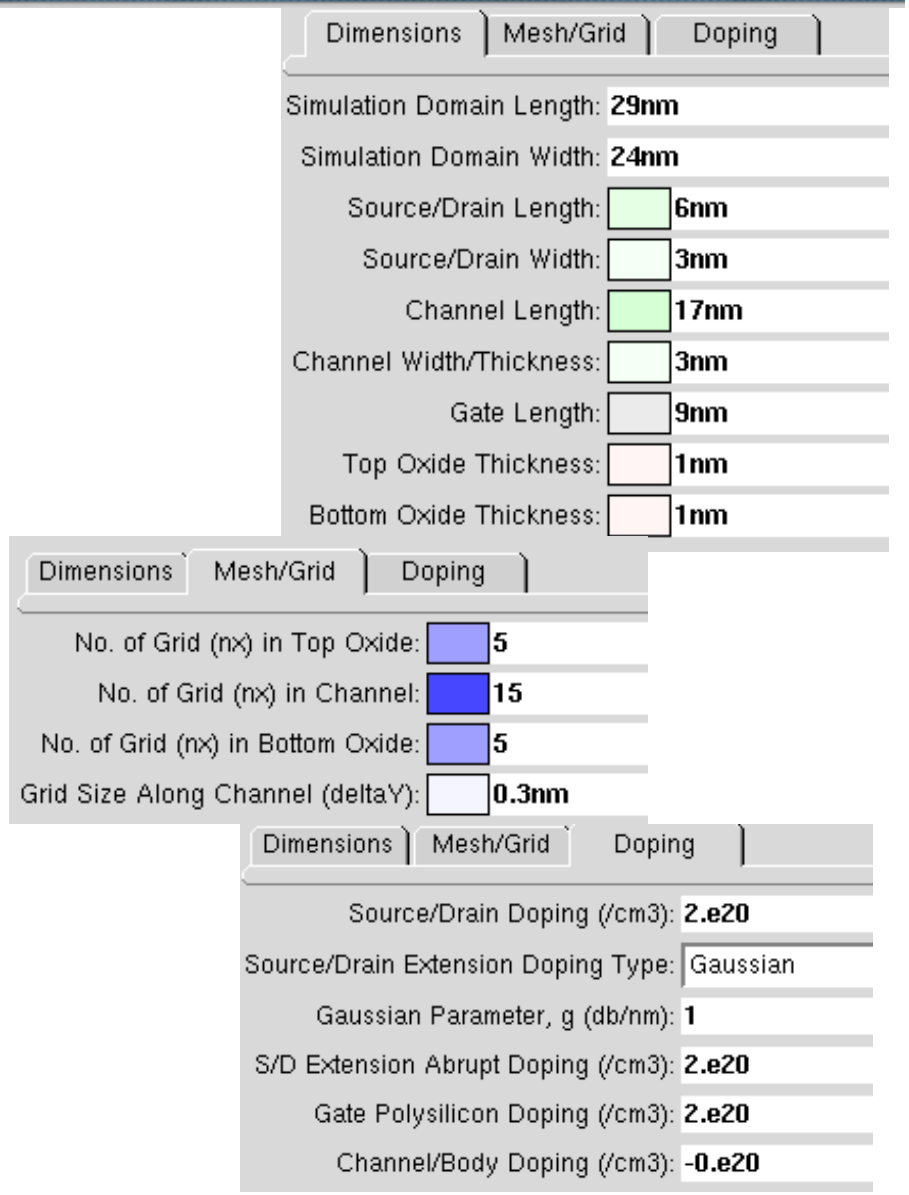
Introducing nanoFET

- Overview
  - Simulates ballistic transport in 2D, double-gated MOSFET devices
  - Four phases of inputs
- Objective
  - Upgrade tool using newly developed software



