Multiscale-Multiphysics modeling of nanostructured devices: The TiberCAD project.

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

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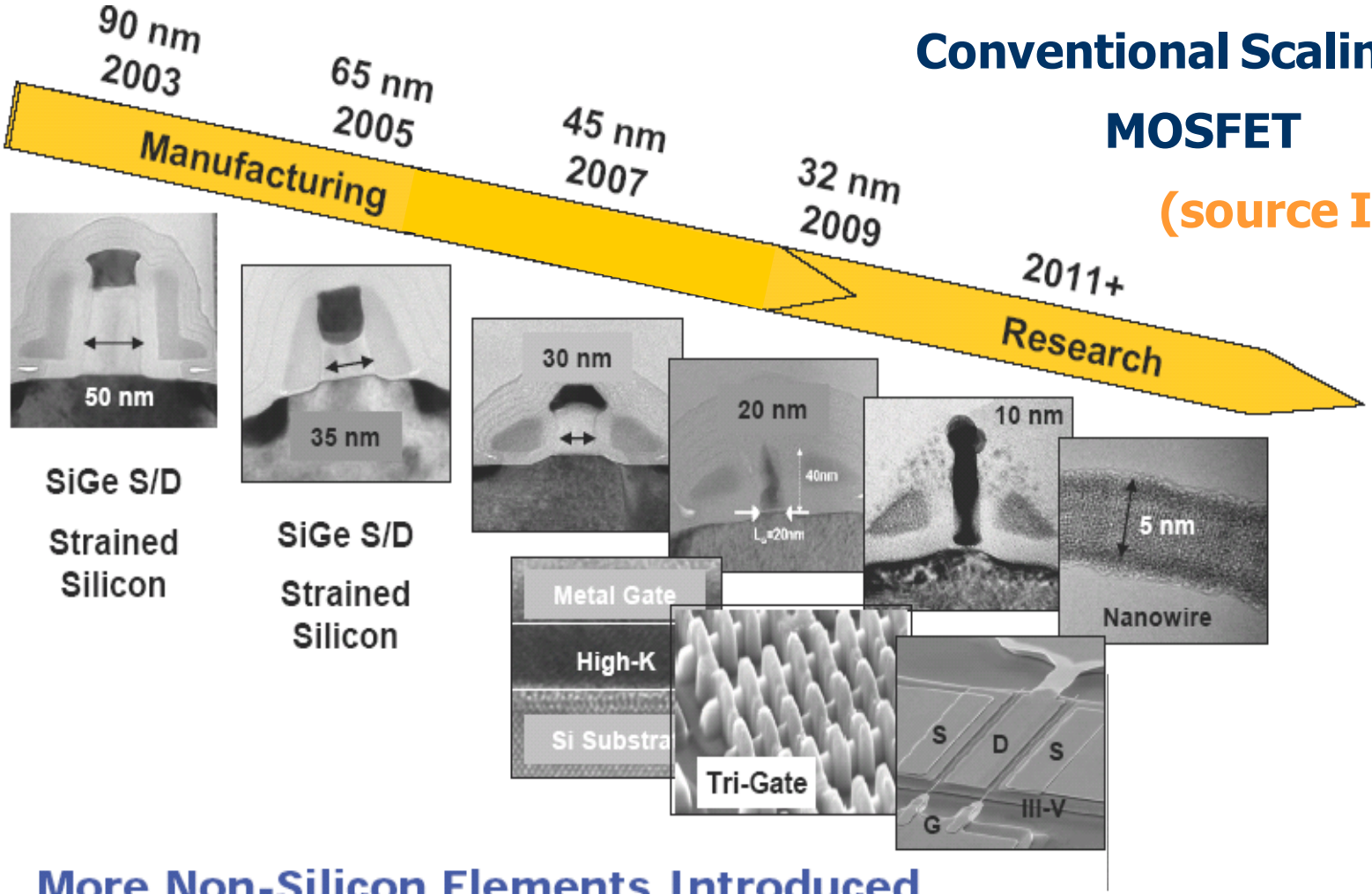
TIBERLAB

University of "Tor Vergata"

The Moore law

2 in 1.5 years

Downscaling example

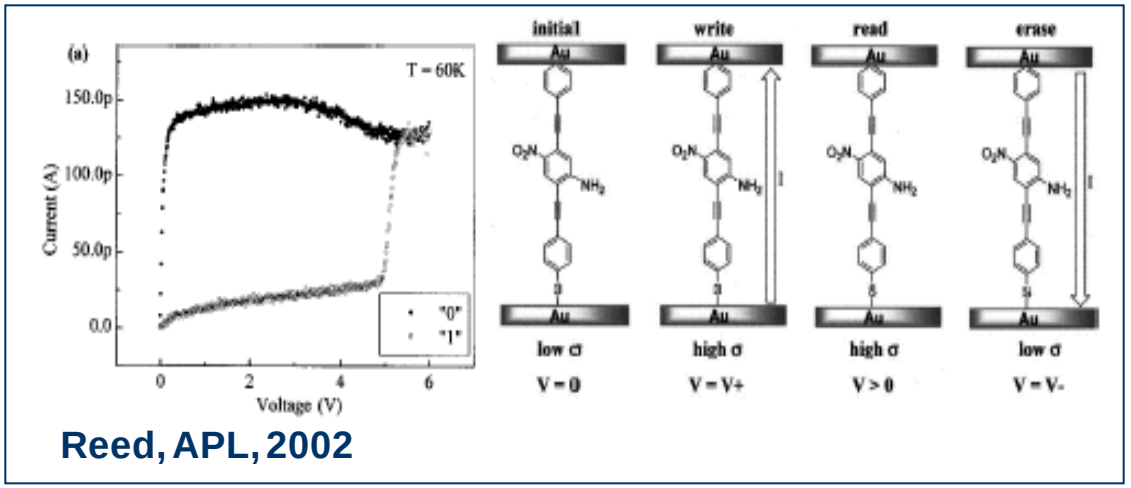


Beyond MOS: molecular electronics

Electron transport across molecules

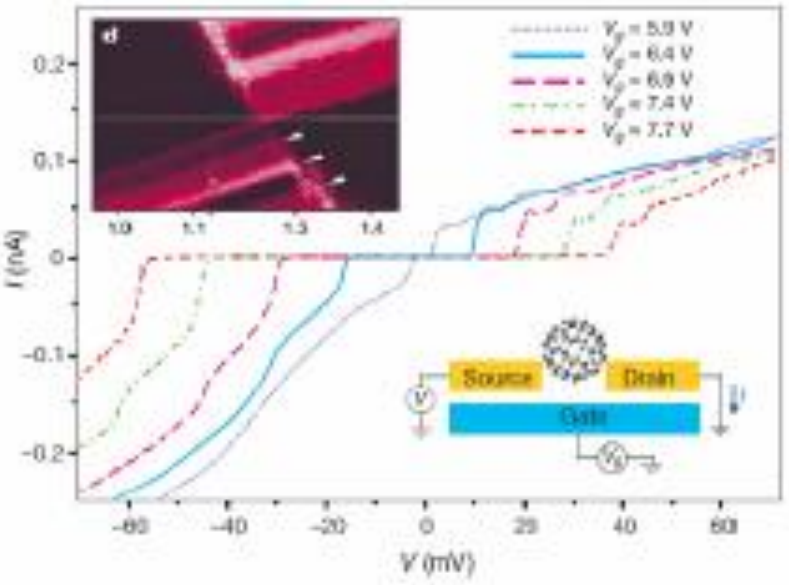
Structural modification

Coulomb blockade

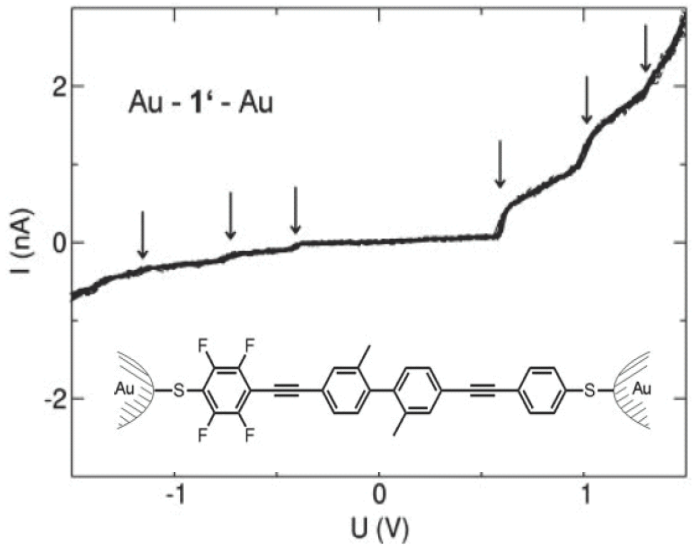


Reed, APL, 2002

H. Park, Science, 2003



Heiko, PNAS, 2005



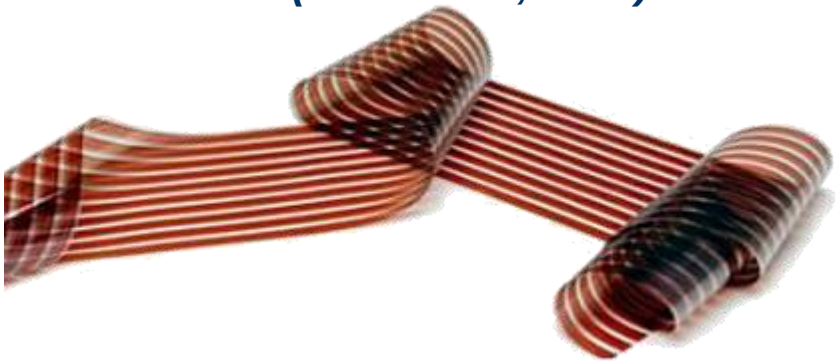
The Obama law

777 in 5 years

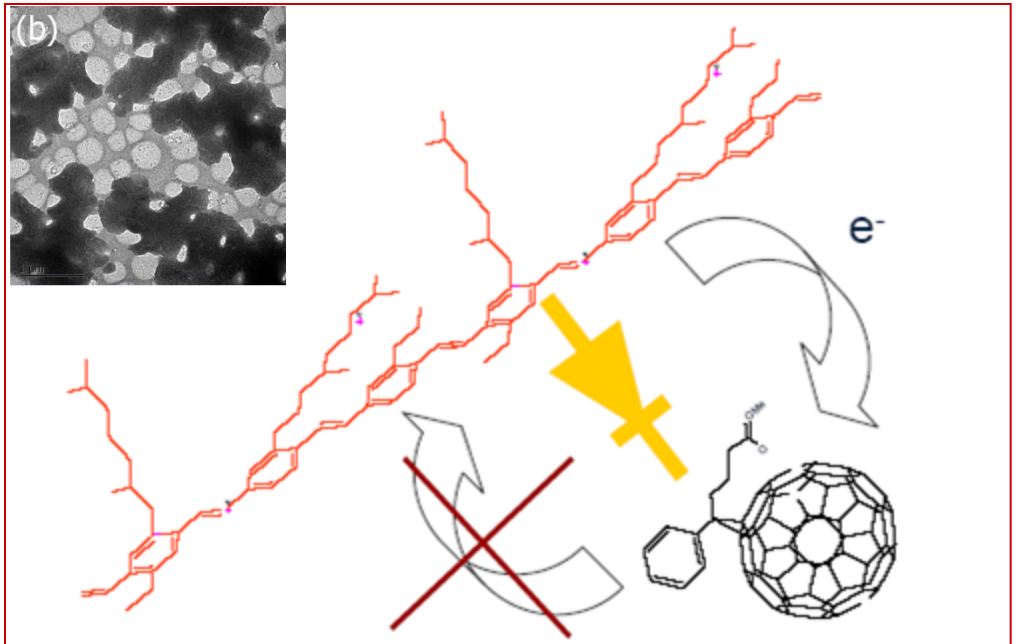
Department of Energy will invest $777 million in Energy Frontier Research Centers (EFRCs) over the next five years

