Coupling Atomistic and Finite Element Approaches for the Simulation of Optoelectronic Devices

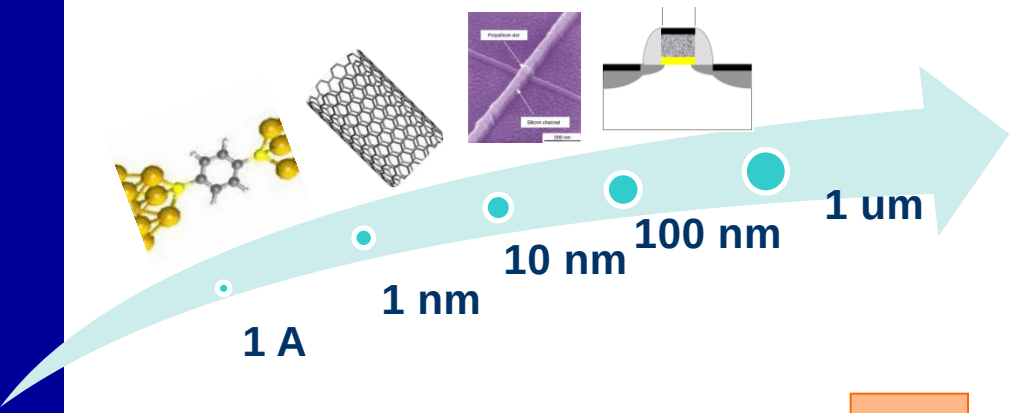
M. Auf der Maur, F. Sacconi, G. Penazzi,
M. Povolotskyi, G. Romano, A. Pecchia,
A. Gagliardi and Aldo Di Carlo

University of Rome "Tor Vergata", Italy
Department of Electronic Engineering

Outline

- Introduction
- The multiscale approach
- Coupling of FEM and atomistic simulations
- Example
- Conclusion

Introduction



Modern optoelectronic device industry pushes for reliable numerical models down to nanometer and sub-nanometer scale. A multiscale/multiphysics approach is needed for the interaction between small active and the larger embracing device regions.

TIBER CAD

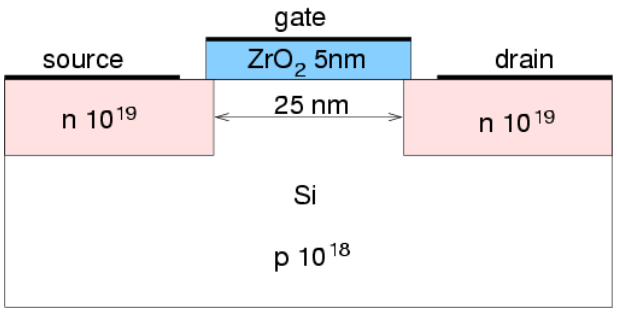
TiberCAD is a TCAD for optoelectronic devices, designed to provide a solution to these needs.

Features:

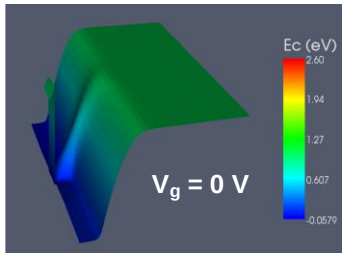
- FEM models: drift diffusion, strain, heating, Shroedinger EFA.
- Atomistic models: empirical tight binding, density functional tight binding.
- DSSC modelling.
- SCC calculations: thermal-drift diffusion, drift-diffusion-quantum charge.

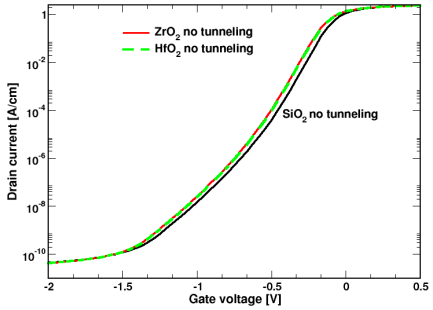
Simulation approaches (Classical)

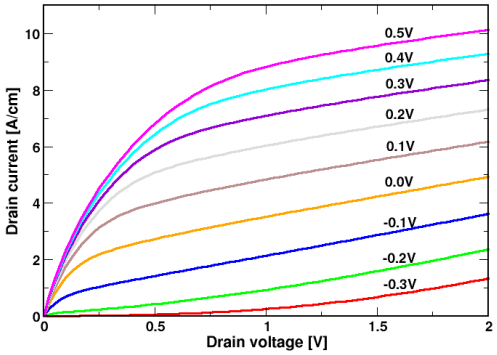
- Approach for 'big' conventional devices:

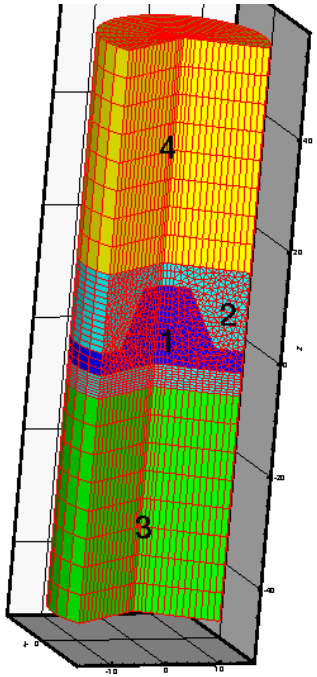


Classical Drift-Diffusion simulations

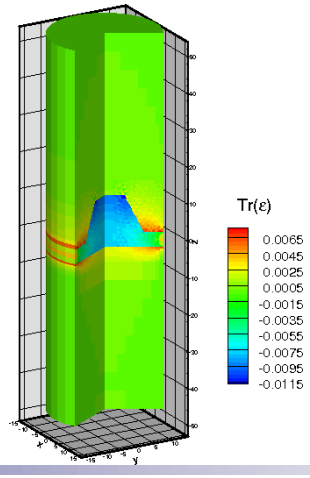


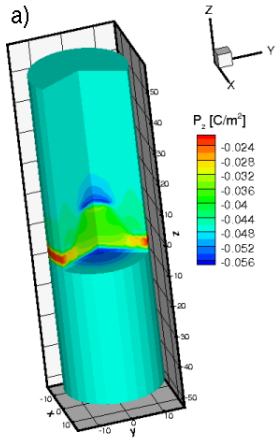


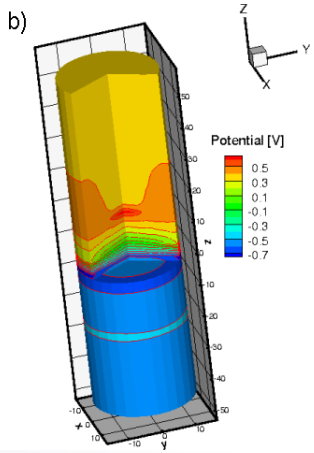




Elasticity theory
Drift-Diffusion

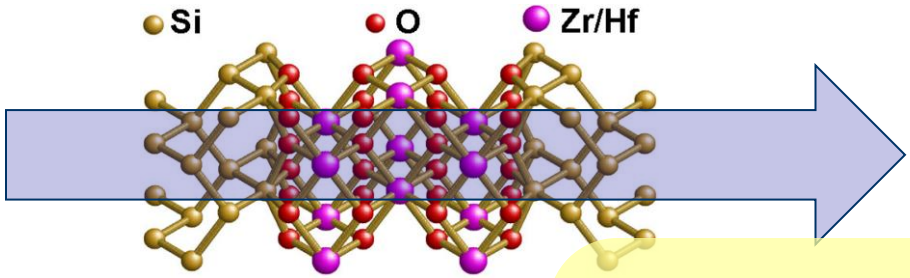




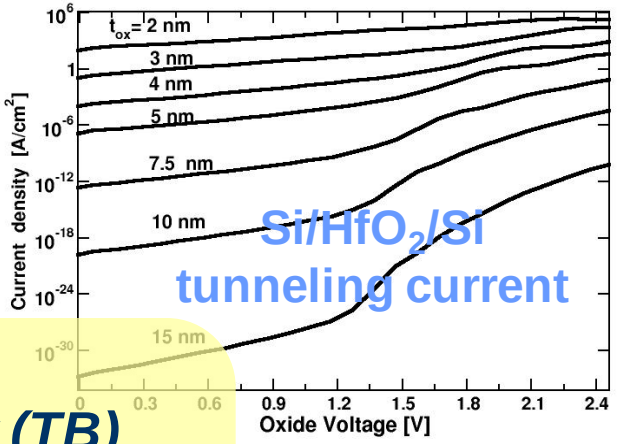


Simulation approaches (Atomistic)