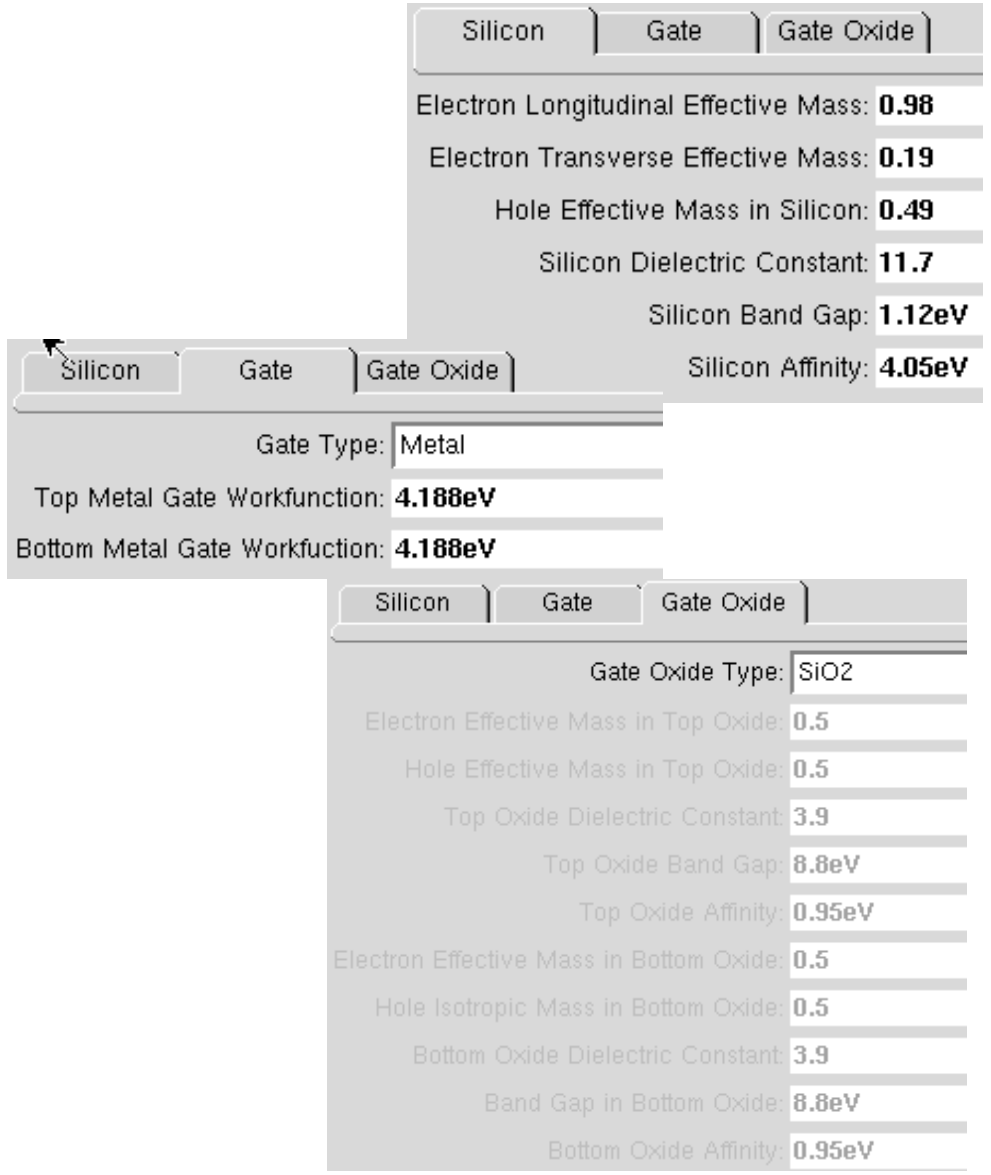
Device Settings

- Dimensions
  - Simulation domain
  - Source/Drain
  - Channel
  - Gate
  - Oxide
- Mesh & Grid
  - No. of grid
  - Grid Size along channel
- Doping
  - Impurity atoms per cm^3