Nanodevices for Renewable Energy

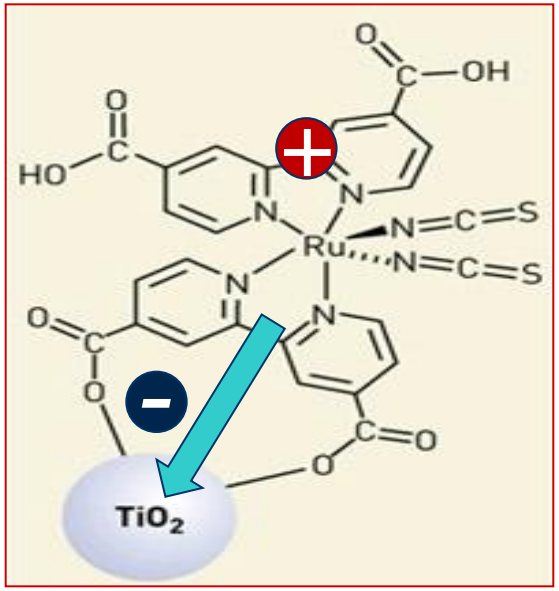
Polimeric Bulk heterojunction solar cell (KONARKA, USA)



Dye Solar Cell (CHOSE, Rome, Italy)

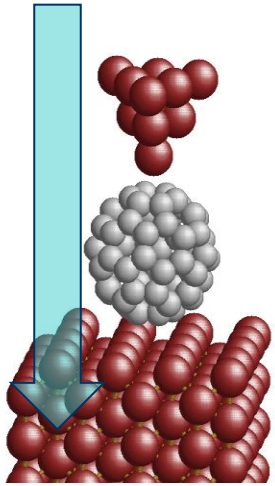


Konarka: molecular diodes for organic photovoltaics



Atomistic methods

At the nanoscale "every atom matters!" (M. Stettler)

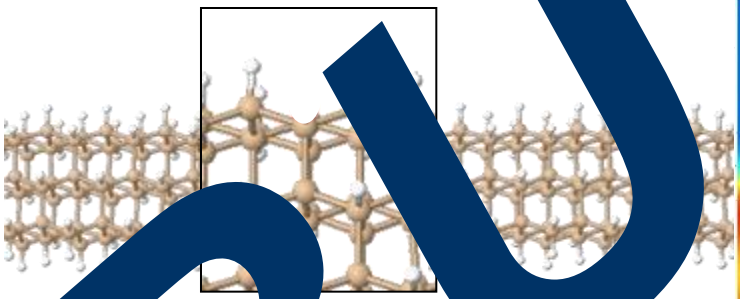


Density Functional TB + NEGF + scattering [PRL 100, 136801 (2008)]

Power dissipated [illegible] the C60 molecule is 10 nW

Power calc[illegible] I x V = 10 μW !!!!

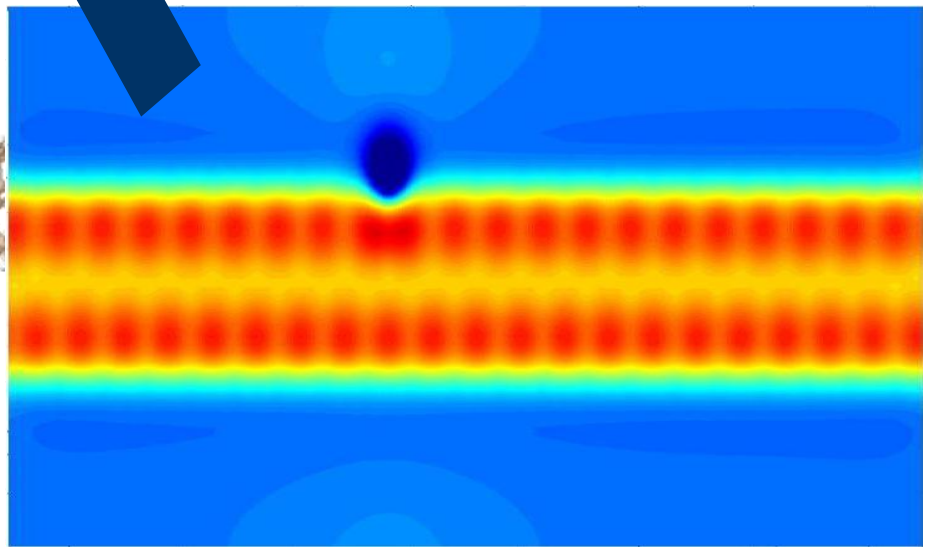
BUT



[illegible]assi[illegible]W with one

- [illegible]gling b[illegible]

- O[illegible]ssiva[illegible] dangling bond

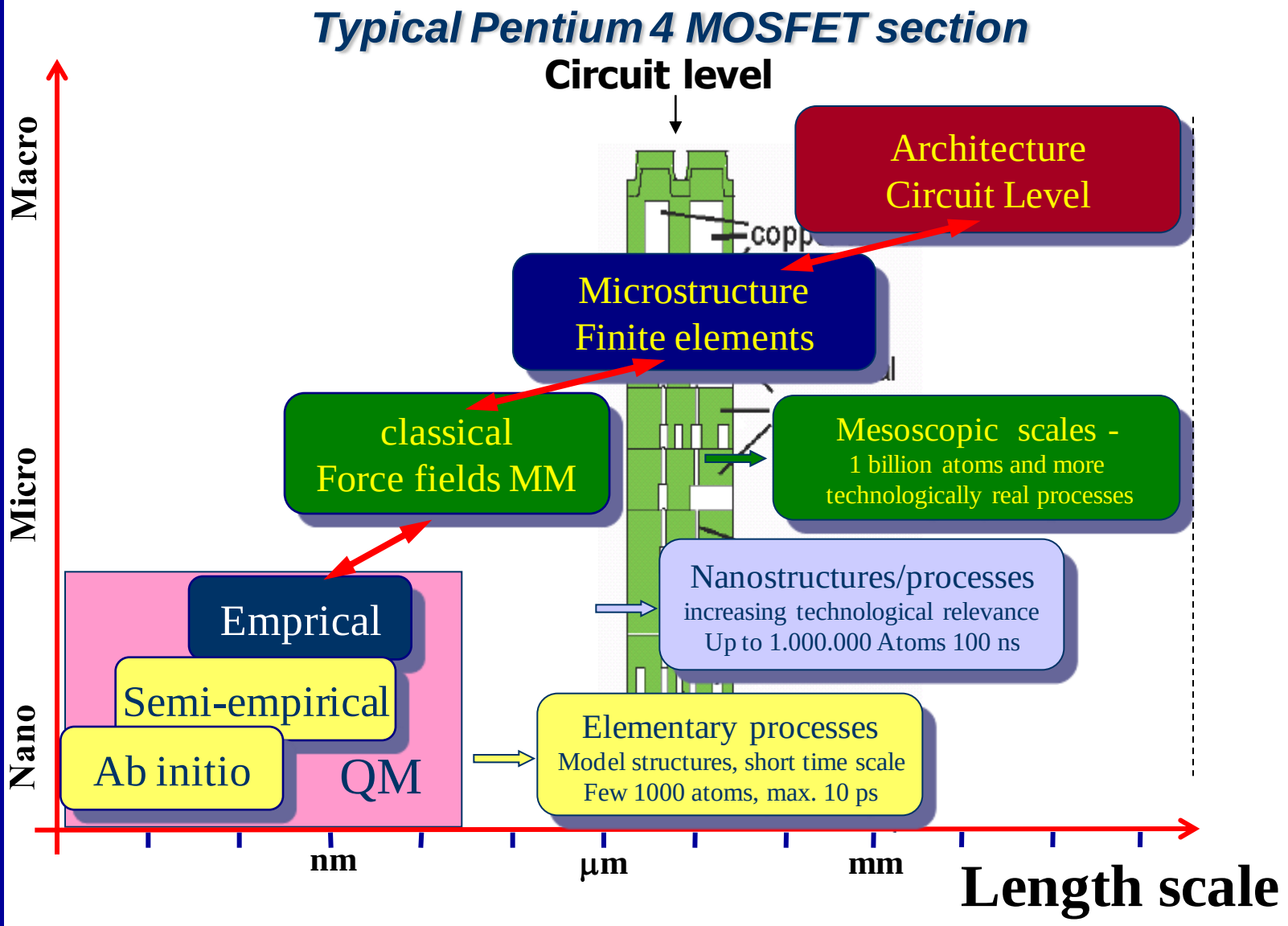


Micro/macro scale

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

- ***Number of atoms cannot grow to 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 !***