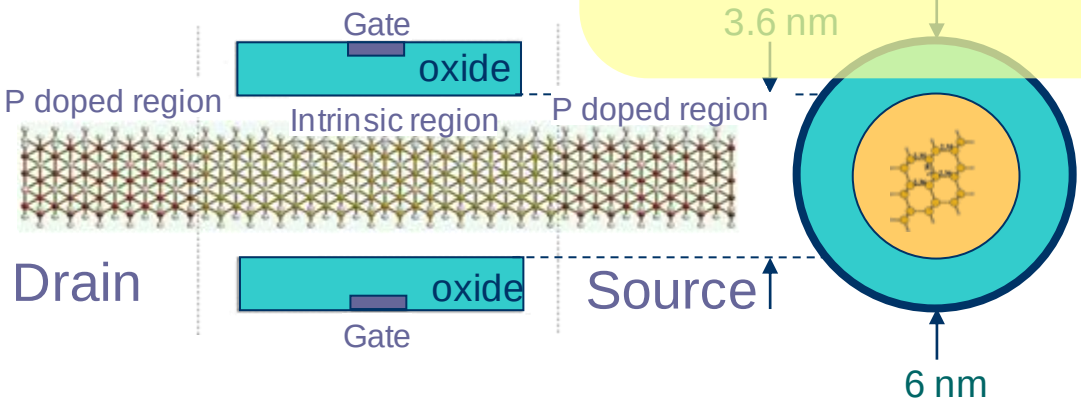
- Approach for nanometer scale devices:

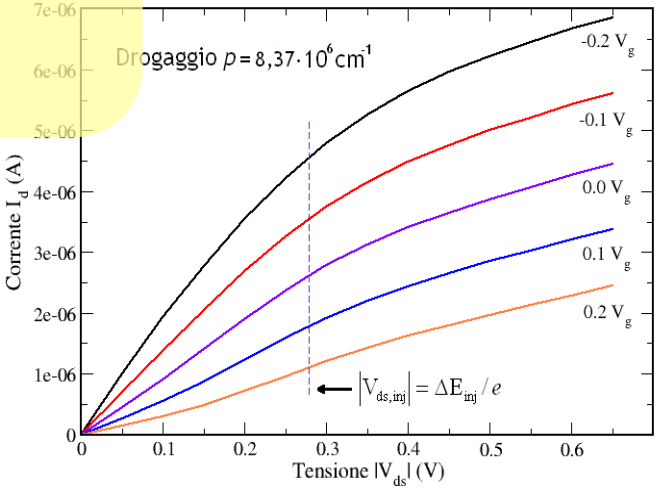


Sacconi et al IEEE TED 2004 and 2007



tight binding (TB)
transfer matrix method
DFT
NEGF





7.7 nm

Micro/macro scale

Many modern devices are based on nanostructures which need a quantum mechanical description, and we know how to do this.

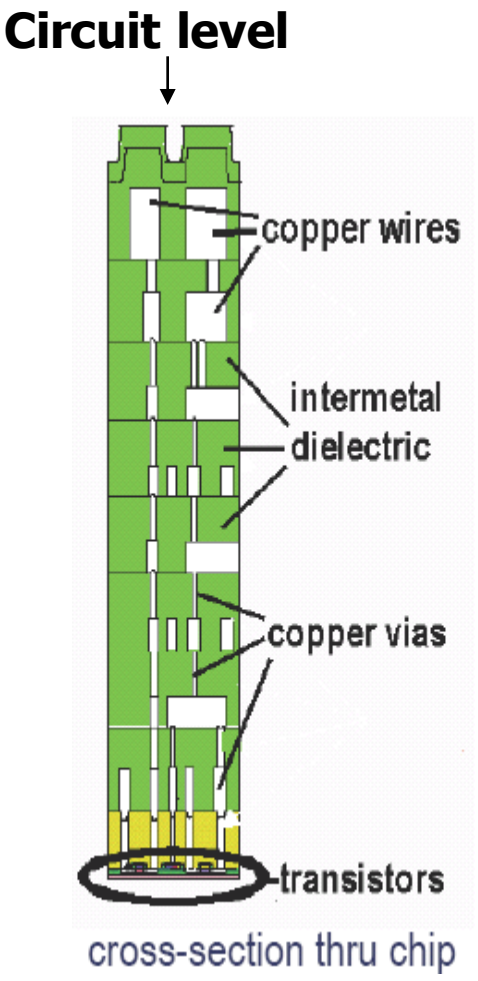
BUT:

In a real device also micro and macro scale should be considered!

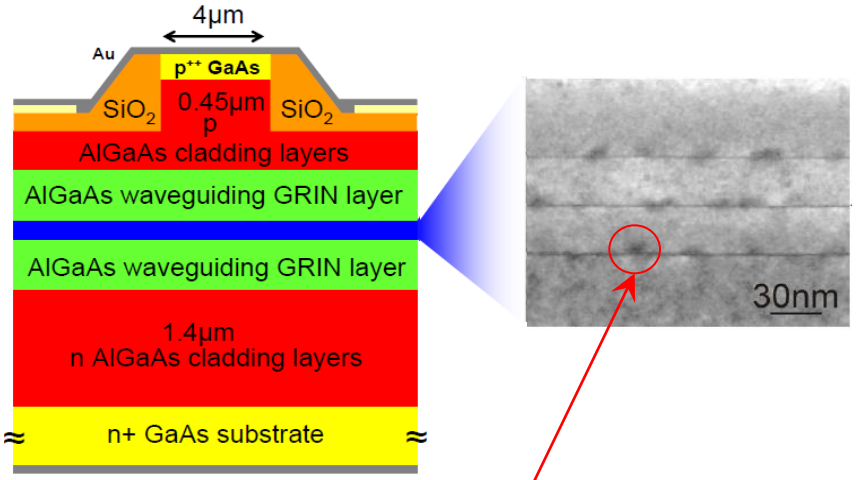
- ***Number of atoms cannot grow too much in simulations***
- ***Device should be accessible from a macro scale***
- ***micro/macro scale details are as important as nanoscale features (temperature distribution, electrostatics, strain, air gap, etc.)***
- ***20 years of experience with Drift-diffusion matters !***

Multiscale structures

Typical Pentium 4 MOSFET section:



