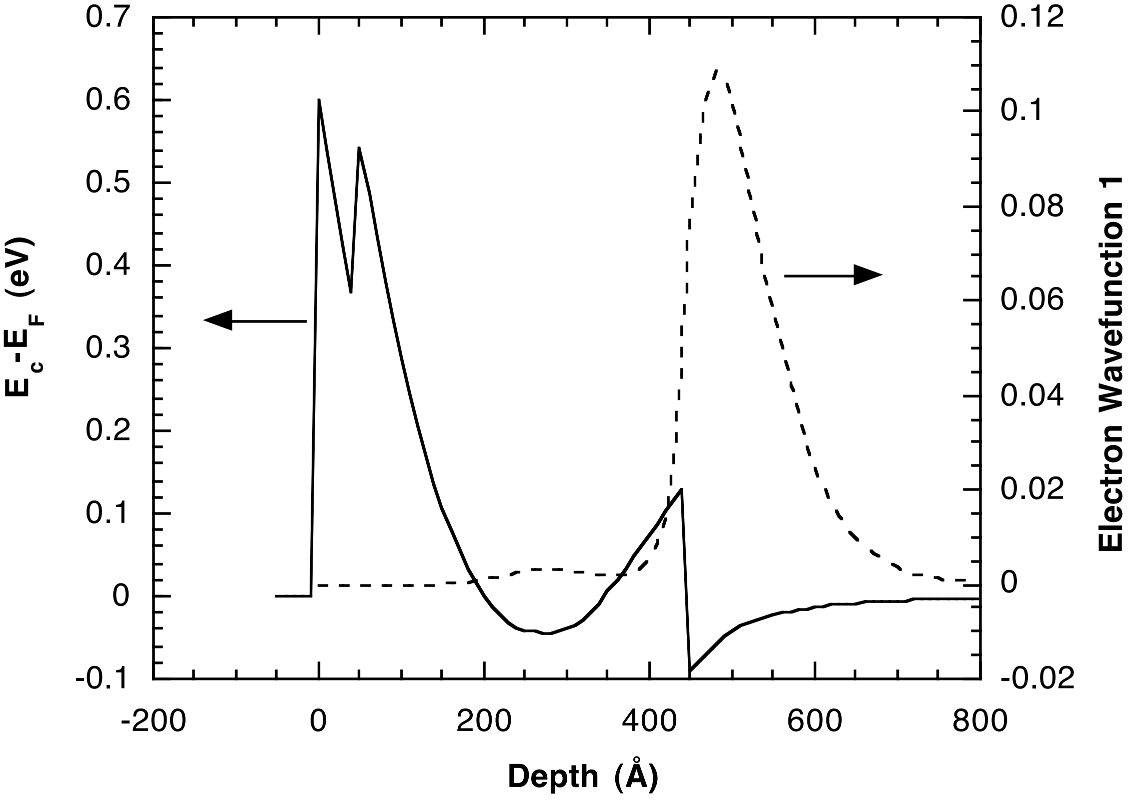
# 1D Poisson/Schrödinger
# User's Manual

## A Band Diagram Calculator



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## General Information

This manual is hugely out of date. My apologies! The basic operation of the program is the same as described here, but the menu driven interface is not there. Everything else should work as described in the manual.

This program uses the method of finite differences to find the one-dimensional band diagram of a semiconductor structure. It can automatically calculate the band diagrams for multiple bias voltages, and can also determine C-V characteristics. It was written with III-V compound semiconductors in mind, but should be general enough to work with other material systems as well. The program is menu driven through a pseudo-Mac interface but the user must provide separate text editing and plotting programs (a shareware text editing program is included in the 1D Poisson distribution).

