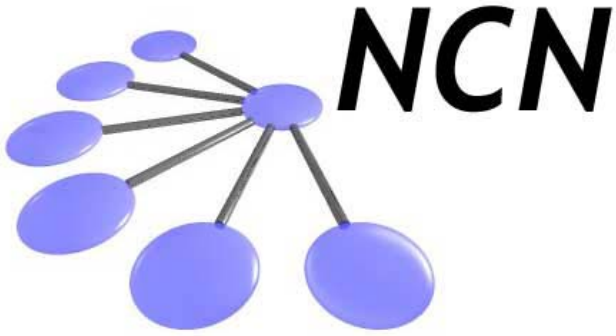
Tutorial 3: NEMO5 Models



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Network for Computational Nanotechnology (NCN)
Electrical and Computer Engineering

PURDUE
UNIVERSITY

A short introduction…

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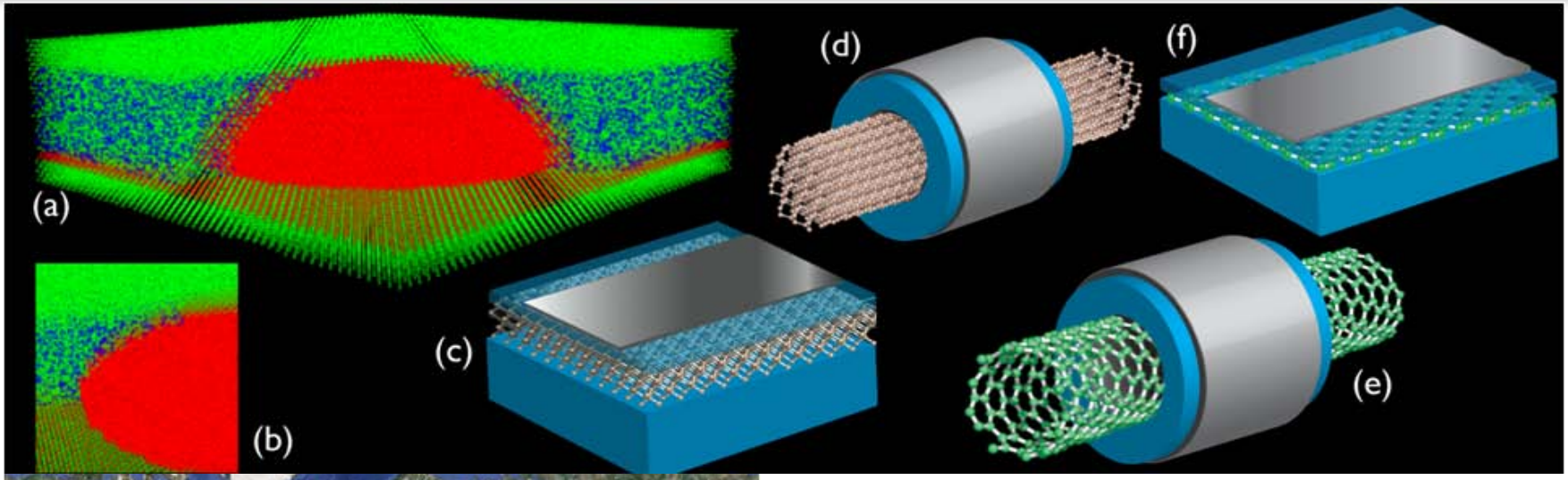


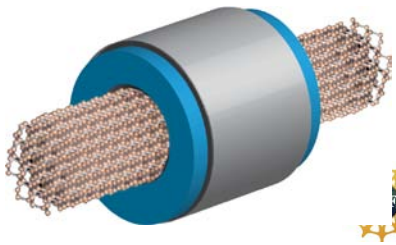
18 years development

- Texas Instruments
- NASA JPL
- Purdue
- Peta-scale Engineering
- Gordon Bell
- Science, Nature Nano

…in this tutorial

...in this tutorial

- Why should one use a atomistic approach today?



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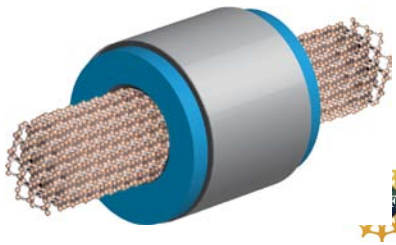
- Why should one use a atomistic approach today?
- What are the models implemented?