The multiscale problem

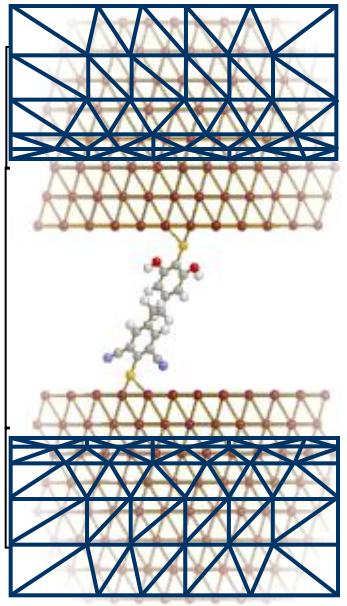


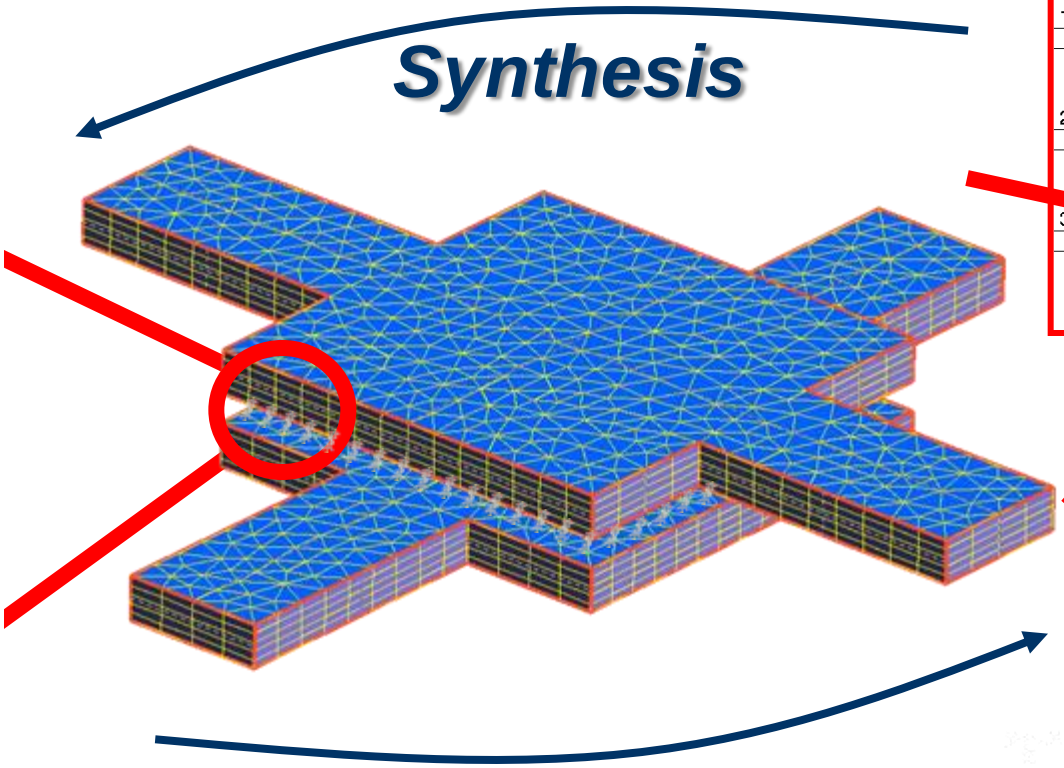
Multiscale simulation approaches

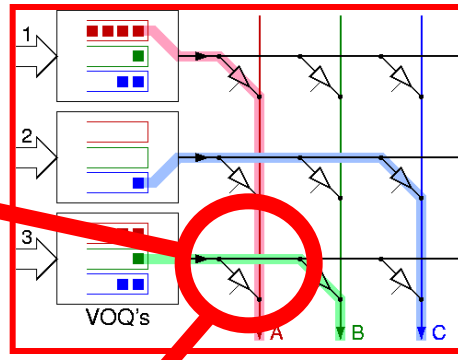
Quantum description

Macro-Microscopic description (Strain, Drift-Diffusion , Heat, etc)

Circuit simulation



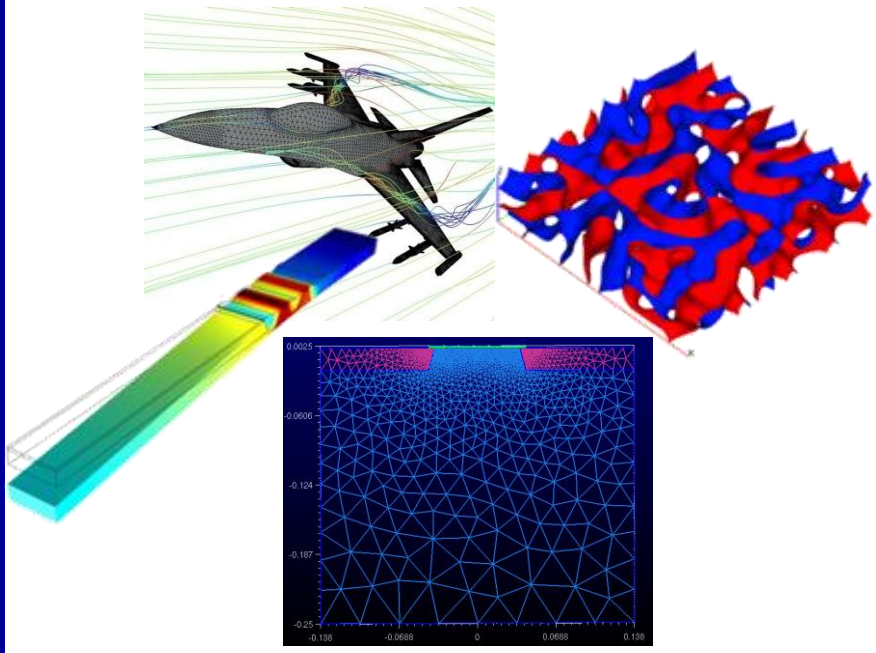




TIBER CAD

www.tibercad.org

Multiscale components



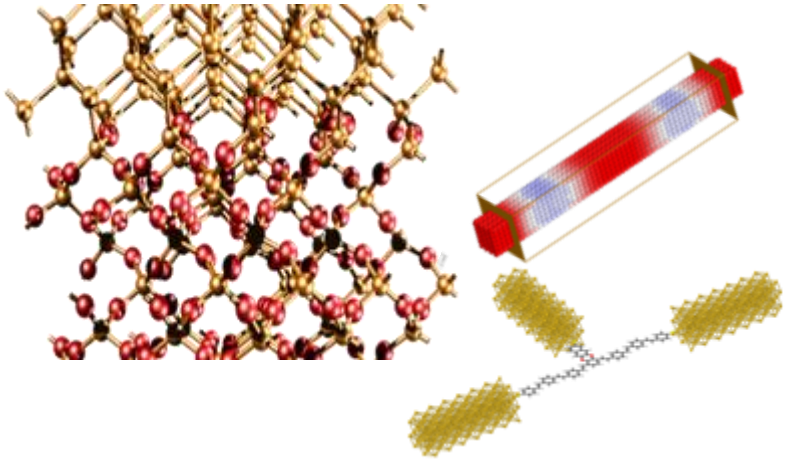
Finite Element Method

- 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 GPL



Atomistic local basis

- Localized basis approach are very well suited for device simulations

- Empirical approaches (ETB)

- Aproximate DFT (DFTB)

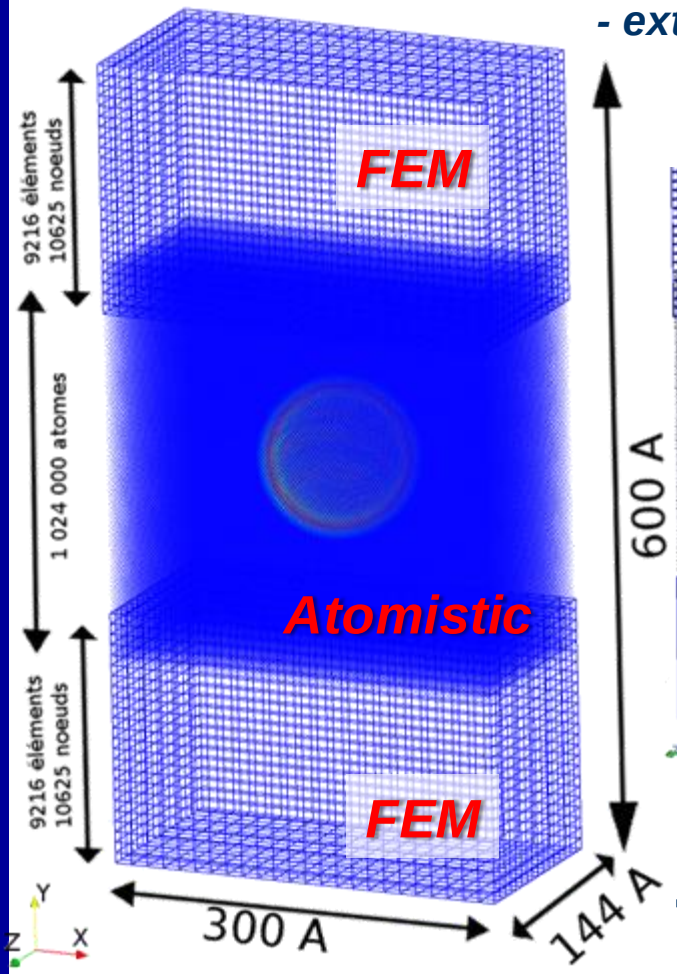
- Full DFT (Siesta, DMOL, etc.)

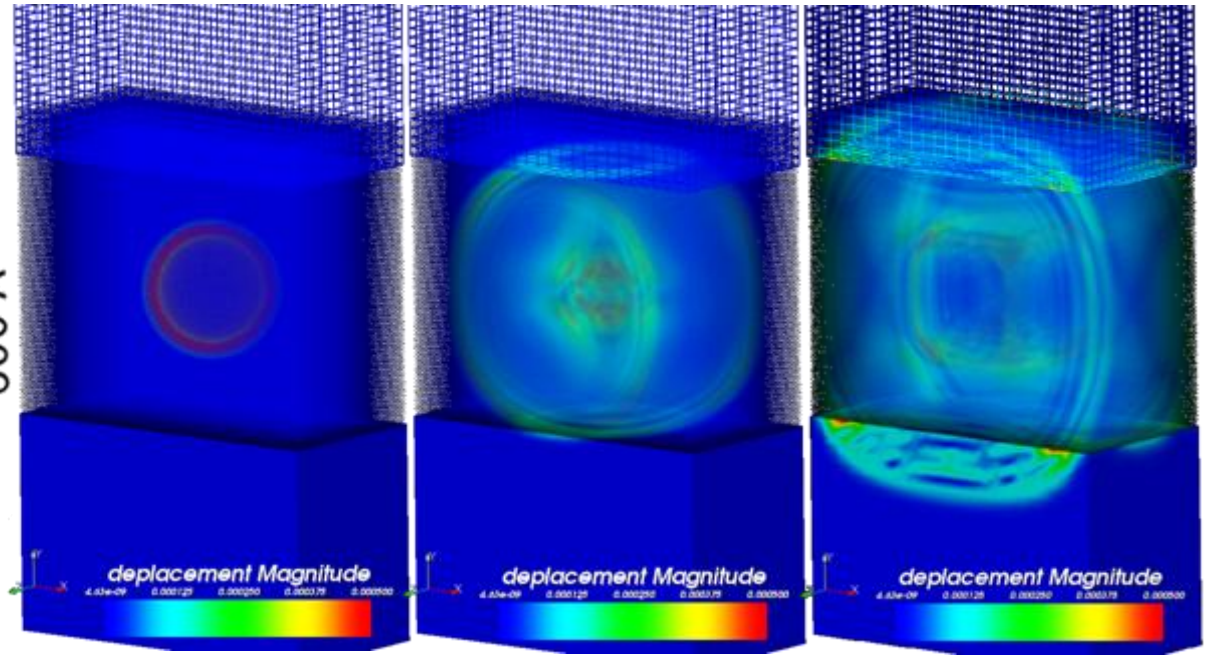
Multiscale methods in material science

Propagation of a shock wave in a crystal

- central region is treated at the atomistic level (MM)

- external part are treated in the continuous approx. (FEM)