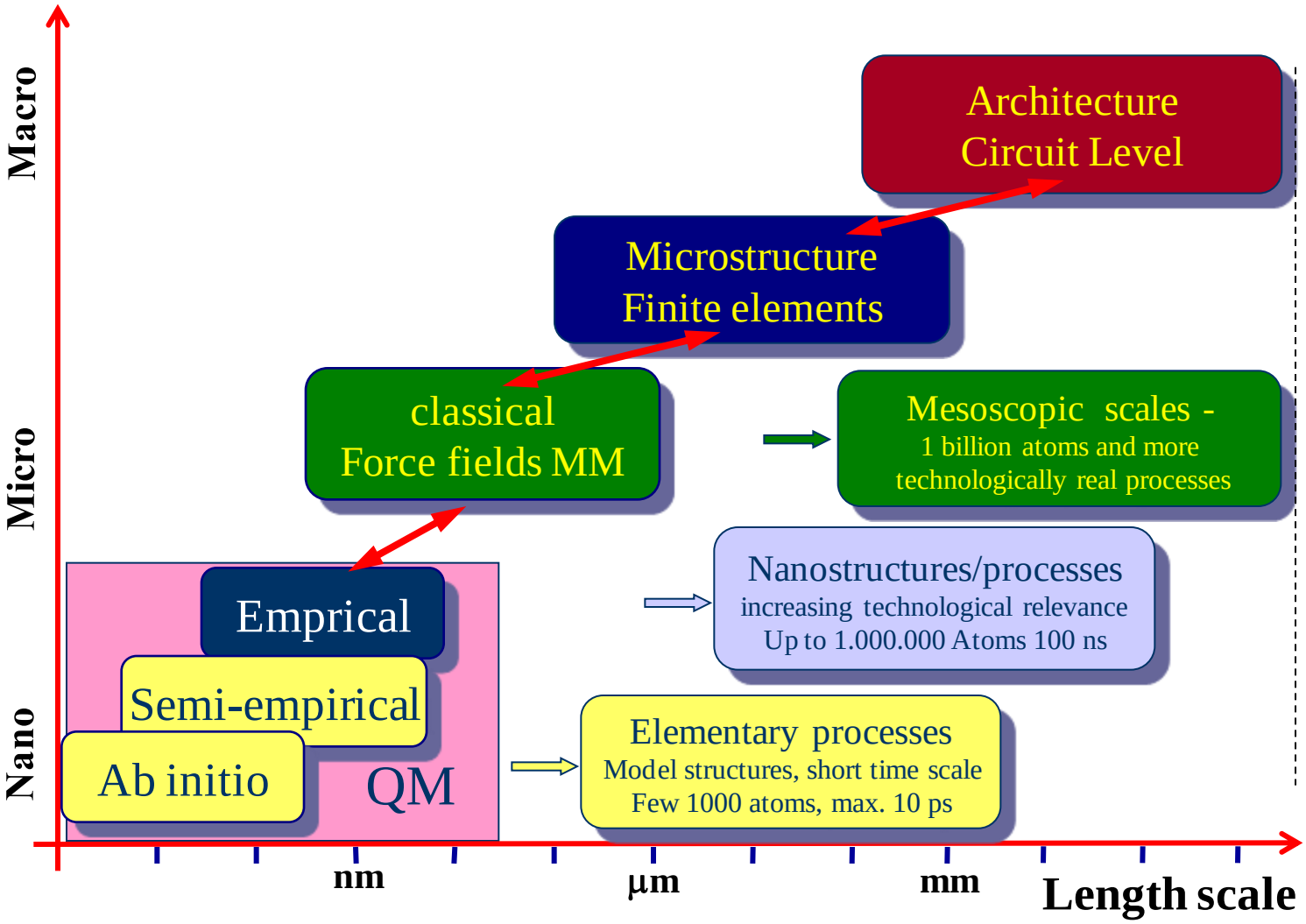
InAs quantum dot LASER:



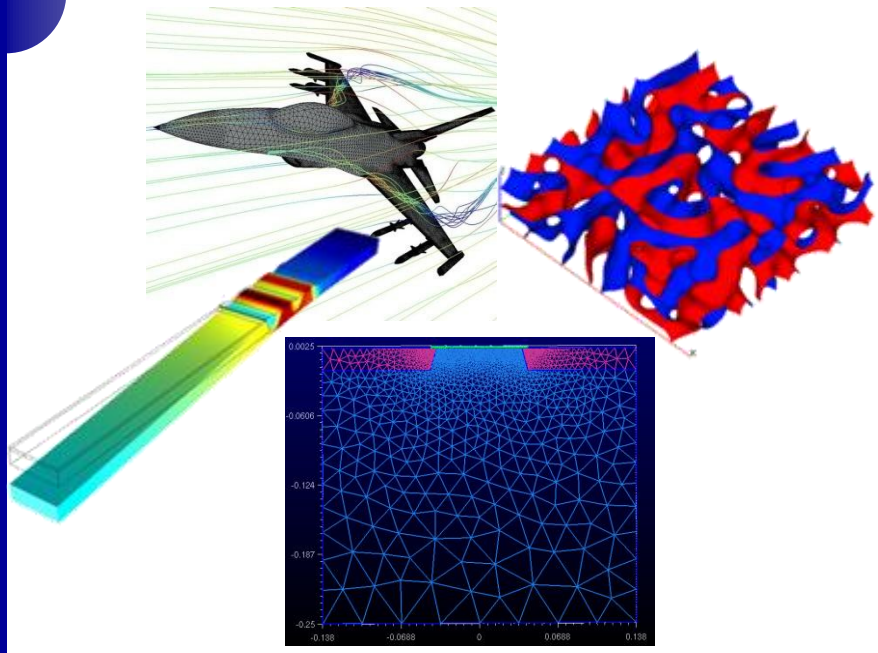
M. Buda et. al., IEEE Journal of Quantum Electronics, 2003

InAs Qdots on several layers embedded in a semiconductor heterostructure

The multiscale problem



Multiscale components



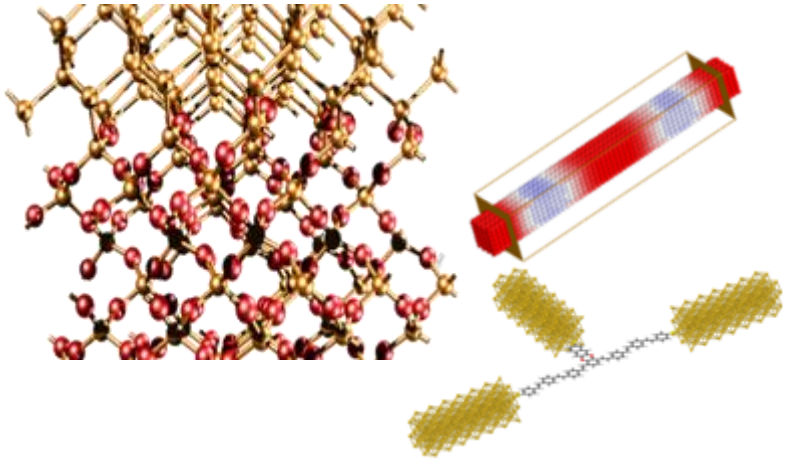
Finite Element Method

- FEM is the method in engineering problems (deformation/strain, heat, Maxwell, etc. etc.)

-Drift-diffusion (DD) like schemes have been solved with box integration methods.

- DD-FEM have been heavily developed in the last 20 years in the Math community (***Hecht, Marrocco, Brezzi, Sacco, Chen)***

- many FEM library in (L)GPL



Atomistic local basis

- Localized basis approach are very well suited for device simulations

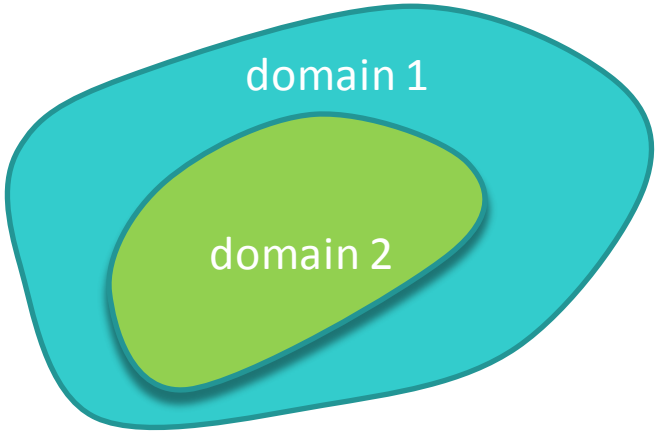
- Empirical approaches (ETB)

- Aproximate DFT (DFTB)

- Full DFT (Siesta, DMOL, etc.)

