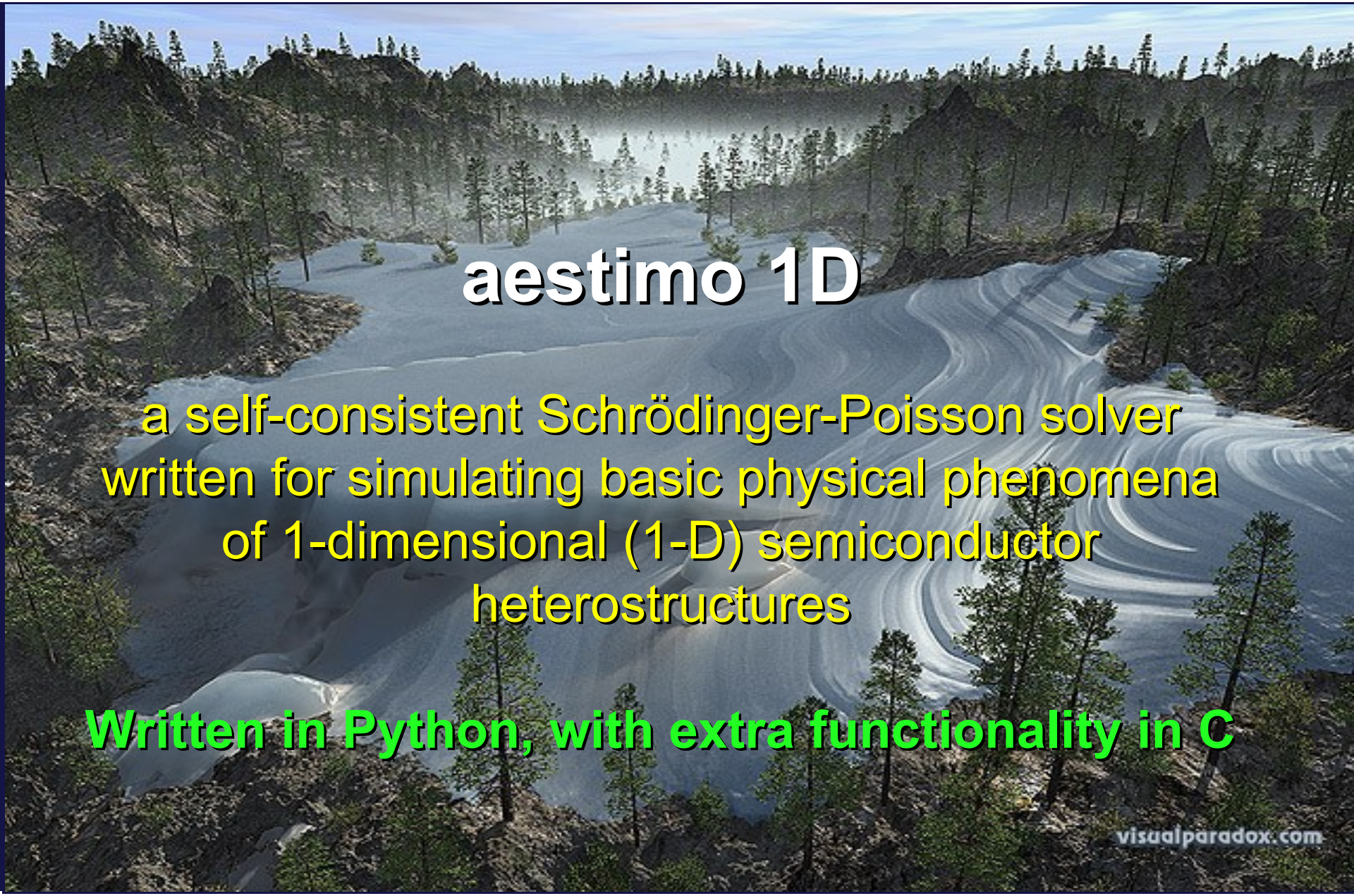


aestimo 1D

a self-consistent Schrödinger-Poisson solver written for simulating basic physical phenomena of 1-dimensional (1-D) semiconductor heterostructures

Written in Python, with extra functionality in C

= started as a hobby by Professor Sefer Bora Lisesivdin from Gazi University, Ankara, Turkey, at the beginning of 2012, and become a usable tool which can be used as a co-tool in an educational and scientific work.