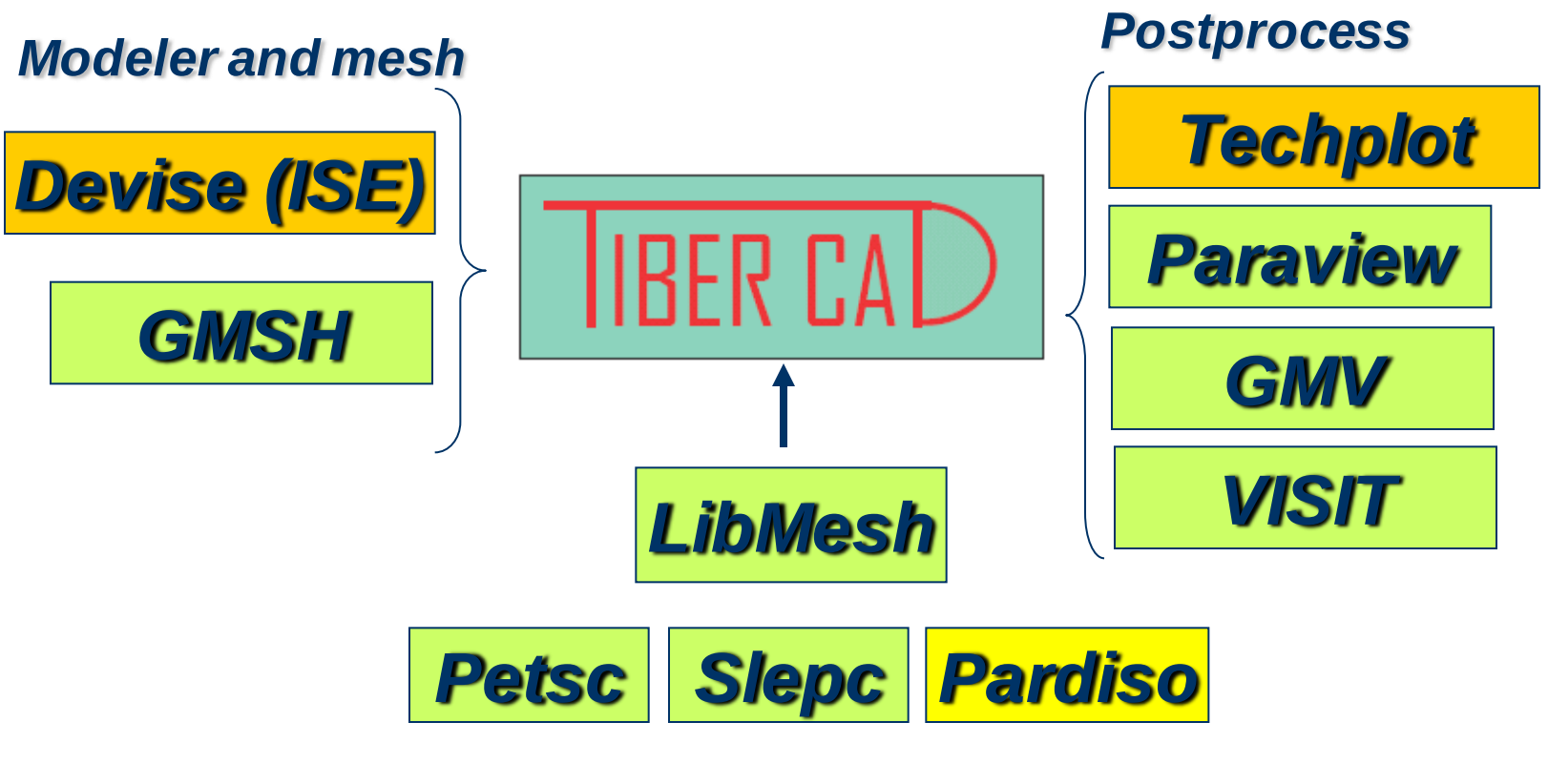




Time

Courtesy of G. Anciaux

TiberCAD structure



Development is done in C++ in Linux, porting to other UNIX-like environments and Windows has been achieved

TiberCAD 1.0 is freely downloadable at www.tibercad.org

TiberCAD models

- Mechanical deformation with any kind of constrain
- Semiconductor Strain including piezoelectric effect
- Drift-Diffusion transport of electrons / holes / excitons / Ions (+ Poisson)
- Heat transport
- Quantum mechanics based with **k·p** envelope function approximation
- Atomistic description via Density functional Theory and Empirical Tight-Binding (sp3d5s*, or any other basis)

- *NEGF(developed but not yet integrated)*
- *Classical molecular mechanics (in progress)*
- *Maxwell solver (in progress)*

TiberCAD features

- *1D, 2D, 3D and cylindrical symmetry*
- *Adaptive meshes*
- *Written to run parallel (but not yet tested)*
- *Input parser with a syntax similar to commercial TCAD*
- *Interfaces with some commercial TCAD*
- *Possibility to link user defined models*

Numerical Implementation

- All PDE based models are discretized by means of the finite element method (FEM) by using Fermi level as variables !
  (in contrast to conventional approaches which uses box integration and densities as variables)
- The linearized equations are discretized using standard Galerkin FEM, using a piecewise linear basis (hat functions)
- Jacobian is asymmetric and ill-conditioned as the diffusion coefficients in the linearized continuity equations are proportional to the particle densities.
- The conditioning is improved by a proper diagonal scaling.
- A M-matrix form of the Jacobian is looked for (proper stabilization procedure)
- The linear system is solved by means of iterative solvers (bi-conjugate gradient with ILU preconditioning), using the open-source library PETSc
- Numeric Gauss integration for integrals

Physical Models: strain (linear)

define shape

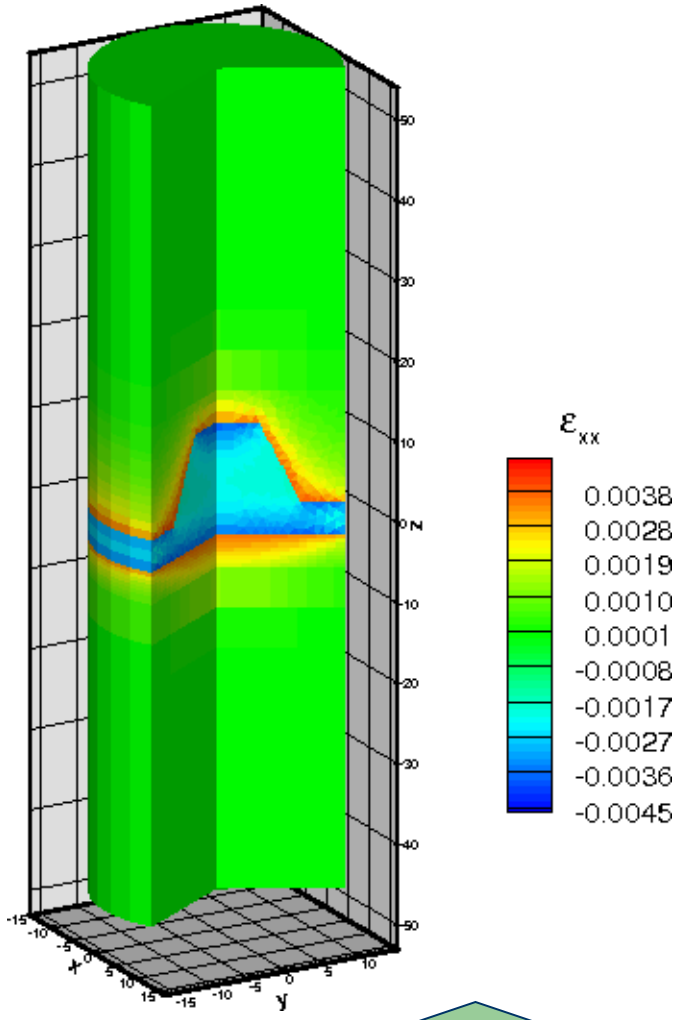
$$\varepsilon_{ij}^{0} = \delta_{ij}\frac{a_i^S - a_i}{a_i}$$

Minimization of the elastic energy

$$\frac{\partial}{\partial x_i}\left(C_{ijkl}(\mathbf{r})\left(\frac{\partial u_k}{\partial x_l} + \varepsilon_{kl}^{n}(\mathbf{r})\right)\right) = 0$$

Strain tensor

$$\varepsilon_{ij}^{n} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)$$



GaN dot in a/AlGaN nanocolumns

Physical Models: strain (non-linear)

Povolotskyi-Di Carlo, JAP **100**, 063514 (2006)

Minimizing the elastic energy with self-consistency cycles

define shape

$$\varepsilon_{ij}^{0} = \delta_{ij}\frac{a_i^S - a_i}{a_i}$$

$$\frac{\partial}{\partial x_i}\left(C_{ijkl}(\mathbf{r})\left(\frac{\partial u_k}{\partial x_l} + \varepsilon_{kl}^{n}(\mathbf{r})\right)\right) = 0$$

$$\varepsilon_{ij}^{n} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) + \varepsilon_{ij}^{n-1}$$

define new shape by moving nodes

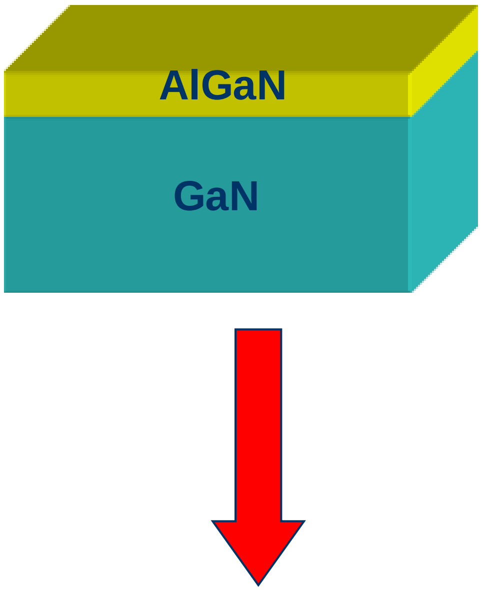
$$\vec{r} \rightarrow \vec{r} + \vec{u}$$