Multiscale methods

OVERLAP METHOD



- the domains are overlapped
- each model computes physical quantities that act as parameters to the other models.

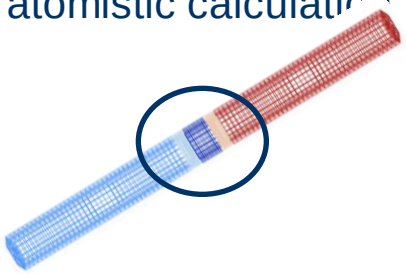
BRIDGE METHOD

- the domains are contiguous and linked through n-1 dimensional regions.
- each domain provides boundary conditions to adjacent domains.

Integration FEM/Atomistic

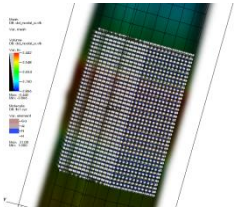
- FEM and atomistic calculations run in the same environment.
- Tools to automatize crystal atomistic structure description and project quantities between atomistic and continuum domain have been developed.

Design geometry and mesh and select region of interest for atomistic calculati



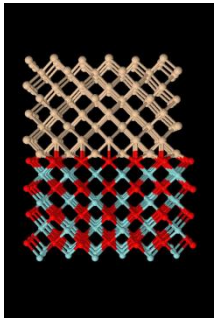
Atomistic structure is generated internally according to device materials

Continuum media and atomistic calculations information exchange within the same environment



Atomistic generator features:

- Manage most useful Bravais lattices (cubic, hexagonal, fcc, bcc)
- Provide any basis
- Manage pseudomorphic heterostructure and commensurable interfaces
- Provides hydrogen passivation model suitable for any crystal
- Generates minimal periodical structure for bulk, 1D and 2D calculations



FEM/Atomistic interaction

Strain:

calculate relative displacement u(x,y,z) and apply displacement to atoms, stretching bond lenght from d_0 to d.

Tight Binding parameters calculated according to Harrison scaling rule:

$$V_{\alpha\beta} = V_{\alpha\beta} \cdot \left(\frac{d_0}{d} \right)^{n_{\alpha\beta}}$$

Potential:

Use FEM potential solution to provide Hamiltonian shifts.

- If no SCC calculation is needed, slow varying potential is projected simply as point potential on atom position.
- If SCC is needed, a projection over an *s*-type orbital with exponential decay is used.

$$V_i = V(r_i)$$

$$V_i = \frac{\tau_i^3}{8\pi} \int V(r_i) e^{-\tau |r - r_i|} dr$$

Charge:

Quantum charge is projected back to FEM grid. An s-type projection with exponential decay is used.

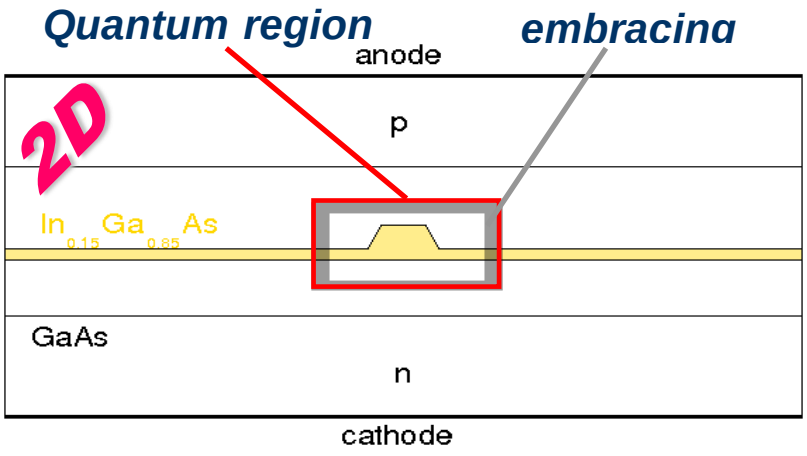
$$n(r) = \sum_i \frac{\tau_i^3}{8\pi} \int \Delta q_i e^{-\tau |r - r_i|} dr$$

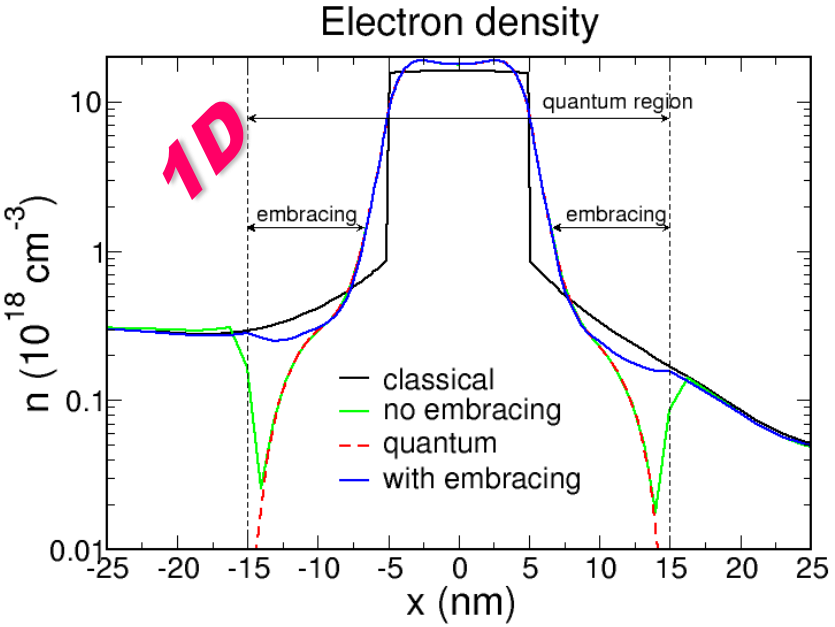
Classical/quantum densities: Embracing

For a smooth transition between classical and quantum density we introduce an automatically generated embracing region where the densities get mixed:

$$n(x) = \lambda(x) \cdot n_Q(x) + [1 - \lambda(x)] \cdot n_{cl}(x)$$

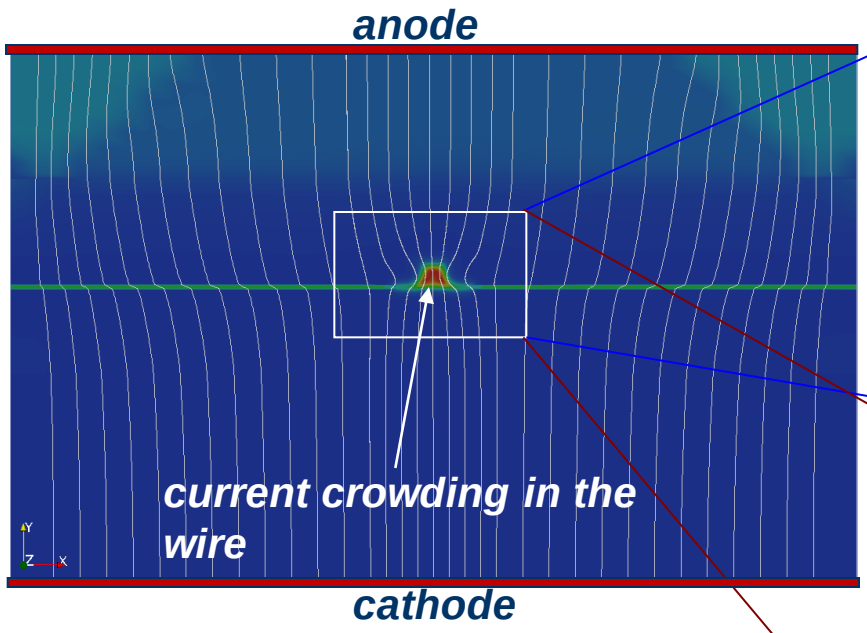
where λ(x) is the solution of a Laplace equation in the embracing region.