A nice feature of the program is that semiconductors are called out by name, and the program automatically retrieves the physical parameters, and will even calculate the parameters for a ternary based on a given x value. Semiconductors within the materials file are organized into families so that parameters such as band offsets are defined within a family, and do not interfere with definitions in other families. The mobile charge concentrations are calculated using Boltzmann statistics, with the addition of the Unger approximation for mild degeneracy and the Sommerfeld approximation for deep degeneracy, and dopant ionization is also considered. If requested the mobile charge can be calculated from a solution of Schrödinger's equation. The program calculates the conduction and valence bands, and the hole and electron concentrations. Dopant ionization is included for both shallow and deep level dopants. This allows materials such as semi-insulating GaAs to be treated, and some of the effects of DX centers can also be simulated. Current flow is not calculated, so the structure can be simulated only in thermal equilibrium. In the current version of the program, three possible boundary conditions can be defined for the surface and substrate, Schottky barrier, ohmic contact, and energy band slope=0. If a Schottky barrier is used the program can simulate the effect of an applied bias which does not cause significant current flow. For example, a GaAs/AlGaAs MODFET could be simulated in reverse bias and in forward bias for vg<0.6V. (A rather kludgy way of simulating structures under bias can be done with this program by assigning different Fermi levels to layers in the biased structure, but this is only valid where the current flow is small enough to be ignored, as in a reversed biased p-n diode.) If an ohmic contact boundary condition is specified, the applied bias must match the Fermi level in the adjacent layer. The slope=0 boundary condition is used when only a certain region of interest is to be simulated. For instance, in an n-N heterojunction, the interesting effects occur close to the junction, so it is not necessary to simulate the whole wafer from surface to back surface.

There are versions of the program for Mac, PC and Linux. The 1D Poisson solver does not have any nice text editing or graphing capabilities, so you will also need a text program, and a graphing program such as KaleidaGraph.

### Getting Started

The input to the 1D Poisson program is a text file which contains the information necessary to simulate the structure. This file is created using a text editing program, and several example files are included with the distribution of 1D Poisson. It is strongly suggested that you copy one of the examples as a template for your own file. Input files should have the extension .txt.

An example file is shown below:

```
# test comment
surface  schottky=0.6   v1
GaAs     t=150    Nd=1e18
AlGaAs   t=200    Nd=1e18     x=.3
AlGaAs   t=50     x=.3
GaAs     t=150
AlGaAs   t=500    x=.3
AlGaAs   t=2500   x=.3  dy=50 Na=1e17
substrate

fullyionized
#v1 0.0 -1.0 -0.5
v1 0.0
schrodingerstart=50
schrodingerstop=2000
implant  donor  dose=2e12  Rp=860  drp=440
implant  acceptor  dose=1e11  Rp=.075um  drp=20nm
temp=300K
dy=10
```

The first thing to notice is that comments are indicated by a # in the first column, and can be placed anywhere in the file. Blank lines are ignored. The layer information is input between the delimiters 'surface' and 'substrate', with each line corresponding to a layer. The layers are listed starting at the surface and proceeding to the substrate.

The boundary conditions used for the simulation are defined on the surface and substrate delimiter lines. The possible boundary conditions are: schottky, ohmic, and slope=0. If a Schottky barrier is defined at the surface or substrate, the barrier height must be specified by including it on the specification line, as shown above. With a Schottky barrier, you also have the option of specifying an applied bias. To do this you include a voltage source number on the line as shown. In this case the source is "v1" but it could be anything from "v1" to "v10". You will specify the value of v1 later. If you have defined both the surface and substrate as Schottky barriers, you can attach bias voltages to both and bias them separately. The other two boundary conditions are not so flexible. The ohmic specifier sets the value of $E_c$-$E_f$ at the boundary to the value necessary for charge neutrality at the boundary. The slope=0 specifier sets the slope of the bands equal to zero at the boundary. Please note that an arbitrary slope is not allowed, only a zero slope.

Now consider the lines specifying the layers. Each line consists of several fields of information separated by either spaces or tabs. The first field on each layer line must contain the name of the semiconductor making up that layer. This name is used to search the file "materials" to find the default physical parameters for that layer. The parameters retrieved are: Energy gap, band offset, relative dielectric constant, donor and acceptor levels, deep donor and deep acceptor levels, electron, light and heavy hole effective masses, donor, deep donor, acceptor, and deep acceptor concentrations, and the polarization. *The values retrieved are only defaults; any of the values can be overridden by information on the rest of the line*. The remaining fields on the input line can be in any order, and have the following form: keyword=number. Notice that there are no spaces by the equals sign. The information contained in these fields completes the specification of the layer, and can be used to override the data read from the materials file. A list of the possible keywords is given in Appendix 1.