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- Why should one use a atomistic approach today?
- What are the models implemented?
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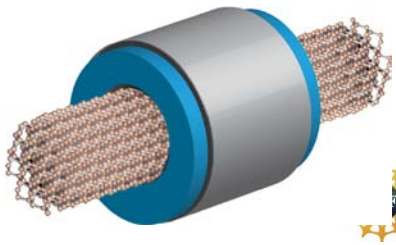

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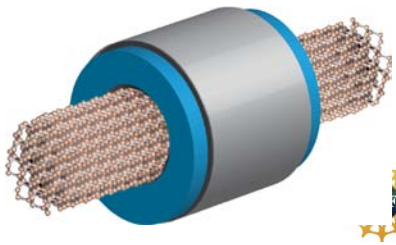
- Example of simulations



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- Why should one use a atomistic approach today?
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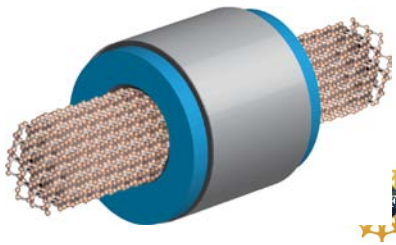
- Example of simulations
- Exercises



Why an Atomistic approach?

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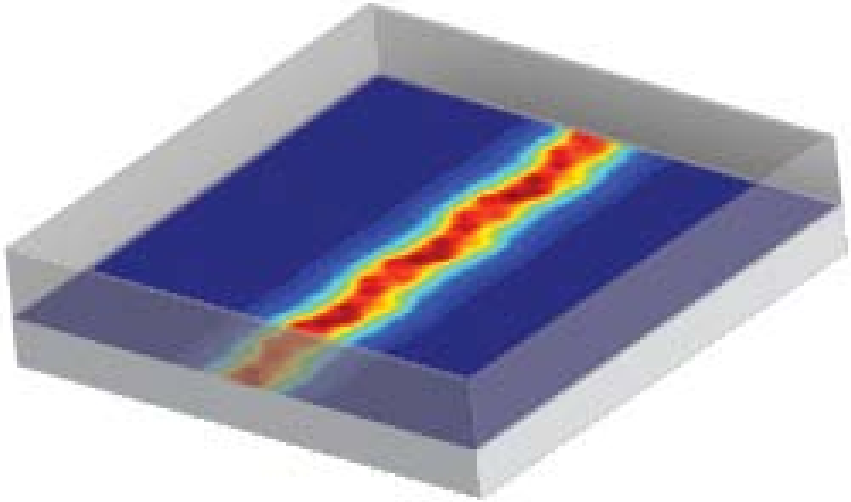
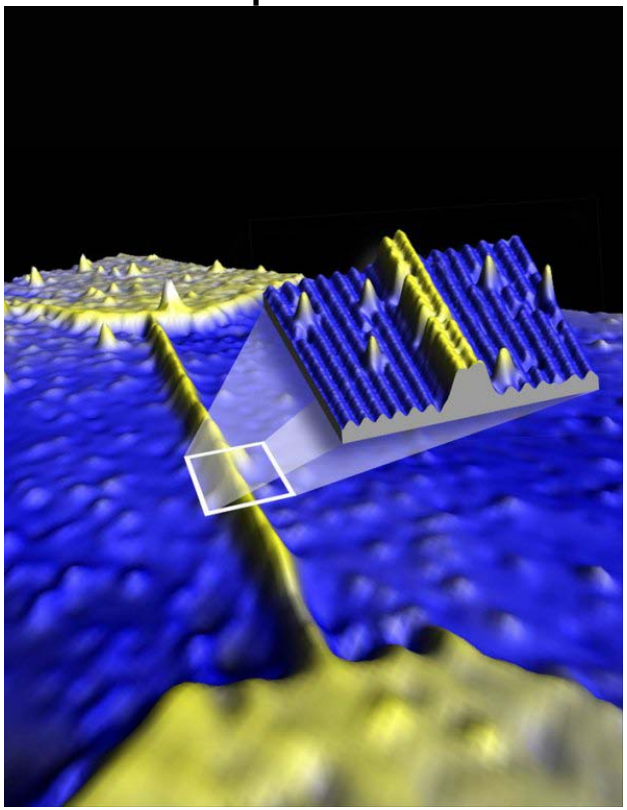
- The miniaturization of devices has reached the point where the number of atoms is countable.