= other developers, programmers, contributors:
* Hamza Hebal, University of Djilali Lyabes Sidi Bel Abes, Algeria
* Robert Steed
* Beyza Sarikavak-Lisesivdin
* Zbigniew Koziol (http://www.linkedin.com)

= The main site:

http://aestimo.ndct.org/doku.php

= A mailing list exists for developers and users

Current features

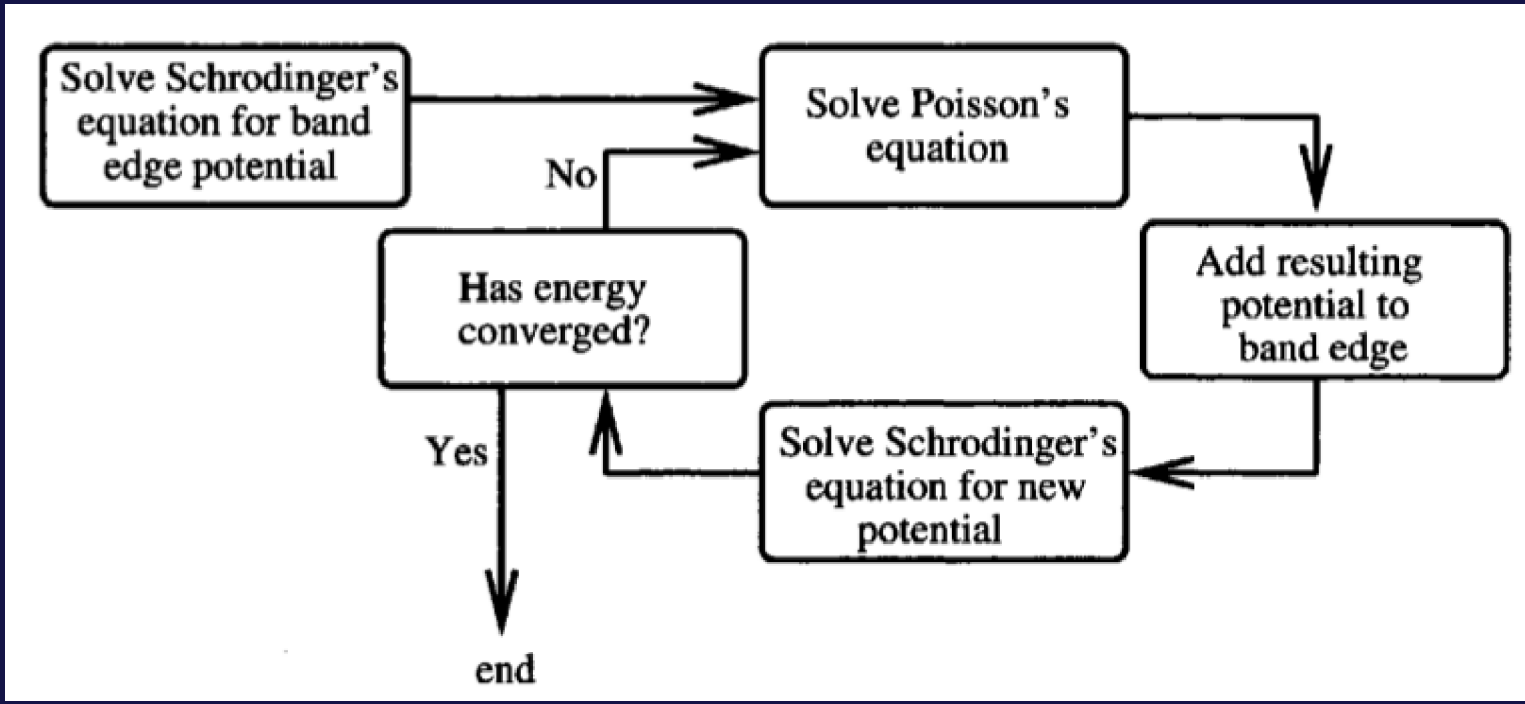
Material and alloys: GaAs, AlAs , InAs, InP, AlP, GaP, AlGaAs, InGaAs, InGaP and AlInP

Band structure for gamma electrons and heavy, light and split-off holes,

Effective-mass method for electrons and 3×3 k.p method for holes,

Carrier concentrations for gamma electrons and heavy, light and split-off holes, Exchange interaction

Electric field distribution, Electron wavefunctions, Non-parabolicity



Block diagram illustrating the process of self-consistent iteration (Figure 3.35 in Harrison; Paul Harrison, Quantum Wells, Wires and Dots. Theoretical and Computational Physics of Nanos-structures. Wiley-Interscience, 2005.