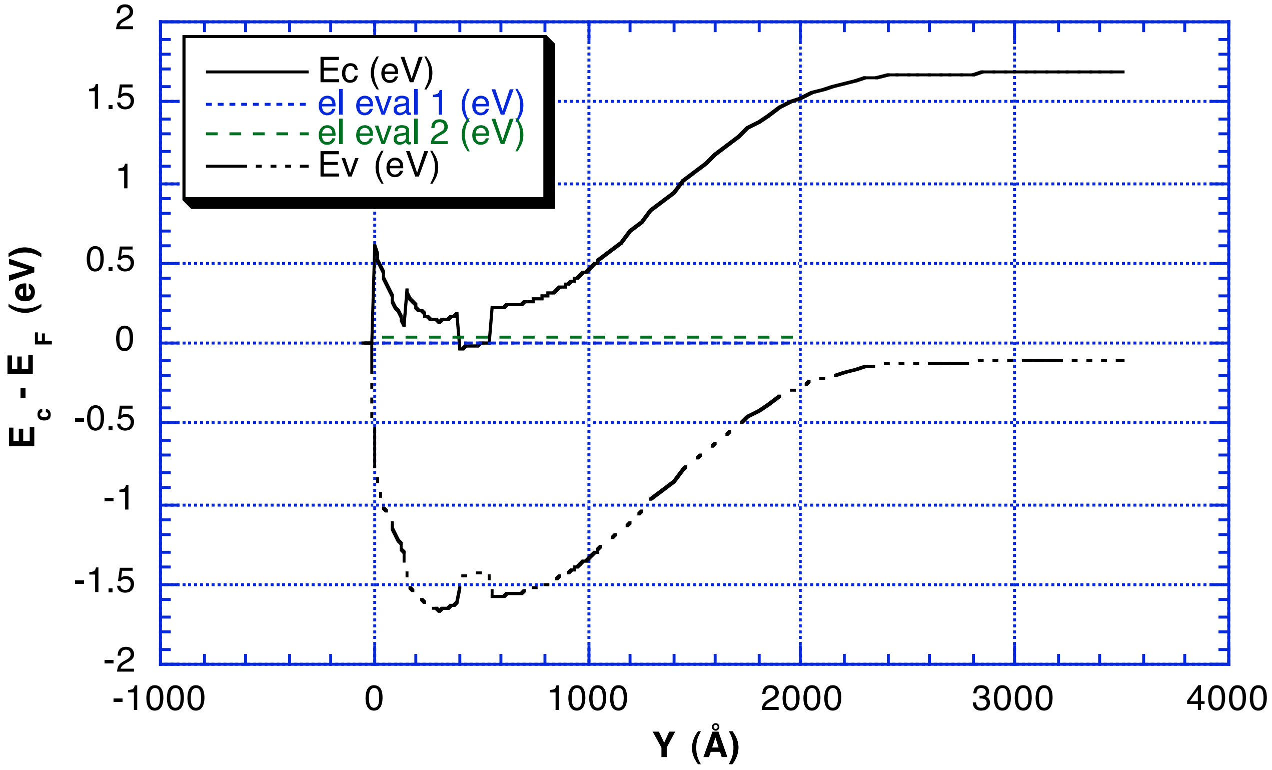
The remainder of the input file, after the layer specifications, contains information defining the simulation. This is the place were things like the temperature, bias voltage and other important parameters are defined. Here there is only one keyword per line, and a complete list of possible keywords is found in Appendix 2.

## Running the Simulation

When you have completed your input file, you are ready to run your simulation. Sorry, but the program runs with text menus, where information will be printed on the screen rather than in dialog boxes.

To start the 1D Poisson solver, simply double click on the application's icon. When the program has started, several text menu items will be printed. All operations are based upon an input file, so the first thing to do is to choose an input file using one of the first two menu items. If you are confident that your input file is correct, choose 'Select and Run Input File' by typing a 1, and you will then be asked to type your input file name, and the program then runs a simulation based on that file. If you are less secure in the accuracy of your input file, choose '**Select Input File**' which merely selects the input file. If you try to do anything before choosing an input file, you will be asked, nicely of course, to choose an input file. The next menu item, '**What is the Current Input File?**' will produce a printout of the layers of the current input file, which allows you to verify that the program read your file correctly. As you might expect, the next menu item '**Run**