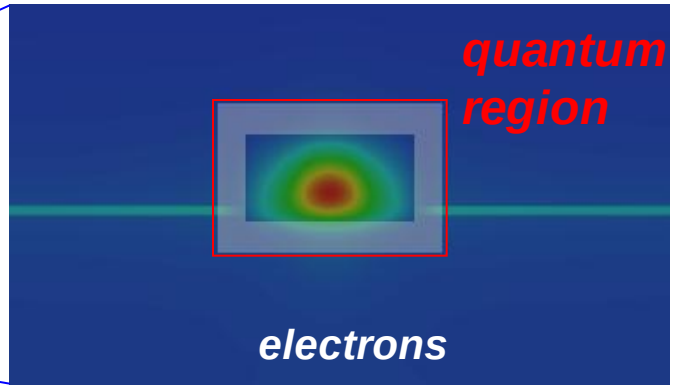


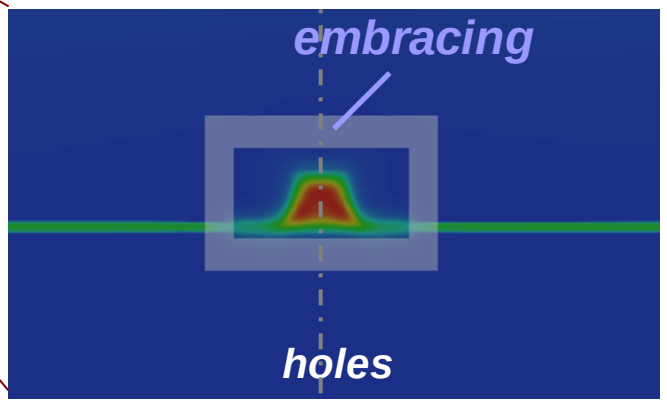


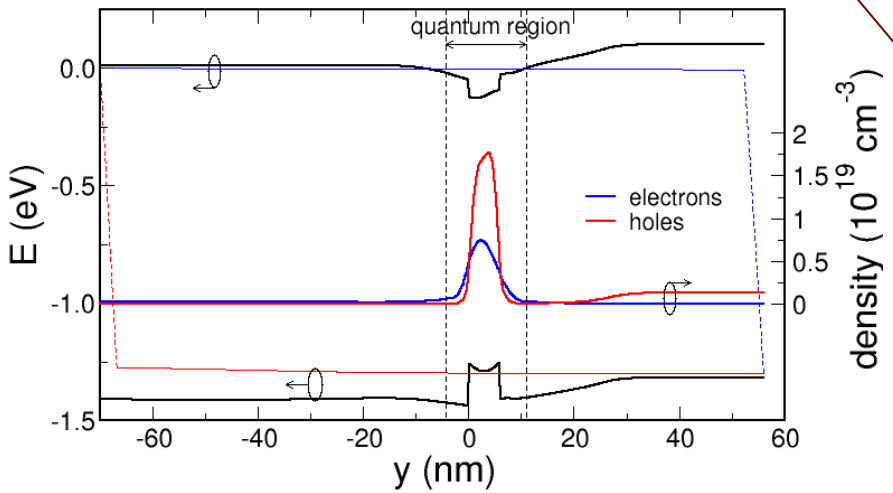
K.P quantum model

InGaAs Quantum wire







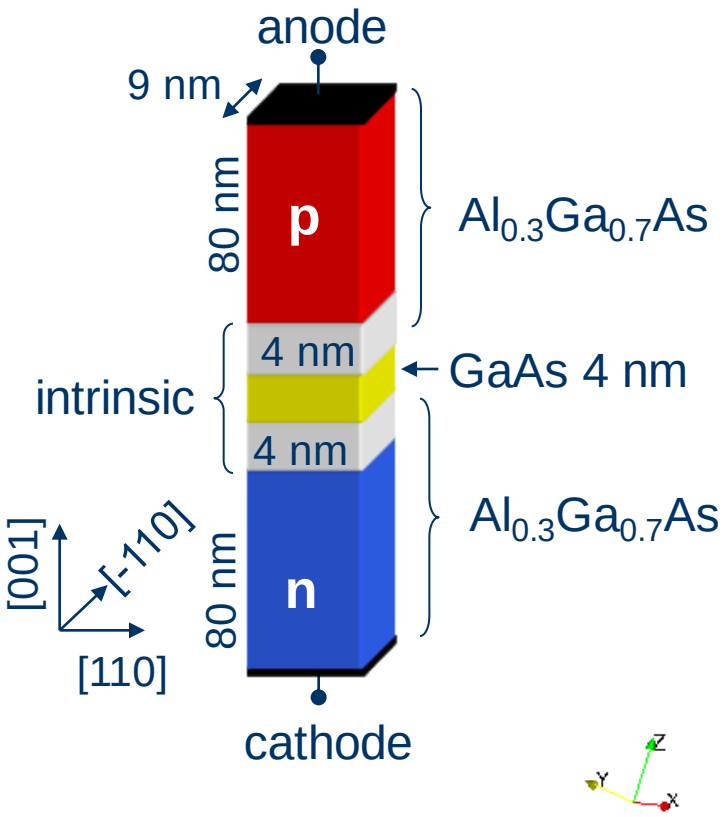


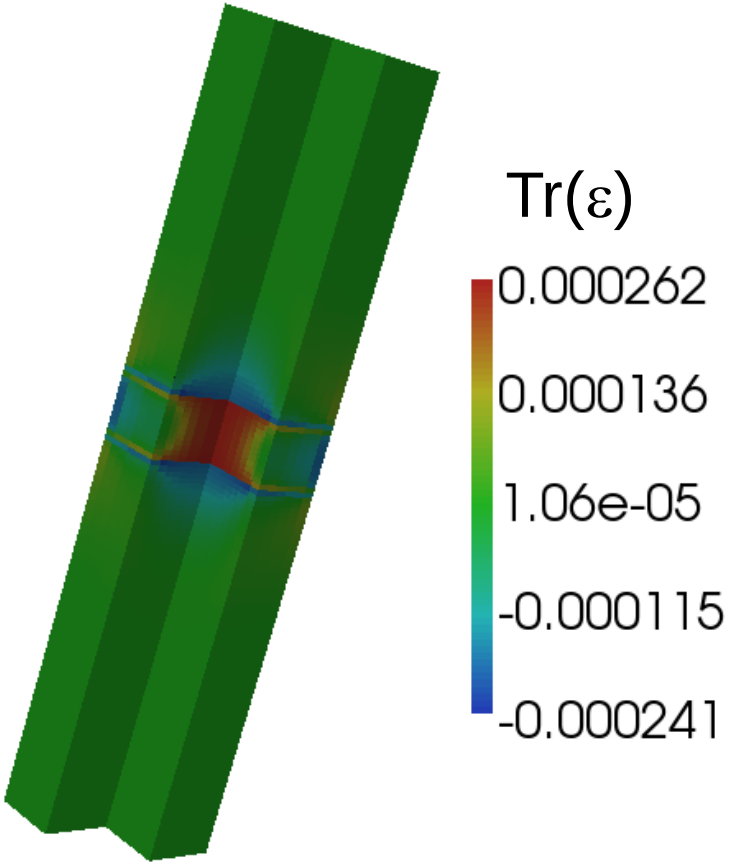
Selfconsistent densities at Vb = 1.3 V

K.P quantum model

AlGaAs/GaAs nanocolumn

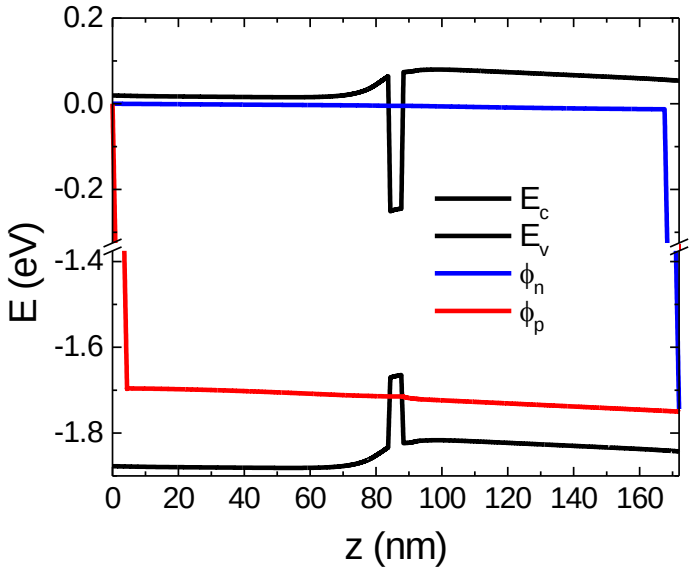
- AlGaAs/GaAs nanocolumn with quadratic base
  - solve strain, drift-diffusion, EFA, TB