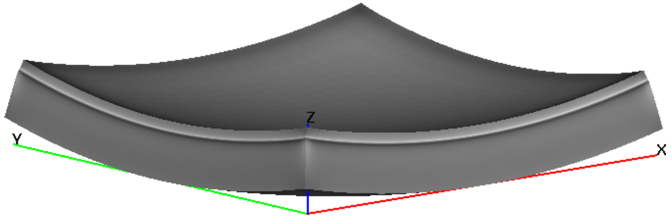
$$\|\vec{u}\| > \delta$$

yes (back to the equilibrium equation)

stop

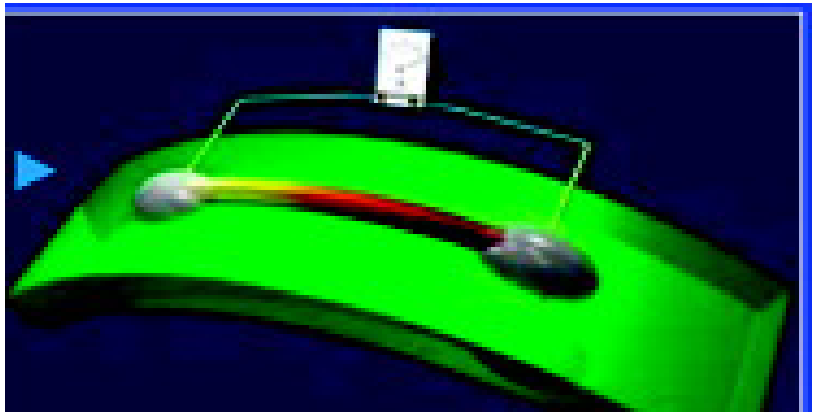
Free-standing AlGaN/GaN





Adaptive grid are used

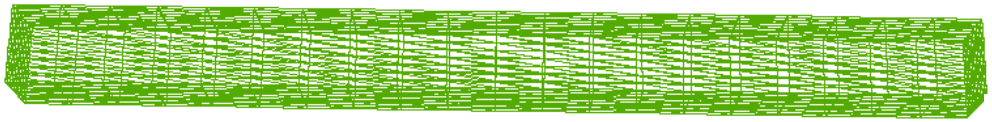
ZnO_2 Wang nanogenerator



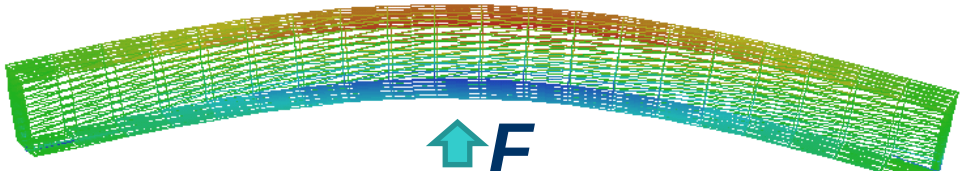
Zhong Lin Wang investigated nanogenerators for converting mechanical energy into electricity.

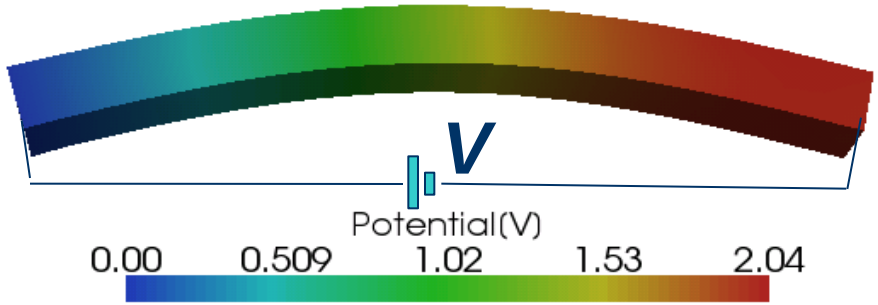
Zhong Lin Wang. Adv. Funct. Mater, 2008.18, 3553-3567

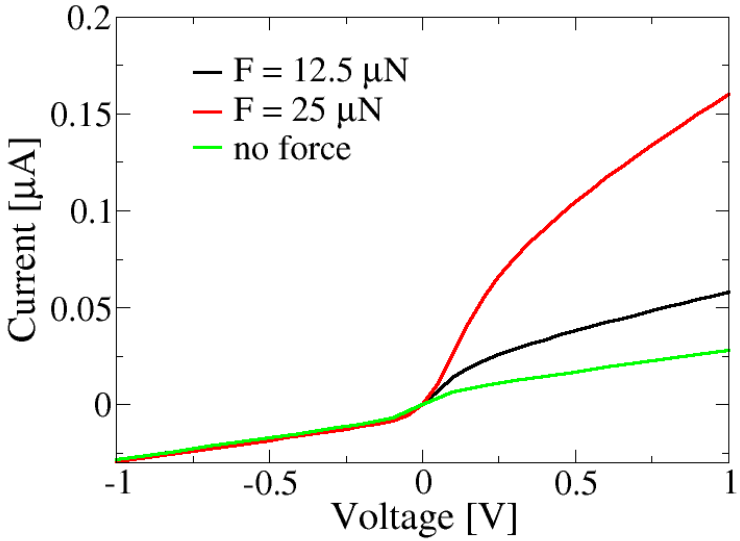
Rusen Yang, et al. Nano Letters , 9 (2009) 3, 1201-1205.



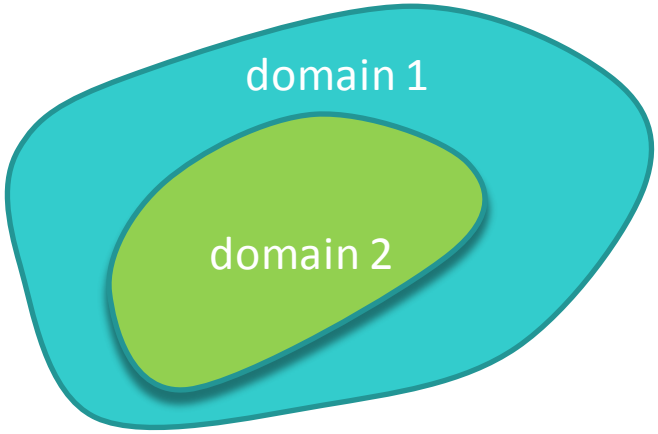
Jun Zhou et al, Nano Letters. (2008)







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.

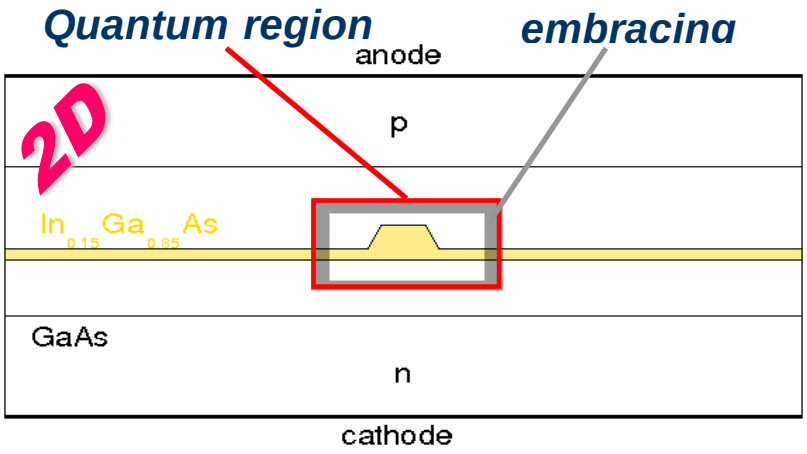
Multiscale simulations: OVERLAP method

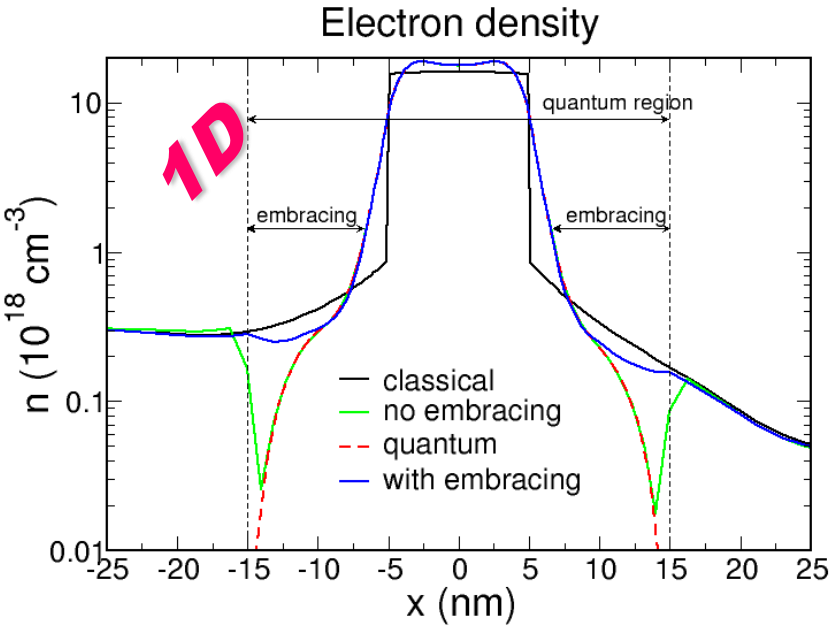
Classical/quantum densities: Embracing

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

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

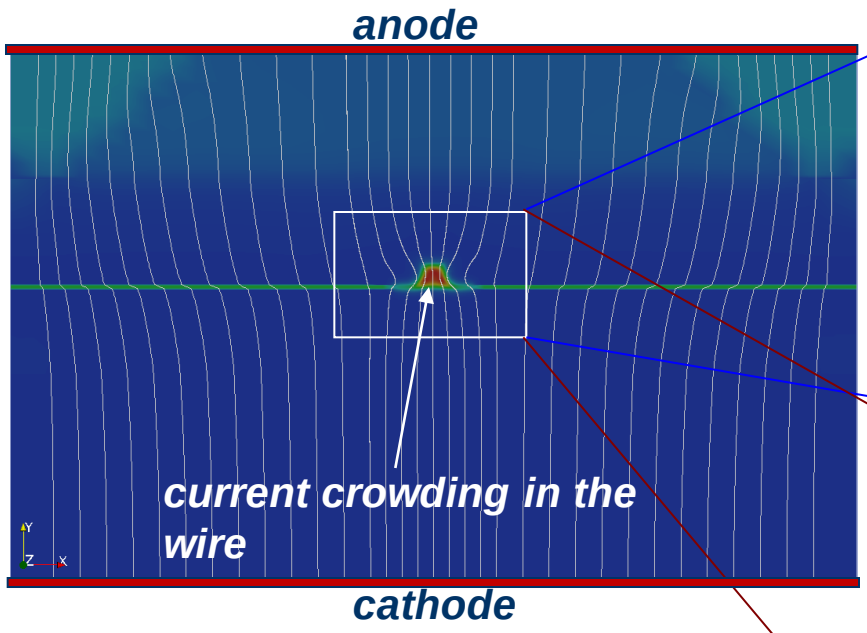
where λ(x) is the solution of a Laplace equation in the embracing region.