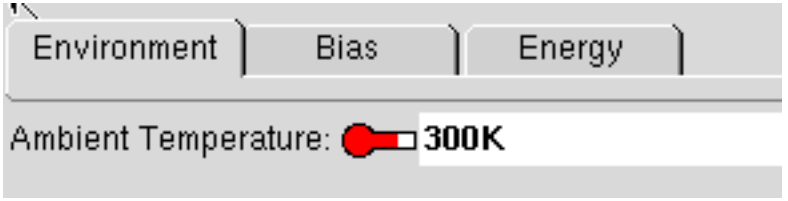
Material Settings

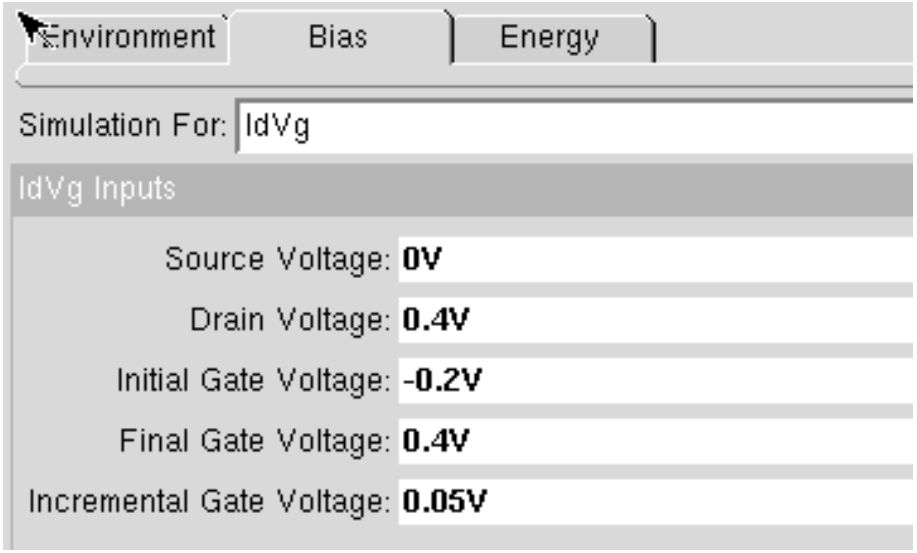
- Silicon
  - Effective Masses
  - Dielectric Constant
  - Band Gap
  - Affinity
- Gate
  - Metal or n-Polysilicon
- Gate Oxide
  - SiO2 or Other Oxide
  - Must specify Other Oxide Parameters

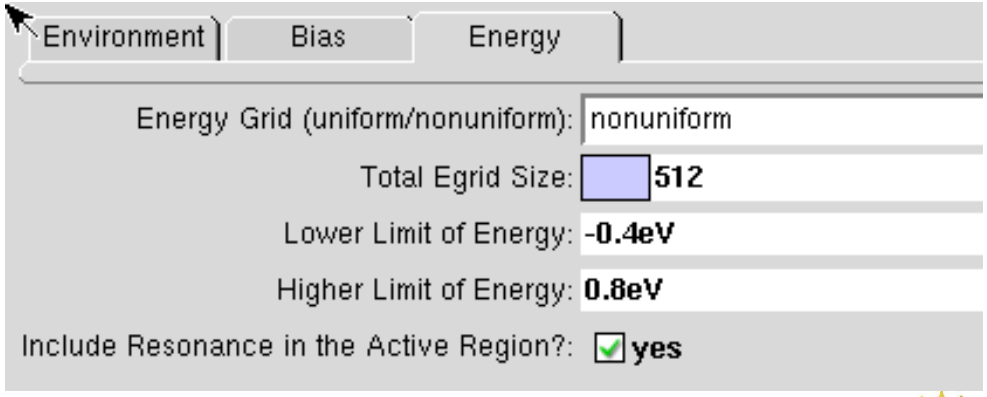


Bias Settings

- Environment
  - Temperature of environment around device
- Bias (applied voltage)
  - IdVg (gate controlled), IdVd (drain controlled), or single bias
  - Incremental gate voltage determines step size between bias points
  - Gate voltage controls both top and bottom gate
- Energy
  - Uniform or nonuniform grid