**Poisson'** starts the simulation. The program goes off and happily, merrily performs the needed calculations. When the error falls below $10^{-5}$ eV (or the user selected value), the calculations terminate. If the calculation fails to converge in 100 iterations (or the user selected value), it gives up. If you want to abort the calculations, type "command .". When the calculations are completed, the program creates two or more data files. If your input file was called "input", the files normally created are named "input_out", and "input_status". If you called for a Schrödinger solution, a third file call "input_wave" is created. The _out file contains the conduction band, valence band, electric field, electron and hole concentrations, the fixed charge due to dopants, and if a Schrödinger solution was done, the quantized state energies. This file is set up to be read directly into KaleidaGraph, which is used to plot the results. The plotted band diagram of the example file is shown below:



The _wave file contains the wavefunctions of the quantized states that were found. The _status file contains additional information about simulation run, the sheet concentration of carriers in each layer, and if a Schrödinger solution was performed, the energies of the quantized states. A typical file is shown below:

```
number of iterations to converge =  13
Final correction to bands =  0.595E-05eV
maximum error in poisson equation= -0.436E-04
```

```
Don't worry, be happy! The convergence is good!

Structure Sheet Resistance = 1.053E+03 Ohms/square

 layer sheet concentrations

 surface           schottky
 ----------------------------------------------------------------------
     150Å             gaas  ns= 4.129E+05 cm-2   ps= 1.095E-02 cm-2
 ----------------------------------------------------------------------
     200Å   algaas x=0.300  ns= 2.323E+09 cm-2   ps= 0.000E+00 cm-2
 ----------------------------------------------------------------------
      50Å   algaas x=0.300  ns= 9.239E+09 cm-2   ps= 0.000E+00 cm-2
 ----------------------------------------------------------------------
     150Å             gaas  ns= 6.359E+11 cm-2   ps= 0.000E+00 cm-2
 ----------------------------------------------------------------------
     500Å   algaas x=0.300  ns= 1.040E+10 cm-2   ps= 0.000E+00 cm-2
 ----------------------------------------------------------------------
    2500Å   algaas x=0.300  ns= 1.258E-14 cm-2   ps= 1.085E+12 cm-2
 ----------------------------------------------------------------------
 substrate         slope=0

Temperature = 300.0K
Schrodinger solution from 5.000E+01 Å to 1.950E+03 Å

 The following subband energies were found (E-Ef):

electron eigenvalue  1 =   -1.282950E-03 eV
electron eigenvalue  2 =   44.022609E-03 eV
electron eigenvalue  3 =  117.781349E-03 eV
electron eigenvalue  4 =  157.097727E-03 eV
electron eigenvalue  5 =  192.958638E-03 eV
```

The first lines give information concerning the simulation. The important one to notice is the maximum error in the poisson equation. If this number rises above $10^7$, the simulation is not accurate. It is left to the user as an exercise to find the units of this number. An error above $10^7$ usually implies that the substrate boundary condition is not satisfied properly. The substrate layer must be thick enough to ensure the bands do indeed have a slope of zero. If you requested multiple bias voltages, a separate set of files is generated for each voltage. To distinguish these files, the voltage value is added to the file name, just before the _out, _wave, and _status. If you asked for a C-V run (see appendix 2) a file _CV is created which contains the C-V data.

The fifth menu item is '**Find Quantized States**'. This will find all of the quantized hole and electron states, whether they are occupied or not. This routine uses the results of the Poisson solution, so that simulation must be run first. If a Schrödinger solution was called for in the input file, you will be asked if the range is still OK. If a Schrödinger solution was not called for, you will be asked to provide the start and stop points. Again you are limited to 500 mesh points. The program then needs to know the energy range to search for quantized states (both hole and electron). The defaults range is from the lowest point of the band in the Schrödinger range to the highest point. You will be asked if the defaults are OK, or if you want to define the search range. The program then calculates the quantized states and generates a set of output files as described above. These output files will be named "input_states_out", etc. These files will contain all the quantized states, not just the occupied ones.

The sixth item is '**Materials Menu**', wich will be discussed below, and the final is '**Quit**'. When you are ready to exit the program, either choose '**Quit**'.