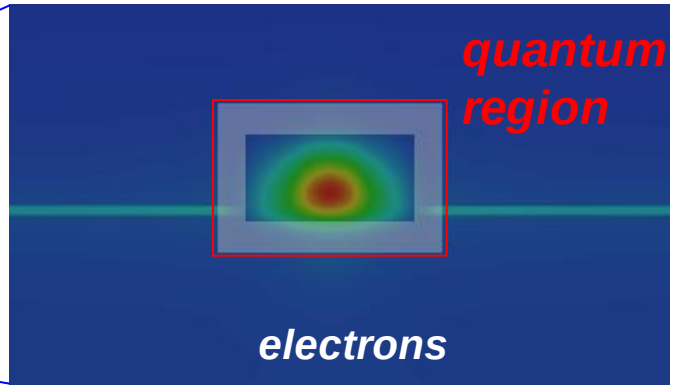


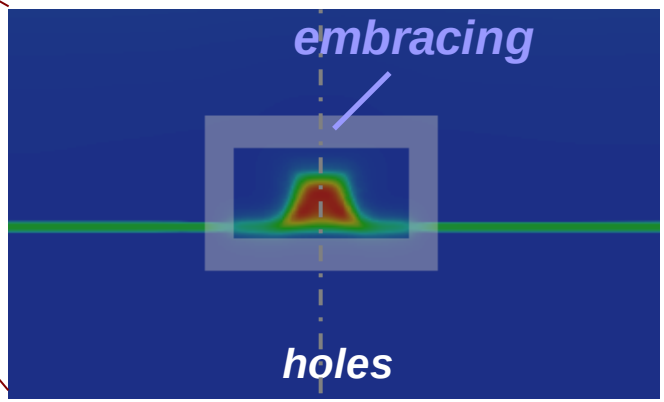


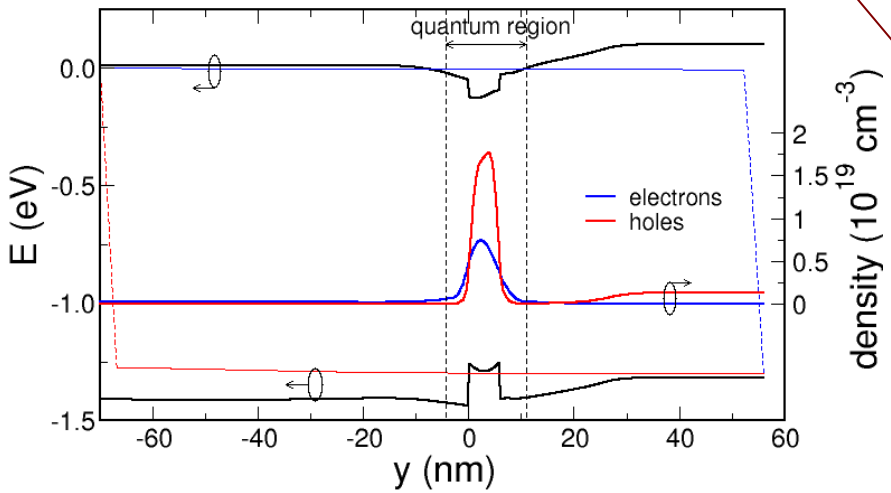
K.P quantum model

InGaAs Quantum wire







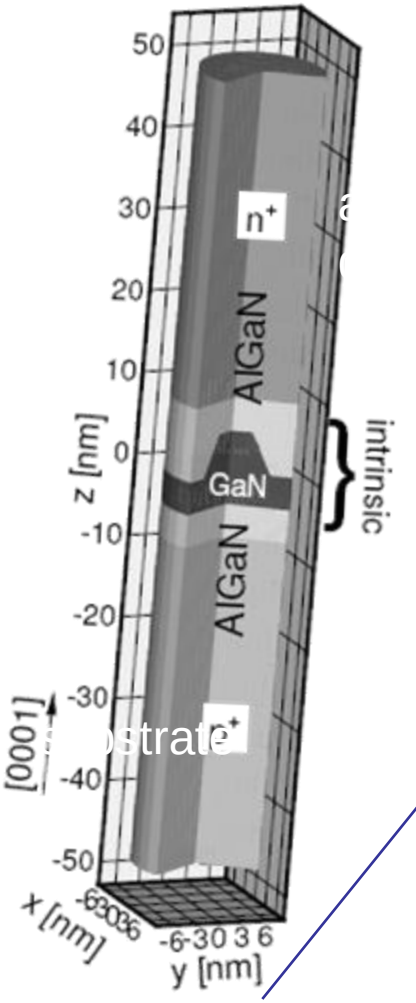


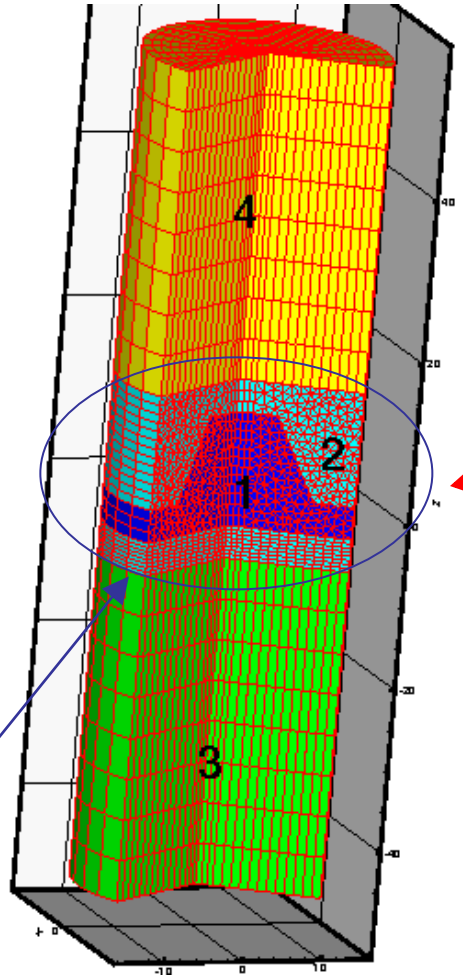
Selfconsistent densities at Vb = 1.3 V

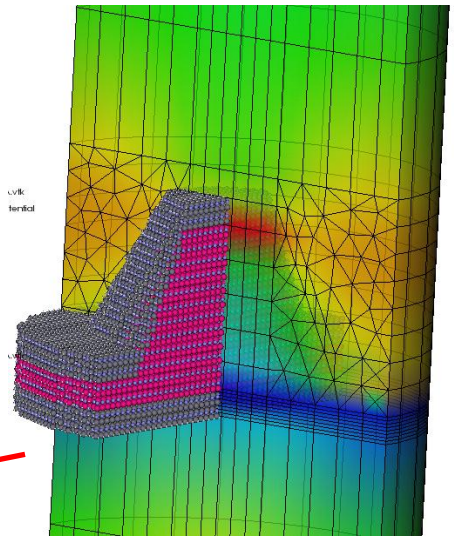
K.P quantum model

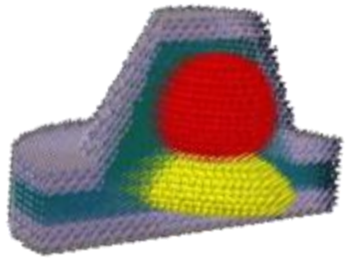
GaN/AlGaN Quantum Dot

Macroscopic ↔ Atomistic projection of potentials and densities

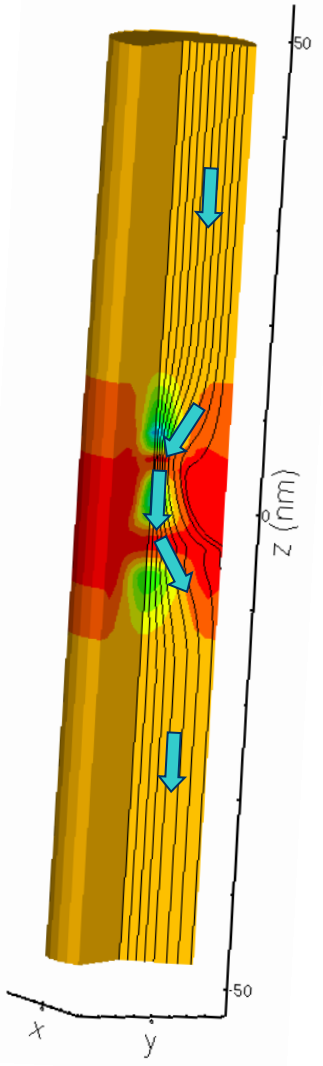








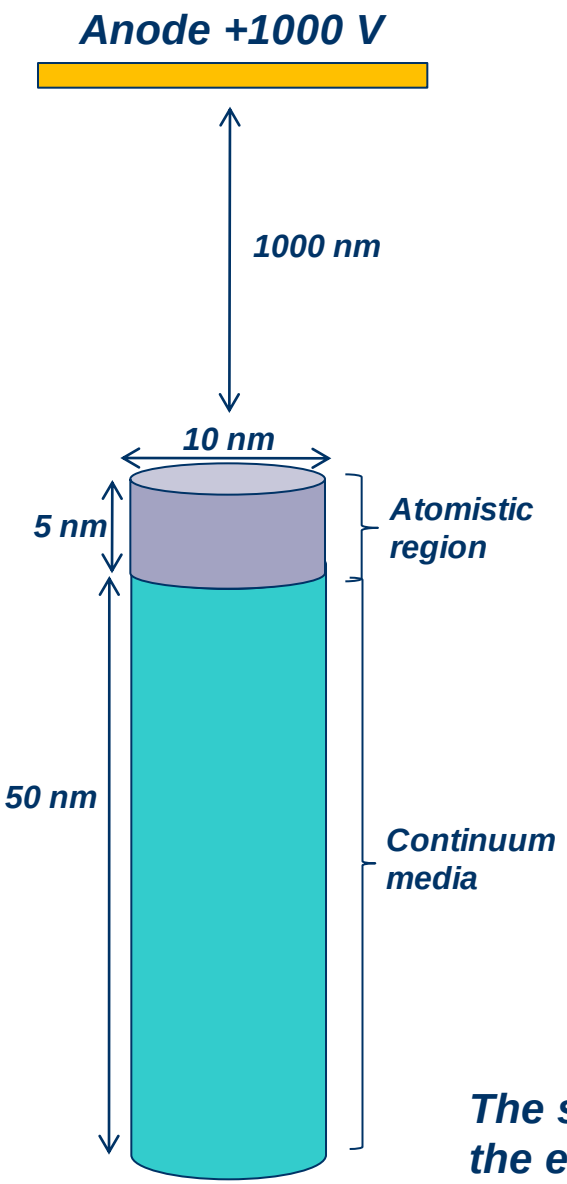
sp3d5s* quantum model

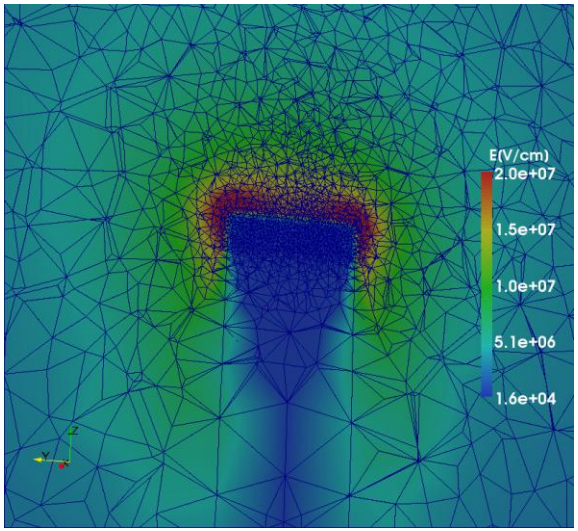


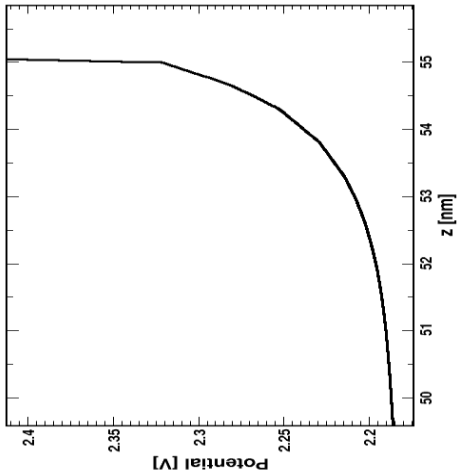
Quantum equation is solved only here (1 + 2)