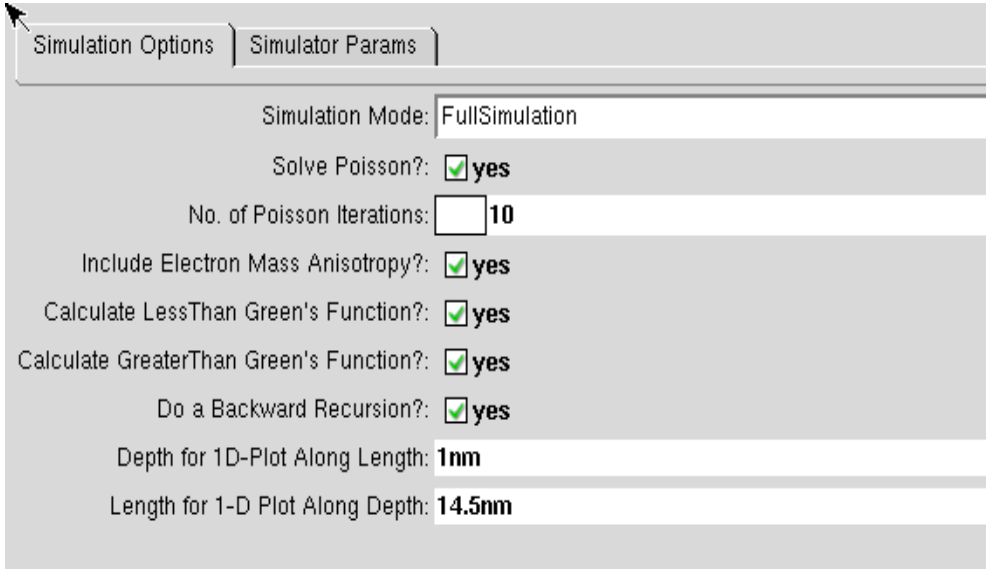


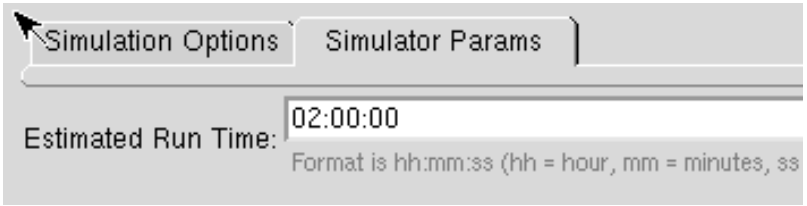




Simulator Settings

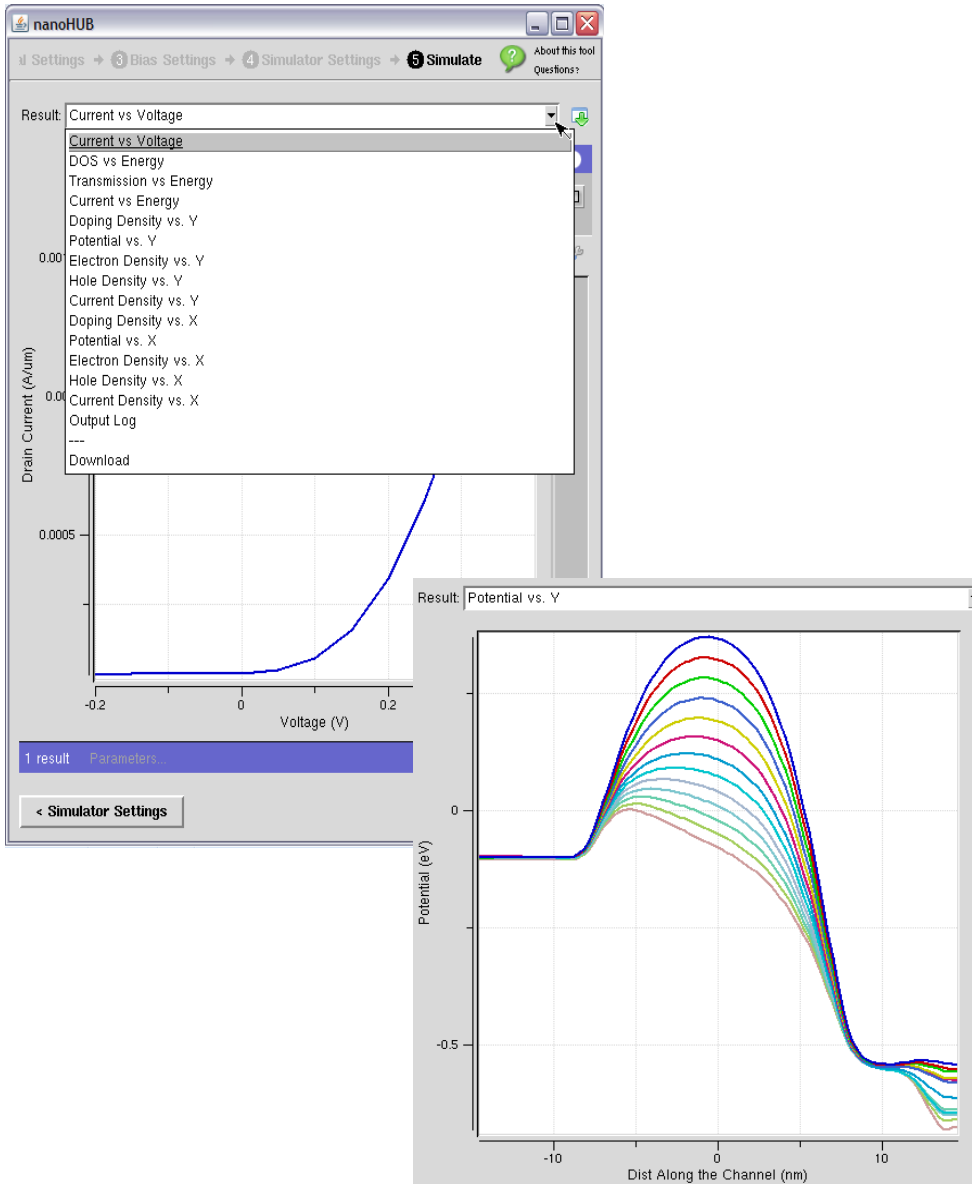
- Simulator Options
  - Full Simulation or Flat Potential
- Simulator Parameters
  - Sets up simulation time