If you do simulations where you want self-consistent solutions of both Poisson's and Schrödinger's equations, sooner or later you will get the dreaded "Danger Will Robinson" message. For those of you not of my generation (sigh, time passes so quickly), not brought up the United States, or not a fan of horrible movie remakes, this message is inspired by a rather bad 1960's science fiction TV show called Lost in Space. There is a robot in the show assigned to protect a kid, Will Robinson. When evil comes near, the robot starts shouting, lights a flashin' and arms a flailin', "Danger Will Robinson, DANGER!!". In this program the message means that your structure does not provide enough confinement to ensure that the carrier wavefunctions correspond to a bound state. This is necessary because in converting from the wavefunction and subband energy to the carrier concentration, the program assumes that the wavefunction is 0 at the boundaries of the Schrödinger mesh. With this assumption it is possible to use the two-dimensional density of states to calculate the number of carriers in each subband. If the wavefunction is not zero, then there is a probably of the carriers being outside the Schrödinger mesh, the carrier concentration calculated is incorrect. The program posts the "Danger Will Robinson" error message if the band edge is less than 10 kT above the Fermi Level. Once an error occurs, the program allows you a couple of options. First you can have the simulation stop when the error occurs by using the "stop on Will Robinson" flag in the input file (see appendix 2). The other option (the default), is to let the program find all the bound states, and then calculate the carrier concentration from carriers in unbound states of higher energy. Your last option is to just ignore the error message by setting the "ignore Will Robinson" flag.

A final word on the bane of all numerical analysis: convergence. This program's convergence characteristics are very good, with the exception of simulations involving dopant ionization at temperatures below 50K. This applies to both shallow and deep levels. These simulations take many iterations to converge, and sometimes will not converge in the default 100 iterations. You can try increasing the number of iterations, but this is at best a painful solution. Often, the convergence error will be in the 1e-4 range after 100 iterations, which may be good enough. If the program fails to converge, the fullyionized flag can be set, which takes care of the problem for shallow levels. If deep levels are causing the problem, you can remove the deep level traps by setting

Ndd=0.0 and Nda=0.0.

Now to the Materials Menu. The Materials menu allows you access to the contents of the materials file. The first menu item is '**List Materials**'. This lists the names of all of the materials contained in the file. The third menu item is '**List Physical Parameters**'. If you select this item, you will be asked for a material name, and the physical parameters will then be listed. If you want the parameters for a ternary, you must supply the x value. For instance: "AlGaAs x=.3". If you want to add or change material parameter information you must edit the materials file directly. It's a pain, and details are given in another file given in the distribution file. But never fear, once the information is in the material file, you can retrieve all of it by simply calling out the material's name.

One final caution: This program simply finds a solution to Poisson's and Schrödinger's equations based on the input file you give it. It is all just mathematics, so beware! It's up to you to check that the answer you get makes physical sense. If the boundary conditions of either the Poisson or Schrödinger mesh are not correct, you will get a wrong answer. So be sure to include a sufficiently thick layer at a slope=0 boundary that the slope of the bands in the physical structure is indeed zero. If not, the program will calculate an answer that is mathematically correct but physically incorrect.

This concludes the user manual for this program. Any suggestions or comments concerning this program would be greatly appreciated. Send these to:

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**References:**

I hope to one day rewrite the manual to include more detail on what formulas are used in the caclulations, but for now I can point you to a couple of papers my collaborators and I have published, which lead to the 1D Poisson program. Hopefully these papers answer the basic questions.

1. G.L. Snider, I.-H. Tan, and E.L. Hu, "Electron states in mesa-etched one-dimensional quantum well wires", *J. of Applied Physics*, Vol. **68**, pp. 2849, 15 September 1990.
2. I.-H. Tan, G.L. Snider, and E.L. Hu, "A self-consistent solution of Schrödinger-Poisson equations using a nonuniform mesh", *J. of Applied Physics*, Vol. **68**, pp. 4071, 15 October 1990.

## Appendix 1. Keywords for layer specifications

"t=" The layer thickness. The thickness must be specified for each layer. The default unit is angstroms, but nm, um, and mm can be specified. For instance t=500, t=50nm, t=0.05um, and t=5e-5mm are equivalent.

"Nd=" Donor concentration in cm-3

“Na=” Acceptor concentration in cm-3

"Ndd=" Deep donor concentration in cm-3

"Nda=" Deep acceptor concentration in cm-3

"er=" Relative dielectric concentration.

"Eg=" Energy gap in eV.