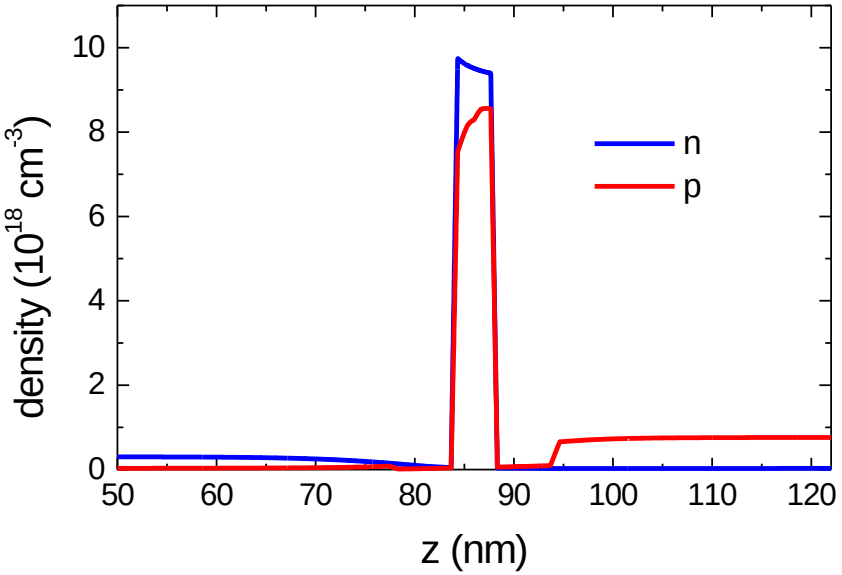




AlGaAs/GaAs nanocolumn

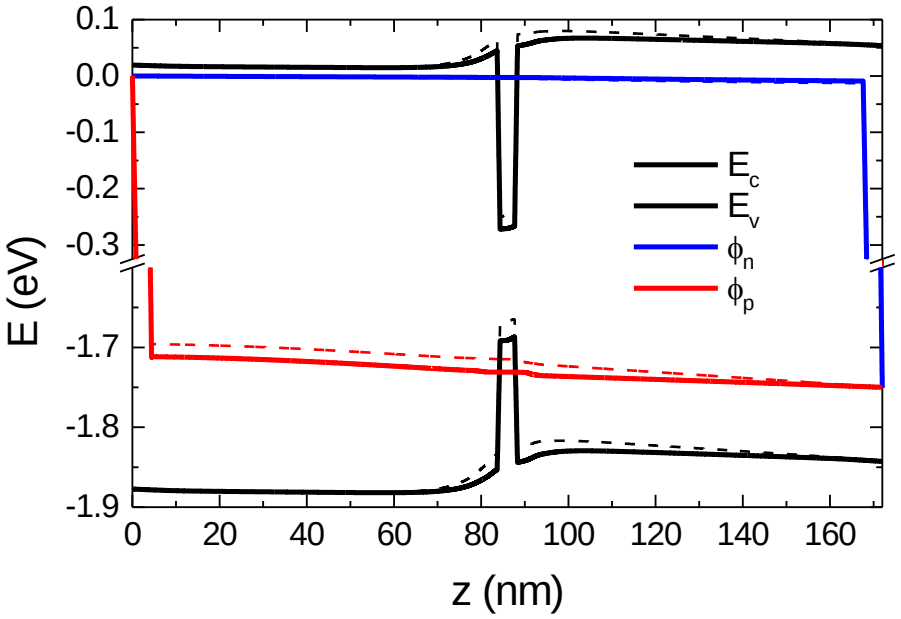
- classical results (1.75 V)

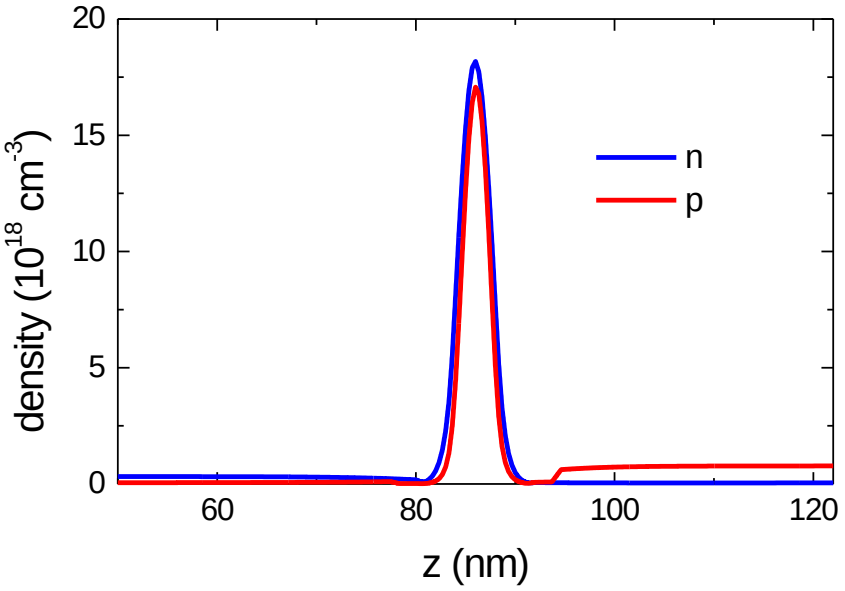


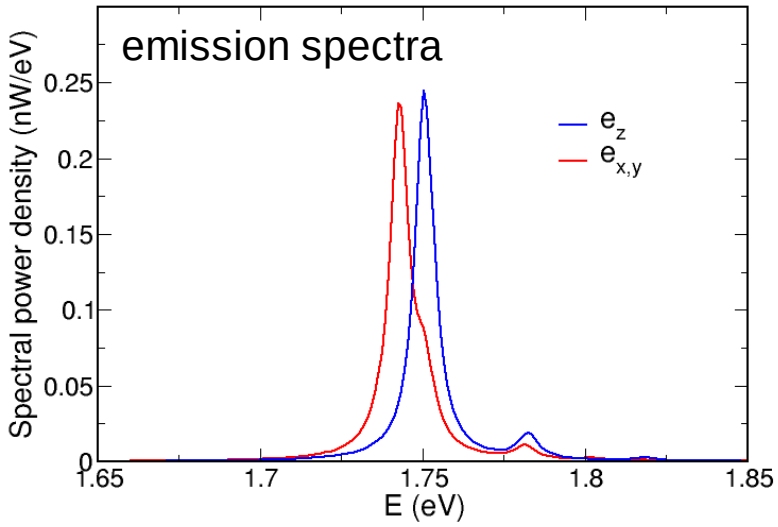


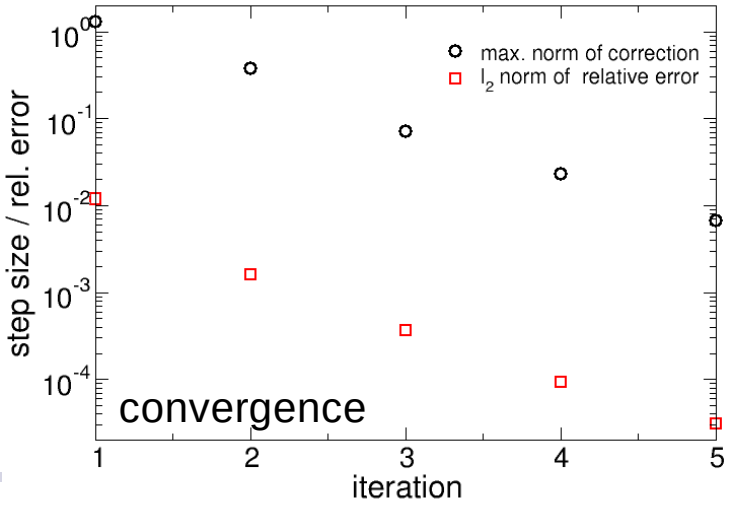
AlGaAs/GaAs nanocolumn

- selfconsistent results (EFA)