Output of nanoFET

- 14 plots
  - Current vs. Voltage
  - Density Of States vs. Energy
  - Current vs. Energy
  - Doping Density vs. Y, vs. X
  - Potential vs. Y, vs. X
  - Electron Density vs. Y, vs. X
  - Hole Density vs. Y, vs. X
  - Current Density vs. Y, vs. X
- Output Log
- Plots are downloadable



Software

Rappture

- **R**apid **App**lication Infrastruc**ture**
- Can be used with C, C++, Fortran, MATLAB, Octave, Perl, Python, and Tcl.
- Creates graphical user interface (GUI)
- Two files:
  - XML tool description
  - Launcher file

NEMO5

- **N**ano**E**lectronics **MO**deling Tools
- Klimeck research group at Purdue
- Two input files:
  - Input deck
  - Material database file

Parts of a Simulation: Rappture

tool.xml

- Extensible markup language
- Input/output description
- Lists characteristics of each parameter

```
- <number id="ChannelLength">
  - <about>
      <label>Channel Length</label>
      <description>Channel Length is considered to be the
        total distance in between the Source and Drain
        regions (Channel Length = 2*(S/D Extension
        Length) + Gate Lengh).</description>
      <color>green</color>
    </about>
    <units>nm</units>
    <min>1nm</min>
    <max>100nm</max>
    <default>17.0nm</default>
  </number>
- <number id="ChannelWidth">
  - <about>
      <label>Channel Width/Thickness</label>
      <color>green</color>
```

Launcher file

- User chooses language
- Three parts
  - Inputs from GUI
  - Algorithm
  - Results back to GUI

```
// Get the current paths (equivalent to UNIX pwd)
    char input_dir[1000];
    char *cwd=getcwd(NULL,0);
    sprintf(input_dir,"%s",cwd);

    char output_dir[1000];
    sprintf(output_dir,".");

    printf("Input directory: %s\n", input_dir);
    printf("Output directory: %s\n", output_dir);


/*##########################################
    READ INPUT FROM lib & STORE IN VARIABLES
##########################################*/
```

Parts of a Simulation: NEMO5

Input Deck

- Specifies material/device and simulation information
- Contains three sections
  - Structure, Solvers, Global

```
Structure
{
      Material
      {
            tag = channel

            name = Si
            crystal_structure = simplecubic
            regions = (2)
            Lattice:a_lattice = 0.300

            Bands:BandEdge:mstar_c_dos = 0.980
      }


      Material
      {
            tag = lead

            name = Si
```

Material Database

- Specifies material parameters
- File provided by NEMO5 developers

```
# Si from Si.mat substrate file


group Si {
        unit_cell = 0.27155;
        type      = "IV";
        group Lattice {
                variables    = "Tkel";
                a_lattice    = 0.54310;
                #a_lattice    = 0.543; #Mathieu
                epsilon_dc   = 11.9;
                c11          = 1.675;
                c12          = 0.650;
                c44          = 0.801;
                c_elastic    = cp_3to1(c11,c12,c44);
                bdp          = -2.1;
                ddp          = -4.8;

                element      = Si;
                Si_mass      = 28.0855;
                Si_mass_ref  = "NIST periodic table";

                #strain_alpha      = 48.5;
                #strain_beta       = 13.8;
                #strain_ref        = "Martin, PRB 1 (1970)";
```