"deltaEc=" Band offset in eV (Base material in each family is defined 0).

"Ed=" Donor ionization energy in eV.

"Ea=" Acceptor ionization energy in eV.

"Edd=" Deep donor ionization energy in eV.

"Eda=" Deep acceptor ionization energy in eV.

"me=" Electron effective mass ($m^*/m_o$).

"mhh=" Heavy hole effective mass($m^*/m_o$).

"mlh=" Light hole effective mass($m^*/m_o$).

"valley=" Number of conduction band valleys.

"dy=" Mesh spacing for this layer.

"Ef=" Fermi level for this layer. This is the rather feeble attempt to allow simulations of biased structures. If you want to simulate a structure where one (or more) layers are biased with respect to some other layers, you can specify the Fermi level in each layer using the Ef keyword. If Ef is not specified for a layer the Fermi level is set to zero. Please notice that the argument to Ef is in electron volts, so if you have an ohmic contact with a bias of 1V, you must set the Fermi level Ef=-1.0. You can also grade the Fermi level in a layer by specifying the Fermi level at the top and bottom of the layer. For example, if you want to grade the Fermi level from 1eV to 2eV, use the form "Ef=1.0,2.0".

"no electrons", "no holes", "electrons", "holes" The program's default is to calculate hole and electron concentrations for the entire structure. In some cases this leads to artifacts in the data, such as the buildup of holes at the surface of an n-type Schottky barrier when there is a large reverse bias. The "no holes" and "no electrons" flags here set the hole or electron concentration to zero for that layer. As explained in Appendix 2, you can also set a default flag to ignore one (or both) type of carrier for the entire structure. In that case, you can re-enable the calculation of carriers for an individual layer using the "electrons" and "holes" flags.

"fullyionized", and "ionize" The program's default is to calculate ionization coeffiecients for both shallow and deep level dopants. As explained in Appendix 2, you can set a default "fullyionized" flag which tell the program to assume that all shallow dopants are fully ionized. The "ionize" keyword on a material definition line overrides this and calculates ionization coefficients for that layer. Conversely the "fullyionized" keyword overrides the ionization calculation for just that layer.

"x=" Ternary x value. If not specified for a ternary layer, the default is x=0. This value is used to calculate the physical parameters of the layer, based on the information stored in the materials file. Linear grading of a layer is implemented using the form: x=0.1-0.3 . This will grade the layer from x=0.1 to x=0.3 across the thickness of the layer. Note: in a graded layer, *each mesh point becomes a layer*, so it is easy to exceed the maximum of 500 layers. If that happens, increase dy for that layer.

“pol=” Polarization. This calculates the charge due to changes in polarization. The units of this parameter are Ccm$^{-2}$, and it is up to the user to define whether this includes the piezo component or not.

## Appendix 2. Keywords for Simulation Definition

"temp=" This specifies the temperature to be used in the simulation. In the number following the "=" a K indicates Kelvin, a C indicates degrees Celsius, and the default is Kelvin. If you want to use Fahrenheit, you are out of luck! A temperature of 0K can be used without causing convergence problems.

"vX " This specifies the voltage of source number X, an integer between 1 and 10. "v1 2.0" will set voltage source 1 to 2 volts. As mentioned before, the surface and the substrate can be biased independently, but more possibilities are available for the surface voltage. The line "v1 0.0 -2.0 -.5" will run five simulations where the surface bias go from 0V to -2V in -.5V steps. Separate output files will be generated for each bias condition.

“CV Voltage”

"CV" and "CV only" These specifiers are used to calculate the capacitance of the structure at the gate voltage of the simulation. To use these functions, the surface boundary condition must be a Schottky barrier. An additional output file, "input.CV" is created which contains the gate voltage and the capacitance at that gate voltage. If the "CV" keyword is used in conjunction with multiple gate voltages, the CV file will contain the data for a CV plot (see the example file "MOS cap.ex"), and output files will be generated for each gate voltage. This is very useful if you want to fill all unused space on your hard disk. If you use the key phrase "CV only", full output files are generated only for the starting gate voltage, while the CV file will contain the capacitance at all the requested gate voltages. Caution must be exercised when running CV simulations. If the gate voltage is too large, carriers can accumulate at the surface of the structure. This accumulation is not real, it is just an artifact of the simulation. Unfortunately, working around this problem is a bit of a pain. All I can suggest, if you want a CV plot over a large voltage range, is to break-up the simulation into several simulations, each with a smaller voltage range, and set the Fermi level of the surface layer so that there is no surface accumulation in that voltage range.