For solving Schrodinger equation, shooting method is used

.

Table 1: The computational schemes implemented

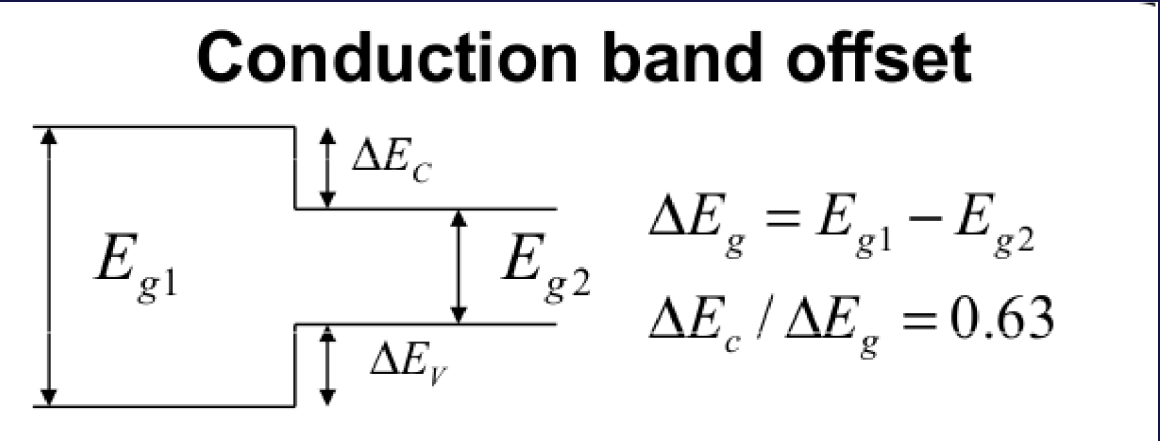
computation_scheme	Model
0	Schrödinger
1	Schrödinger + nonparabolicity
2	Schrödinger-Poisson
3	Schrödinger-Poisson with nonparabolicity
4	Schrödinger-Exchange interaction
5	Schrödinger-Poisson + Exchange interaction
6	Schrödinger-Poisson + Exchange interaction with nonparabolicity

The problem (?)

How to construct band alignement?

- band offset parameters to align energy gaps at heterostructure junction (nextnano for instance) or the concept of affinity energy (Synopsys, for instance)?

-In principle, both methods are available, though one only is officially implemented