Working with Inputs

- Used same tool.xml
- Launcher file
  - Completed reading inputs from GUI

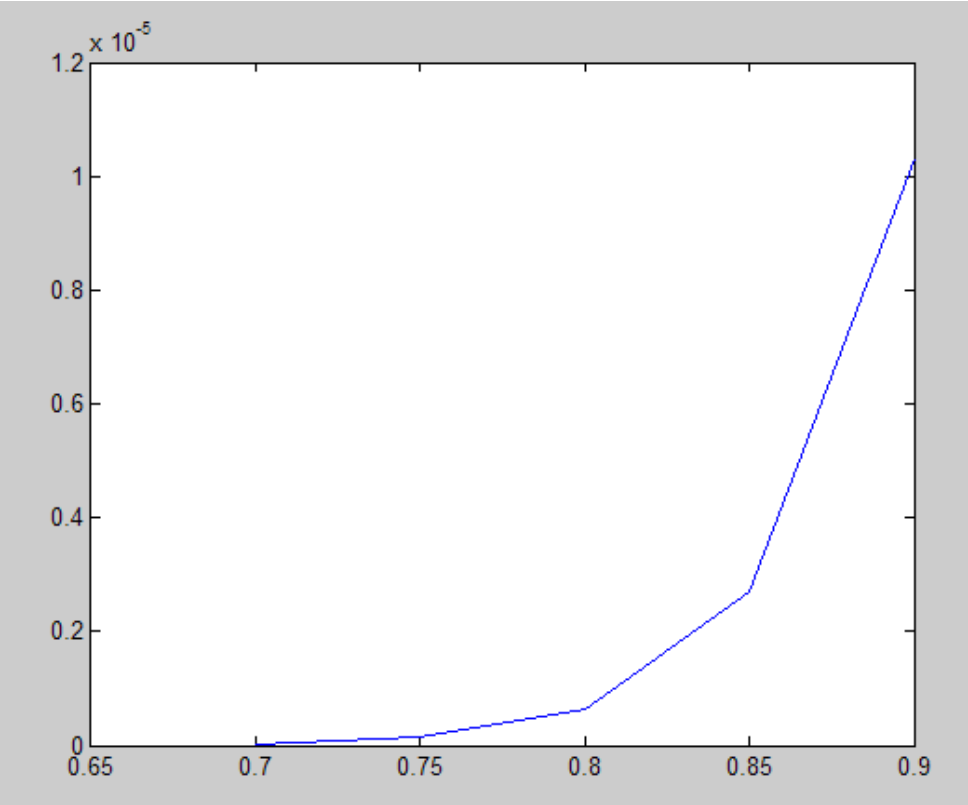
```
//Phase: Device Settings, Group: Dimensions
    rpGetString(lib,"input.phase(DevPhase).group(param).number(Ly).current", &data);
      Ly = rpConvertDbl(data, "nm", &err);
      if (err) {printf("Error while retrieving Simulation Domain Length."); exit(1);}
```

  - Working on printing input deck
  - Working with developers
  - Currently, 50% of inputs completed