"dy=" This specifies the default mesh spacing to be used. If a dy is specified for a layer, it will override this value. As always, there are trade-offs associated with the mesh spacing. The number of mesh points used in the simulation is determined by taking the total thickness of each layer as specified in the layer definitions, and dividing it by dy of that layer (The thickness of each layer is rounded to make it an integer multiple of dy). The maximum number of mesh points is 5000. This program works remarkably fast: a 5000 point simulation will typically take less than one minute, but the data file produced will take a long time to plot or otherwise manipulate (depending on your computer, of course!). So you want to keep dy as large as possible while keeping it small enough to accurately resolve thin layers. Keep in mind that you can change the dy for specific layer on the material specification line of the input file. The default unit for dy is angstroms, but um, nm, and mm can be specified. For example "dy=10", "dy=1nm", "dy=0.001um", and "dy=1e-6mm" are equivalent.

"fullyionized" This specifies that all the shallow dopants in the structure are ionized. The ionization of deep levels is always calculated.

"schrodingerstart=", and "schrodingerstop=" If you wish to solve Schrödinger's and Poisson's equations self-consistently in a region, you must specify the boundaries of the region, measured from the surface, using the schrodingerstart and schrodingerstop keywords. Schrödinger's equation is then solved in this region to find the hole or electron concentration. Both heavy hole and light holes are considered, but things like band mixing are not considered. Only one region of schrödinger solution is allowed, and boltzmann statistics is still used outside of the schrödinger region. The Schrödinger solver only finds bound subbands, so if the structure being simulated does not provide sufficient confinement, a warning will be issued. Both the start and the stop point must be specified. If only one is specified, it is ignored. A maximum of 500 mesh points is allowed in the Schrödinger region. You can change the dy within the Schrödinger region by specifying a different dy for layers within the region.

"Implant" You can specify up to 10 ion implants by simply stating the implant type (donor or acceptor), the dose of the implant (in $cm^{-2}$), the ion's projected range (Rp=) and the ion straggle (drp=). As with all spatial coordinates, you can define Rp and drp in Angstroms, nanometers, microns, or millimeters. The program takes these parameters and, using LSS theory, calculates the dopant distribution. Just like in real life, an implant adds dopants to any "grown in" dopants specified in the layer list. If more than one implant is specified, the dopants from each implant are just added, since the implants are on top of one another.

"no holes" and "no electrons" These tell the program to ignore (set =0) one carrier type or the other. This is useful to avoid artifacts in the simulation such as the build-up of holes at the surface of an n-type Schottky barrier with a large reverse bias. These flags set the defaults for the simulation, which can be overridden for individual layers.

"Convergence=XX" and "CVconvergence=XX", where XX is maximum allowed correction, in eV, to the band diagram for the converged structure. These flags allow you to override the convergence criteria for a normal simulation (default=1e-5 eV) or capacitance calculation (default =1e-10 eV).

"Maxiterations=" Allows you to specify the number of iterations allowed before the simulation terminates (default = 100).

"Stop on Will Robinson" This will cause the simulation to terminate if the "Danger Will Robinson" error message occurs. This error indicates that there is insufficient confinement at the edges of the Schrödinger mesh. If this flag is not used, the program will find any bound subbands, and then calculate the electron concentration based on these subbands and the 3D density of states for unconfined electrons.

"Ignore Will Robinson" This flag tells the program to ignore any Will Robinson errors. Usually not a good idea.

"asterix" Cricket Graph (that horrible program!) needs an asterix in the first column of the first line to tell it to read the next line as titles. If you want this asterix, include this flag, or buy a better plotting program. You'll be happier in the long run!

"no Cleanup" The program tries to clean up after itself by deleting old output files before running a simulation. There may be times when you don’t want this. For instance, if the simulation runs several gate voltages, and you wish to change the input file to run some additional gate voltages without deleting the first set. Include this flag to save the first set of output files.

"no status" The status file is a much neglected file that contains lots of good information that few people ever look at. If you don’t want the file, include this flag.