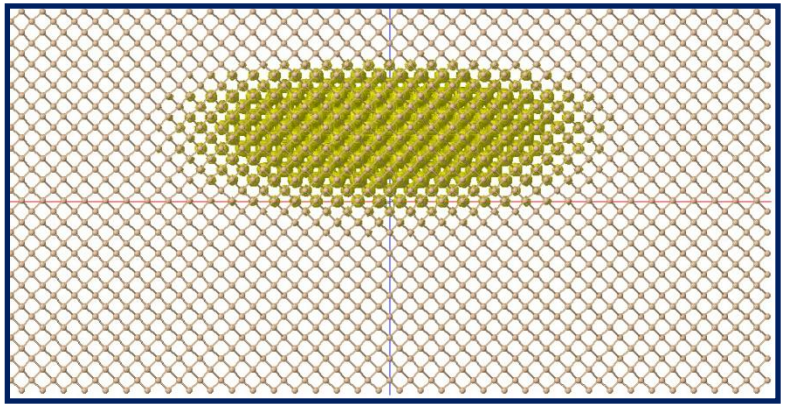
Details in the G. Penazzi talk

SiNanowire for field emission







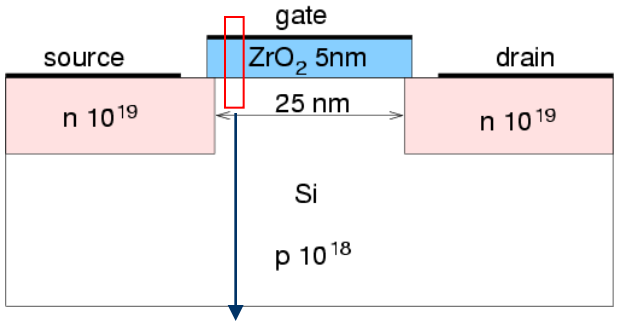


The strong potential drop (tip effect) induced a confinement of the electron state. Field emission is from a localized state

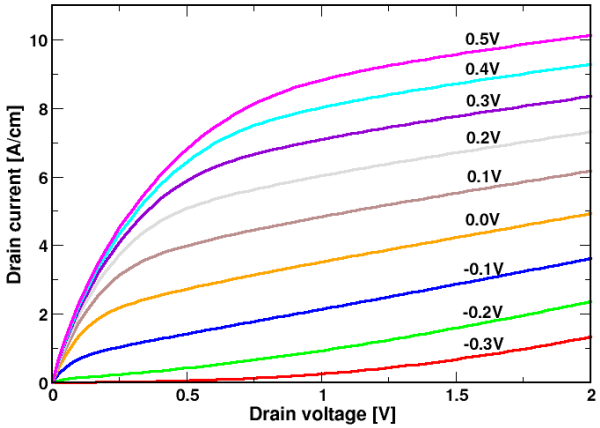
Multiscale simulations: BRIDGE method

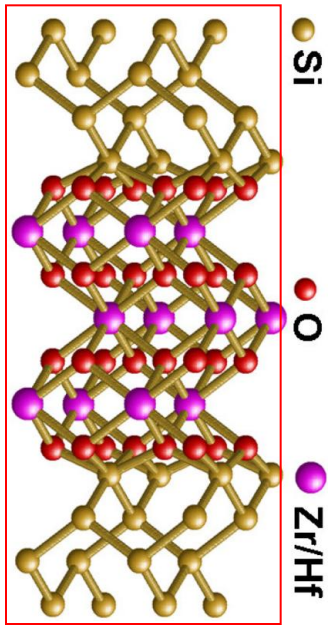
Multiscale simulation example: MOSFET

Drift-diffusion simulation of a 25 nm MOSFET with SiO_2 and high-κ oxide, including gate-tunneling



Classical Drift-Diffusion simulations





Tunneling current calculation based on a atomistic semi-empirical tight-binding description.

How can we merge these two scales ?

M. Auf der Maur et al., J. Comput. Electron., (2007)

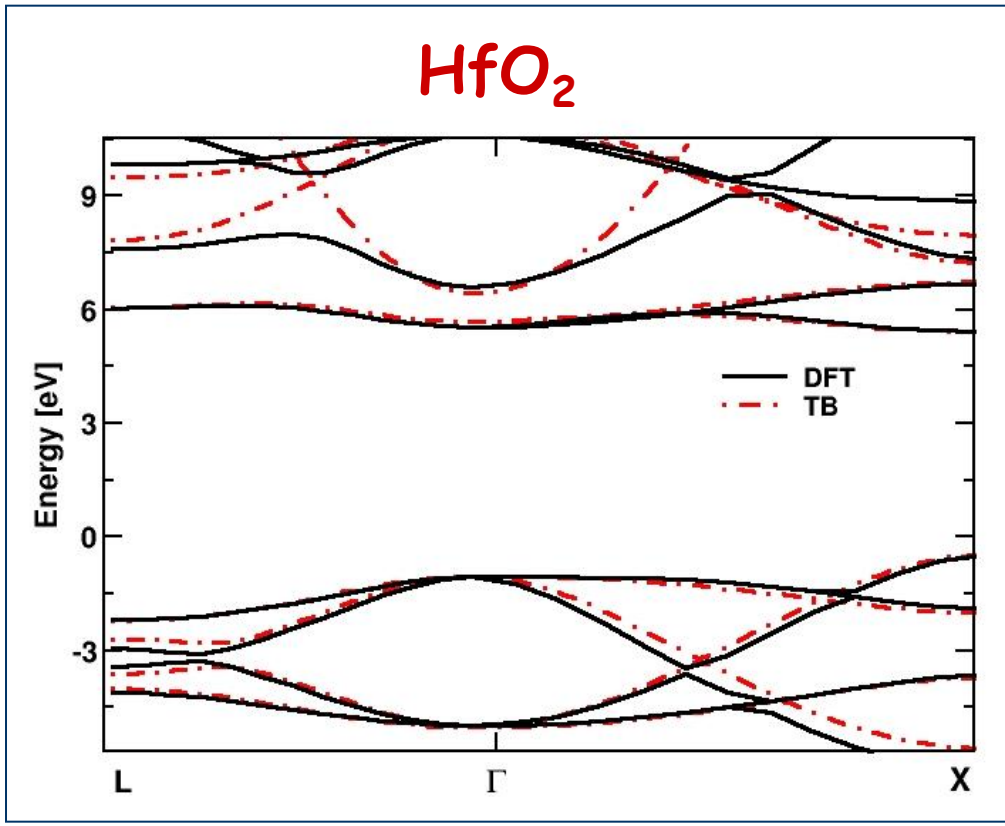
TB parameterization

SiO_2 , HfO_2 and ZrO_2 cubic crystalline forms

- DFT total energy calculation
- optimization of lattice parameters
- energy band dispersions

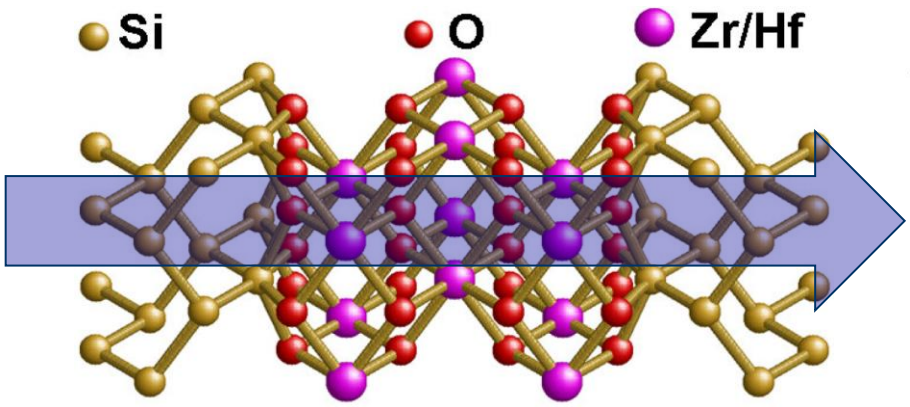
- Effective mass approach cannot the easily applied and a full band calculation is required

- Tight Binding parameterization of SiO_2 , HfO_2 and ZrO_2 has been determined to fit DFT calculations and experimental band gaps. A $sp^3s^*d^5$ model has been used

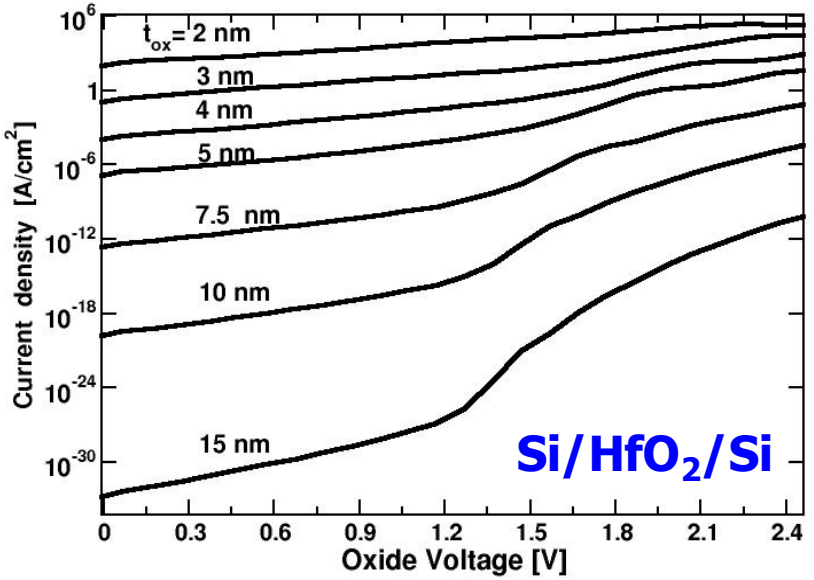


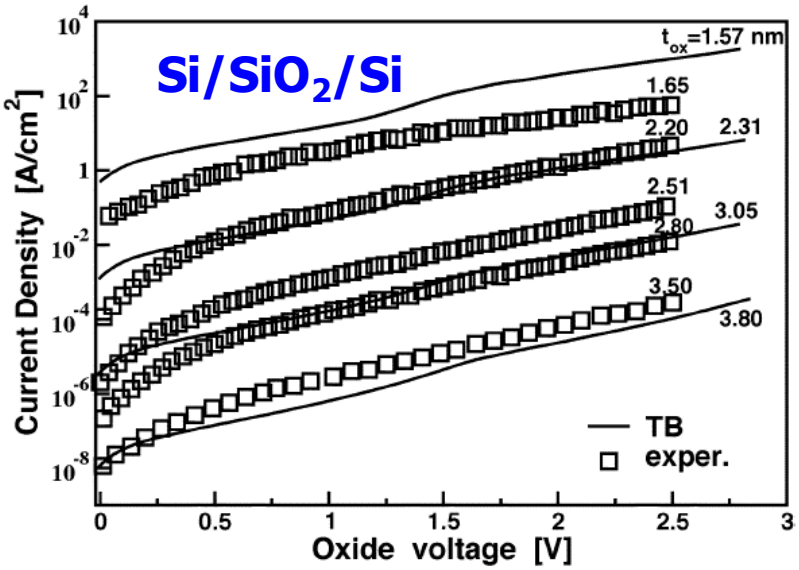
- Calculation of tunneling properties with transfer matrix method in ETB framework