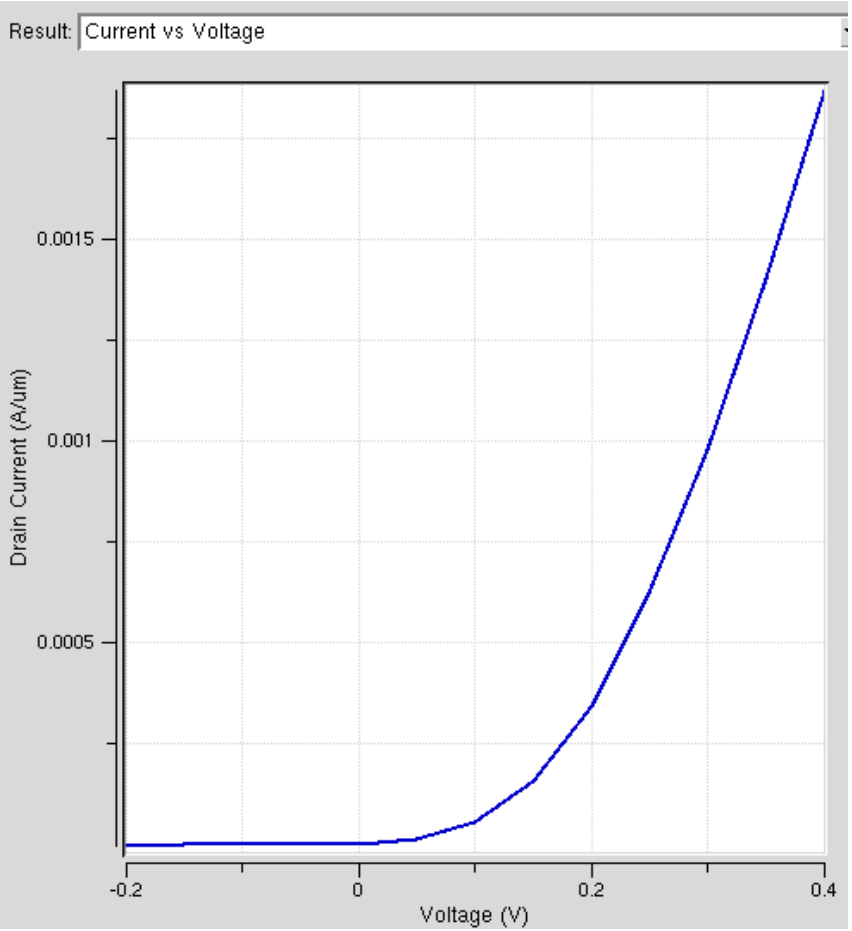
```
    //STRUCTURE

    //Structure/Material/Channel
    fprintf(fpindeck,"Structure\n{\n\tMaterial\n\t{");
    fprintf(fpindeck,"\n\t\ttag = channel\n\n\t\tname = Si\n\t
\tcrystal_structure = simplecubic\n\t\tregions = (2)"); //sections that
won't change (tag, name, crystal structure, and regions)
    fprintf(fpindeck,"\n\t\tLattice:a_lattice = %.3f\n\t}",GridSizeY);
//lattice
```

Current Status

Current Output



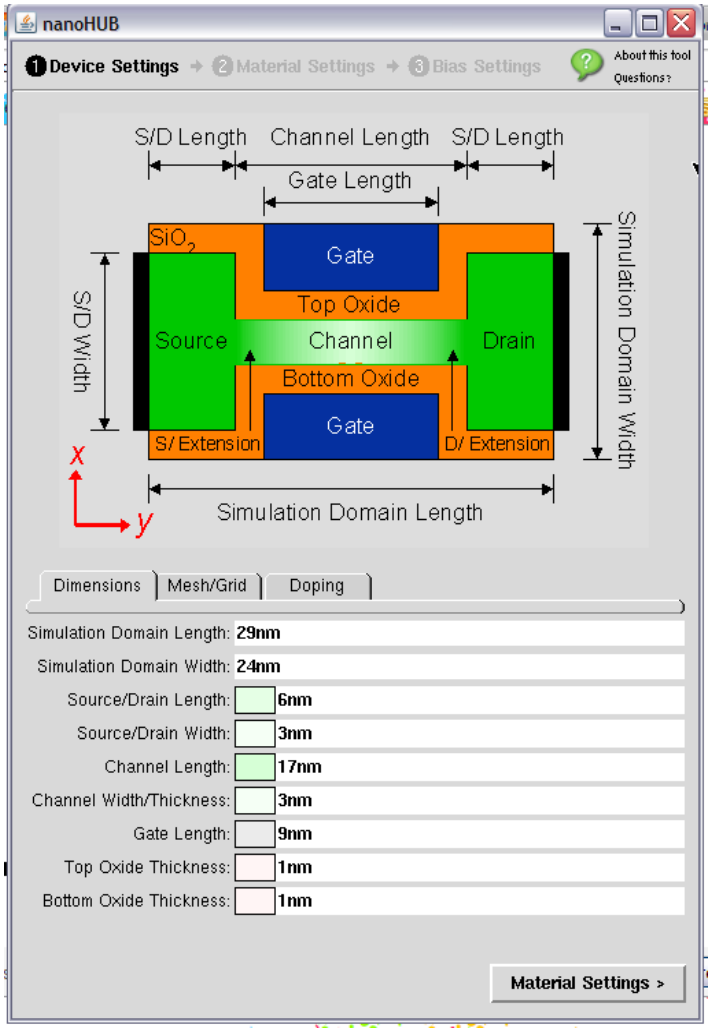
Desired Output



Kelsey Holley

Future Work

- To finish tool
  - Incorporate or remove remaining inputs
  - Run NEMO5 simulation
  - Resulting data must be read back into the launcher file
  - Graphs created and sent to GUI
- Testing of tool
- Create user guide
- Launch on nanoHUB



Questions?