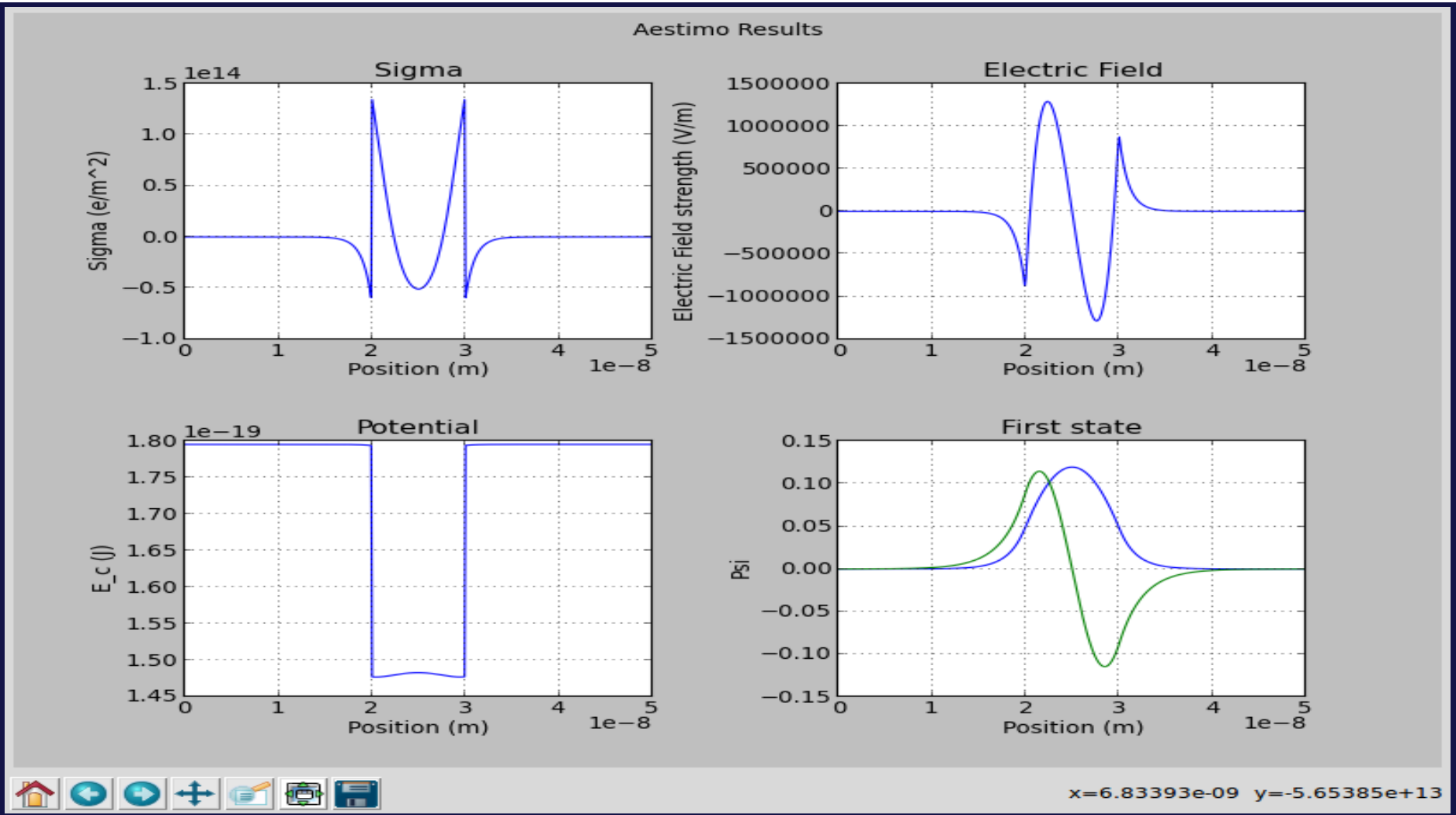


Example device structure definition

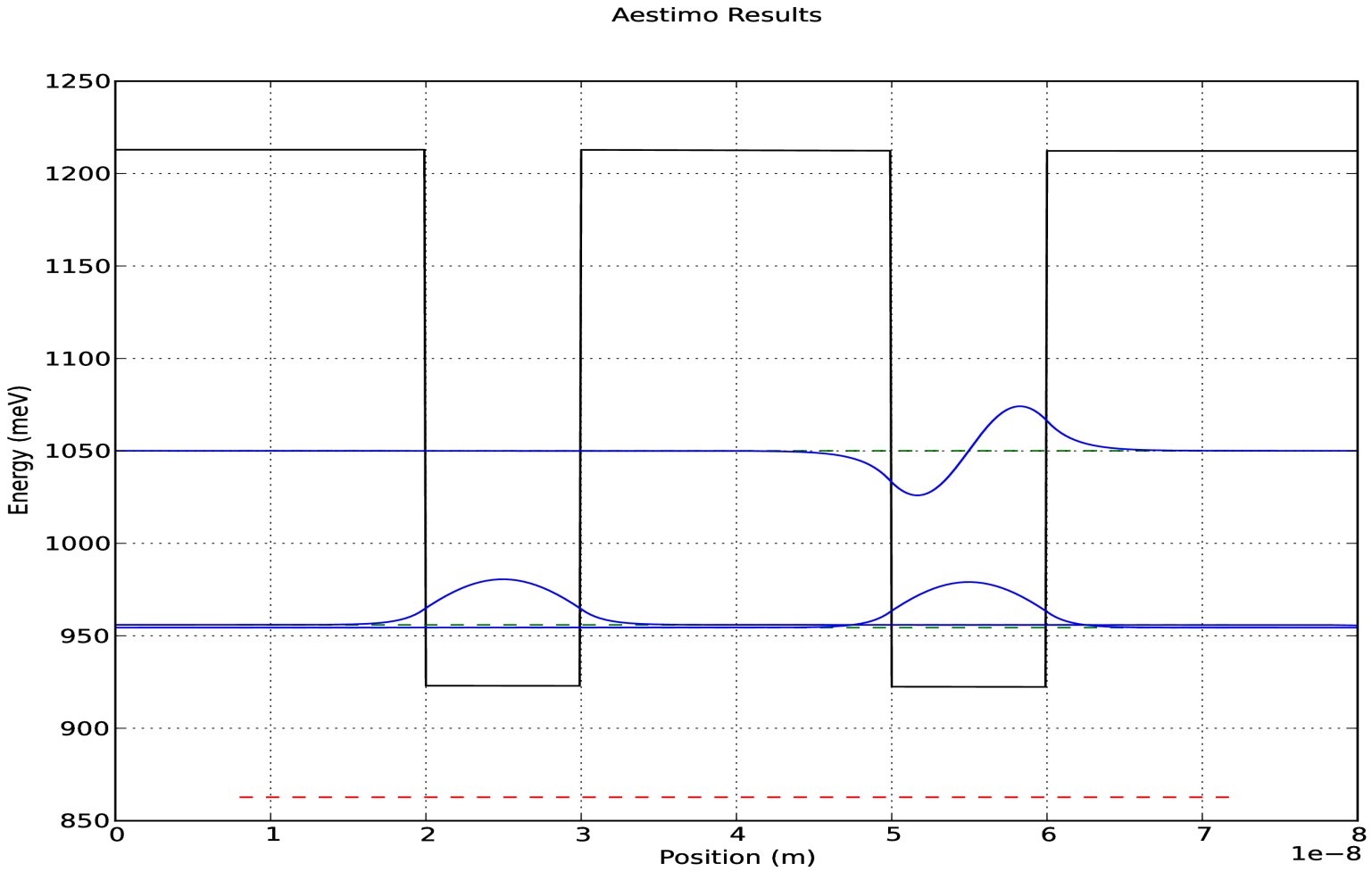
```
material =[[ 20.0, 'AlGaAs', 0.3, 0, 'n'],
           [10.0, 'GaAs', 0, 2e18, 'n'],
           [20.0, 'AlGaAs', 0.3, 0, 'n']]
```

The meaning of it is as follows. Our device consists of three regions (layers). The first region has the width 20 nm, second 10 nm and the third one 20 nm. The first and third regions are of AlGaAs while the second is GaAs. In case of AlGaAs, we assume Al concentration x = 0.3. Only the second region is dopped, with concentration of 2 · 10^18 cm−3 and doping type is n.

The grid (a descrite set of points on which computation is performed) is controled by parameter gridfactor, which sets the maximum value (in nm) of distance between grid points.



Results obtained by running sample-qw-qwdope.py input file, for a single quantum well, doped, of AlGaAs. Figures show charge distribution, electric field, final potential, and two first wave functions.



The first 2 localized wave functions (solid lines) and their corresponding energies (broken lines) for a simple 2-QWs structure obtained with sample-double-qw.py sample input file.

Advantages (some)

- Output datafiles are in plain ASCII (either can be processed by Python itself or tools like Gnuplot)

- One single, custumisable configuration file

- Easy to add new compunds, and modify their physical parameters (if known)

- It should be easy to add new features and physical models (the code itself is of a few tens of kB only)

- Available examples, mailing list for discussions

- Available preliminary User Guide / Tutorial (z. kozioł)

Disadvantages / missing features (some)

- It is in 1D only

- No transport included (neither drift-diffusion nor quantum tunneling),

- No magnetic field

- No strain/stress effects (but probably could be added)

- 3x3 k.p method for holes is known to be not accurate

- Not all possible heterostructerus/compounds can be modelled (type-I only)

- No temperature effects can be studied (unless a substantial work was done for changing code and adding new parameters to database)

- ...

It would be great to find some way of financing for continuing developing this project...

Thank you