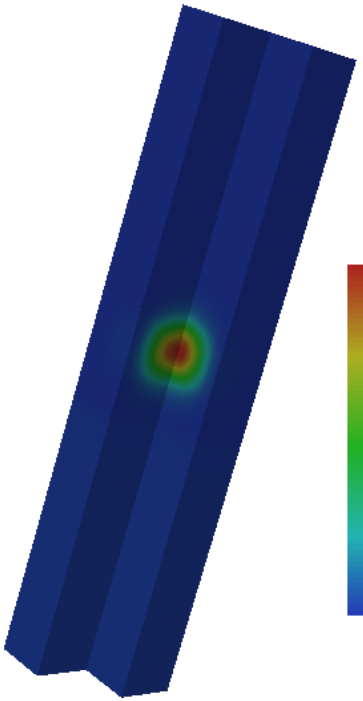


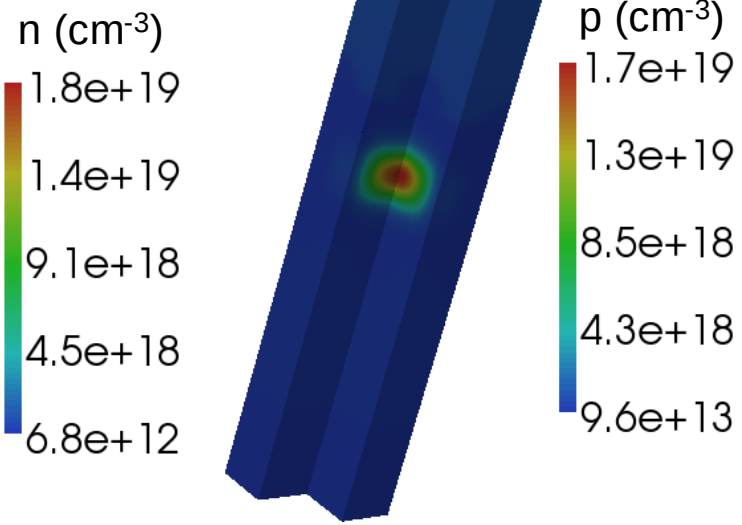


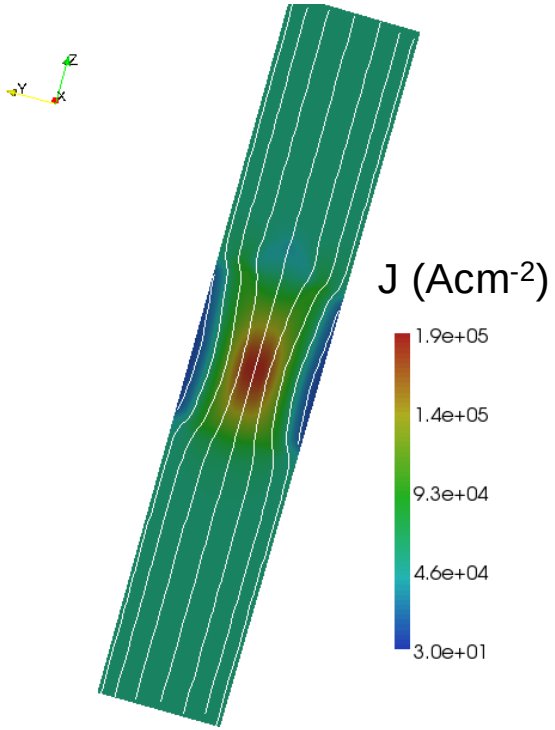


AlGaAs/GaAs nanocolumn

- selfconsistent results (EFA)