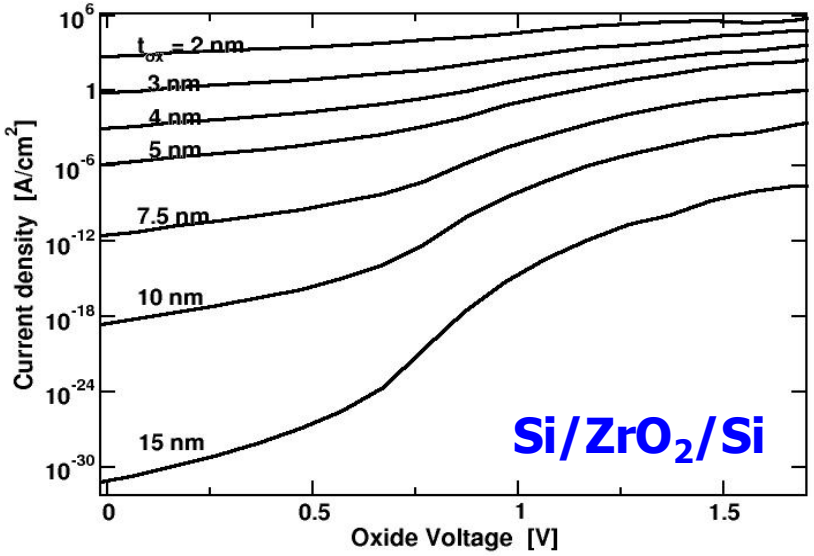
Atomistic description of tunneling current in MOS



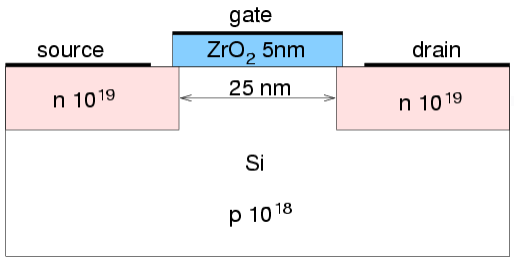
Sacconi et al IEEE TED 2004 and 2007







Bridge method: flux continuity



$$J_y^C(\lambda) = 0$$

$$\mathbf{J}^C = \mu_n n \nabla \phi_n$$

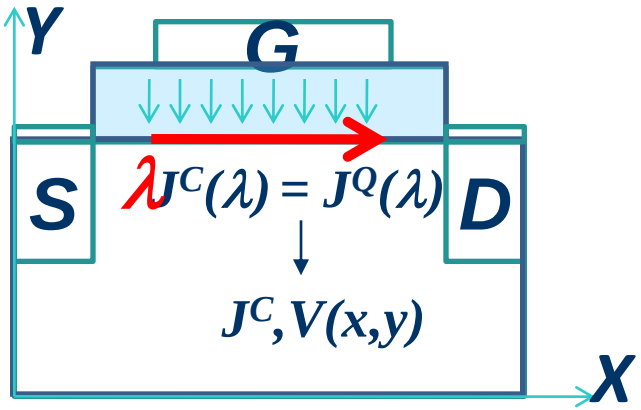
$$\nabla \cdot \mathbf{J}^C = G - R$$

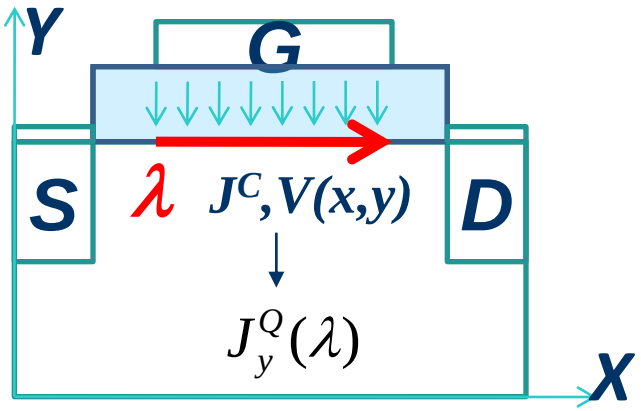
$$\nabla \cdot (\varepsilon \nabla V) = -\rho$$

$V(\lambda)$

$$J_y^Q(\lambda) = f(V(\lambda) - V_G)$$

$$J_y^C(\lambda) = J_y^Q(\lambda)$$





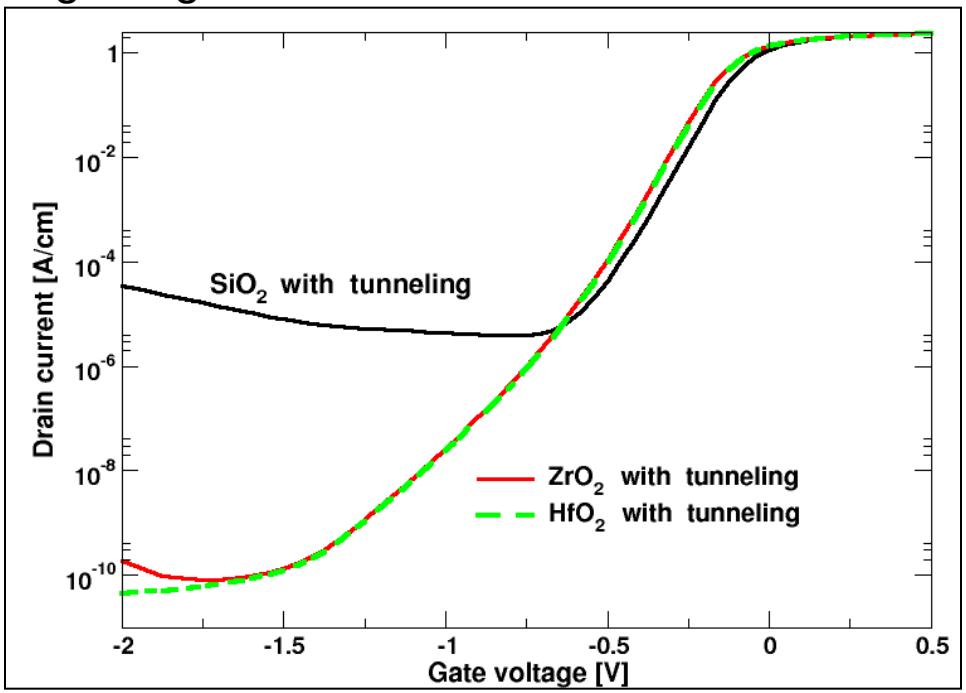
Poisson-Drift-Diffusion is solved in the whole device

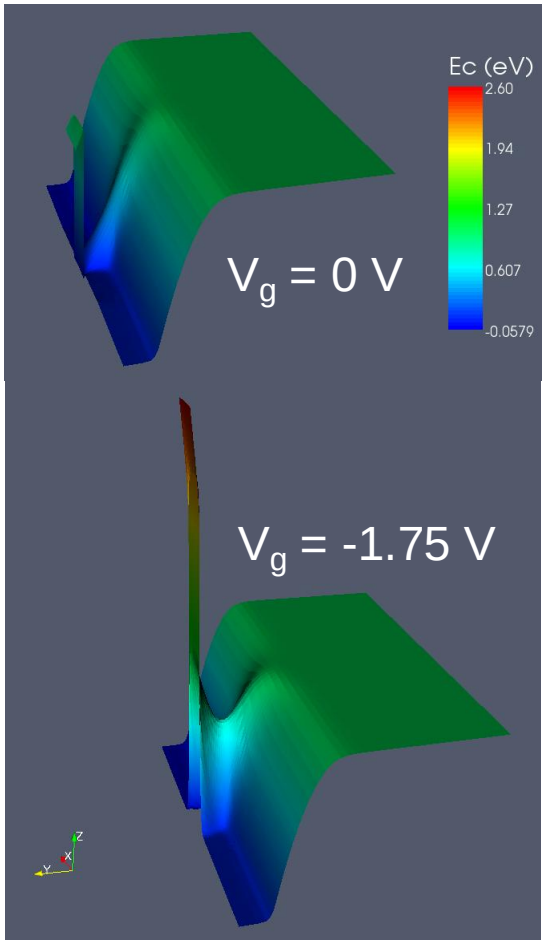
Self consistent cycle

Tunneling current calculated with atomistic tight-binding model is taken as a boundary condition for electron continuity at Si/oxide interface

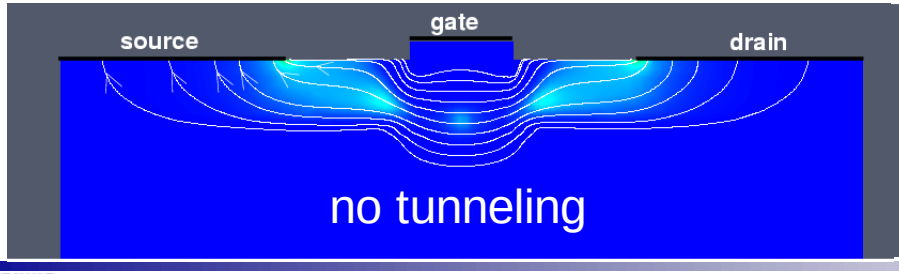
MOSFET: multiscale simulation

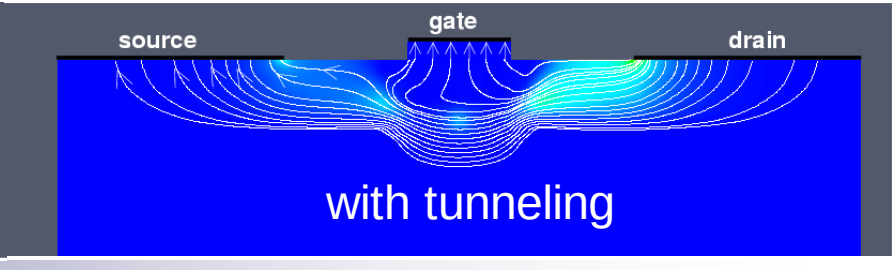
The effect of the oxide tunneling can be seen in the subthreshold characteristic at high negative bias:





Current flow lines at V_{ds} = 0.1 V, V_g = -1.75 V:





Conclusions and outlook

- Multiscale/multiphysics is requested in real modern materials and devices where electronics optics chemistry (and biology) are linked together
- TIberCAD in one of the first attempt to answer this request
- Much effort is still needed to arrive at a consistent multiscale integration for transport simulations such as a coupling between NEGF and DD (IWCE14)

Additional details at http://www.tibercad.org