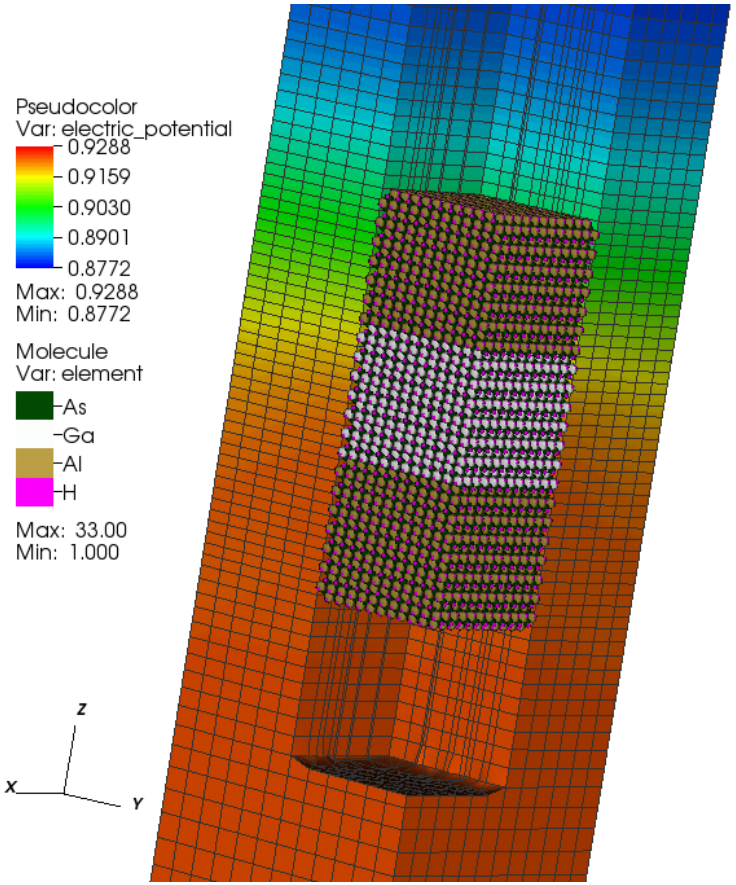


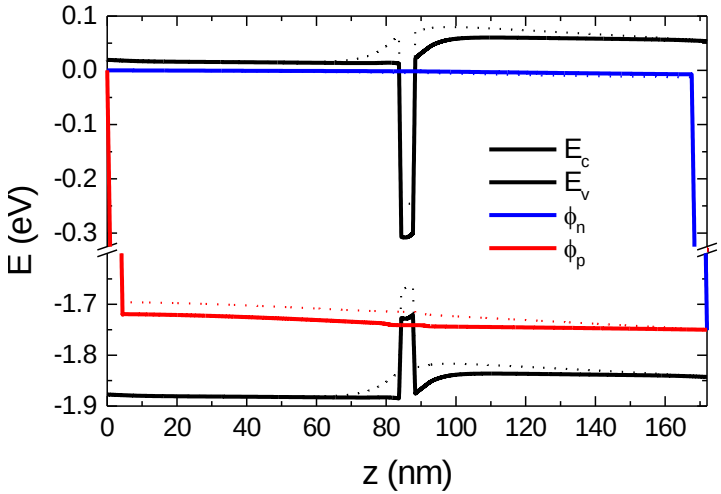


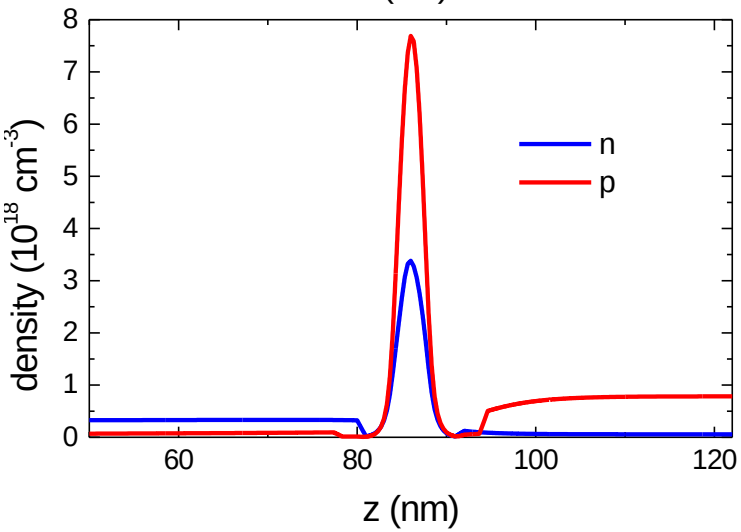
AlGaAs/GaAs nanocolumn

- selfconsistent results (ETB)
  - ETB calculation takes ~ 2h per state (50000 atoms, 20 orbitals/atom)
  - 1 confined electron state, but many dense hole states

    ⇒ ***ETB for electrons, EFA for holes***



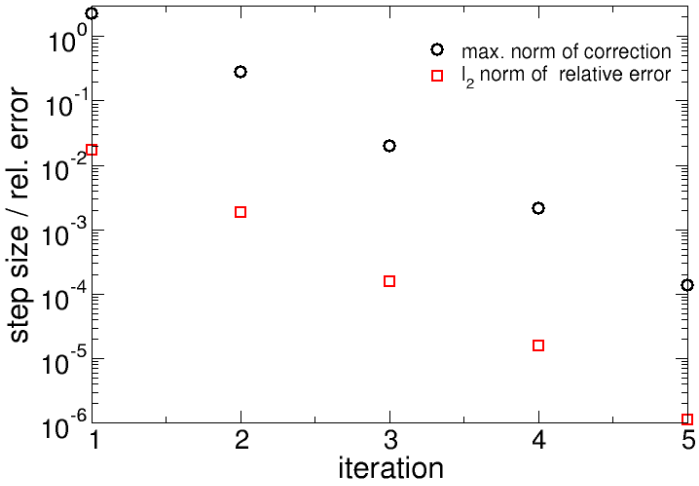


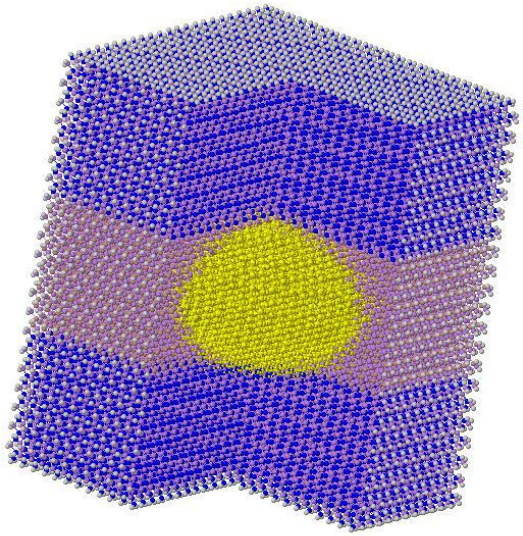


AlGaAs/GaAs nanocolumn

- selfconsistent results (ETB)

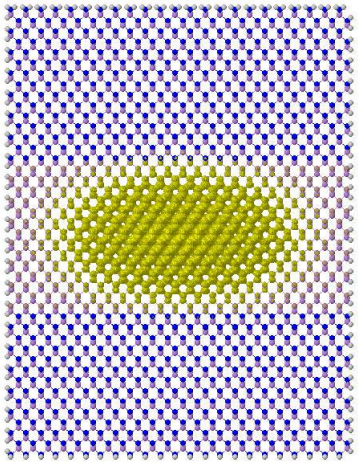
convergence:



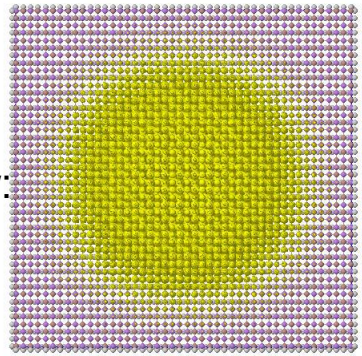


1st electron state

front view:



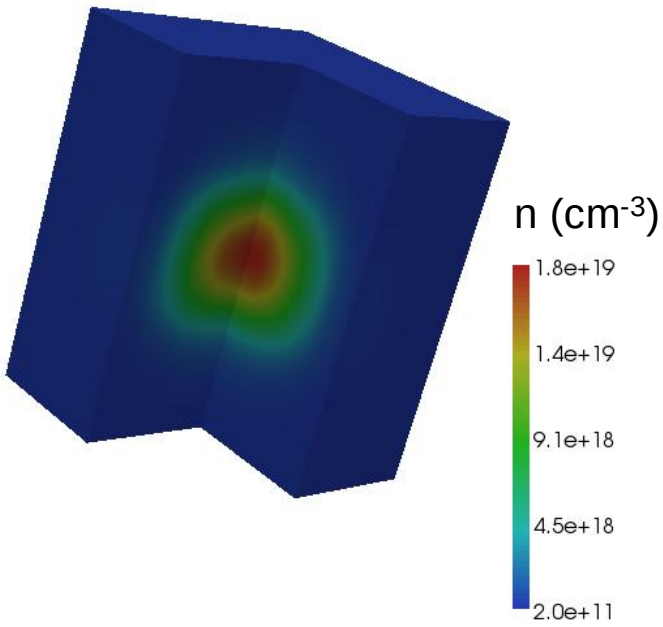
top view:



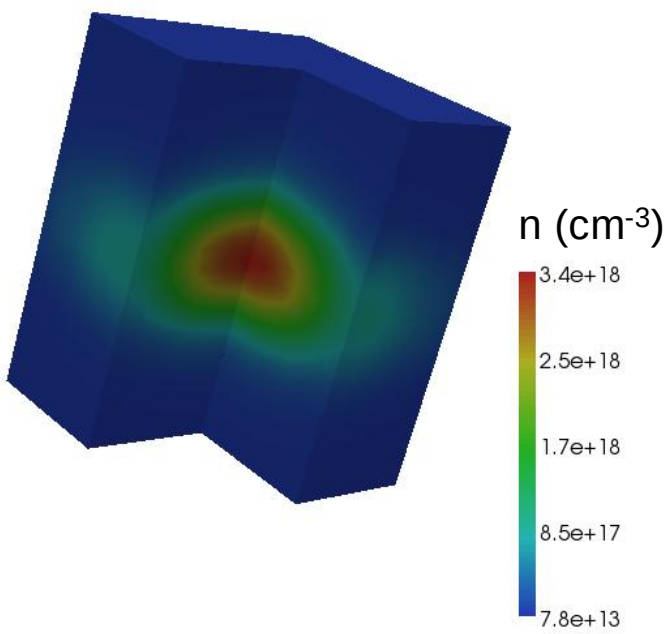
AlGaAs/GaAs nanocolumn

- selfconsistent results: electron density

EFA



ETB



Conclusion

- A multiscale simulation model is needed for modern and future optoelectronic devices
- TiberCAD is now capable of doing selfconsistent Drift-Diffusion/EFA/ETB simulations

- *Coupling of quantum transport (NEGF) and classical transport is still missing*