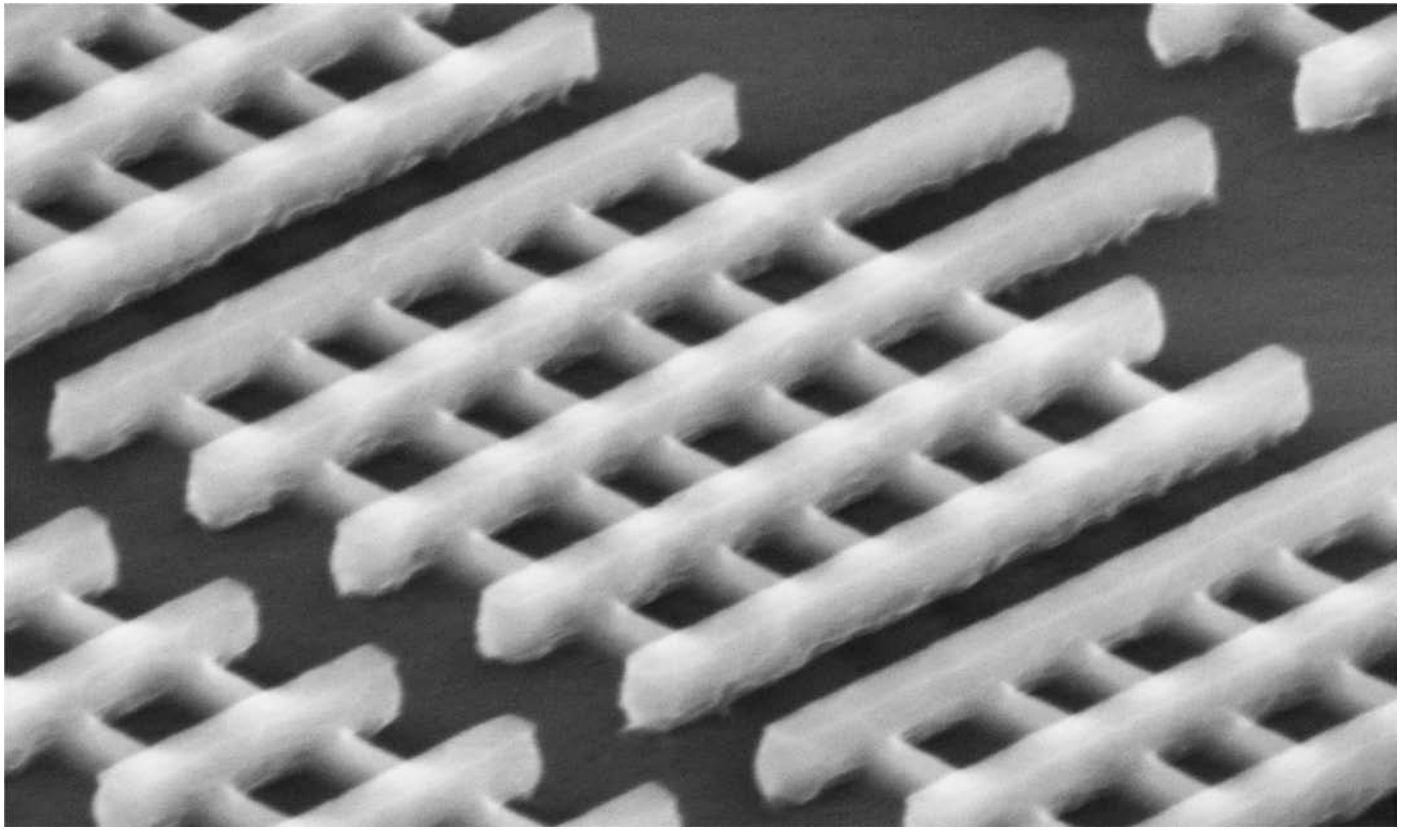


Simulation and STM image of a Silicon wire, only 1 atom tall, 4 atoms wide!!

[1] B. Weber, et al. “Ohm’s Law Survives to the Atomic Scale”, Science 6 January 2012, Vol. 335 no. 6064 pp. 64-67 DOI: 10.1126/science.1214319
[2] http://physicsforme.wordpress.com/2012/01/07/ohms-law-survives-to-the-atomic-scale/

Why an atomistic approach?

- The miniaturization of devices has reached the point where geometries are in 3 dimensions.

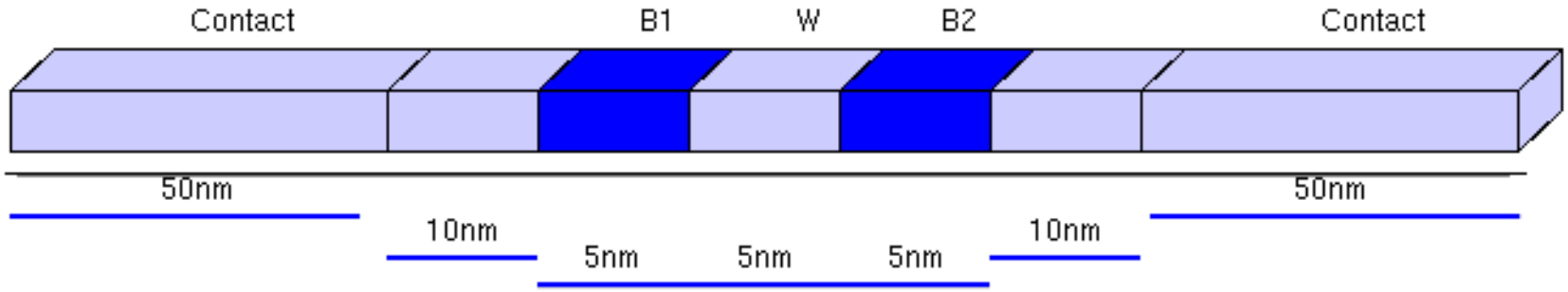


[3] www.intel.com

Multi-Scale approach

Multi-scale and Multi-Physics approaches

- Many modern devices can be considered as constituted of a fully quantum active (small) area and a fully semi-classical (big) area.

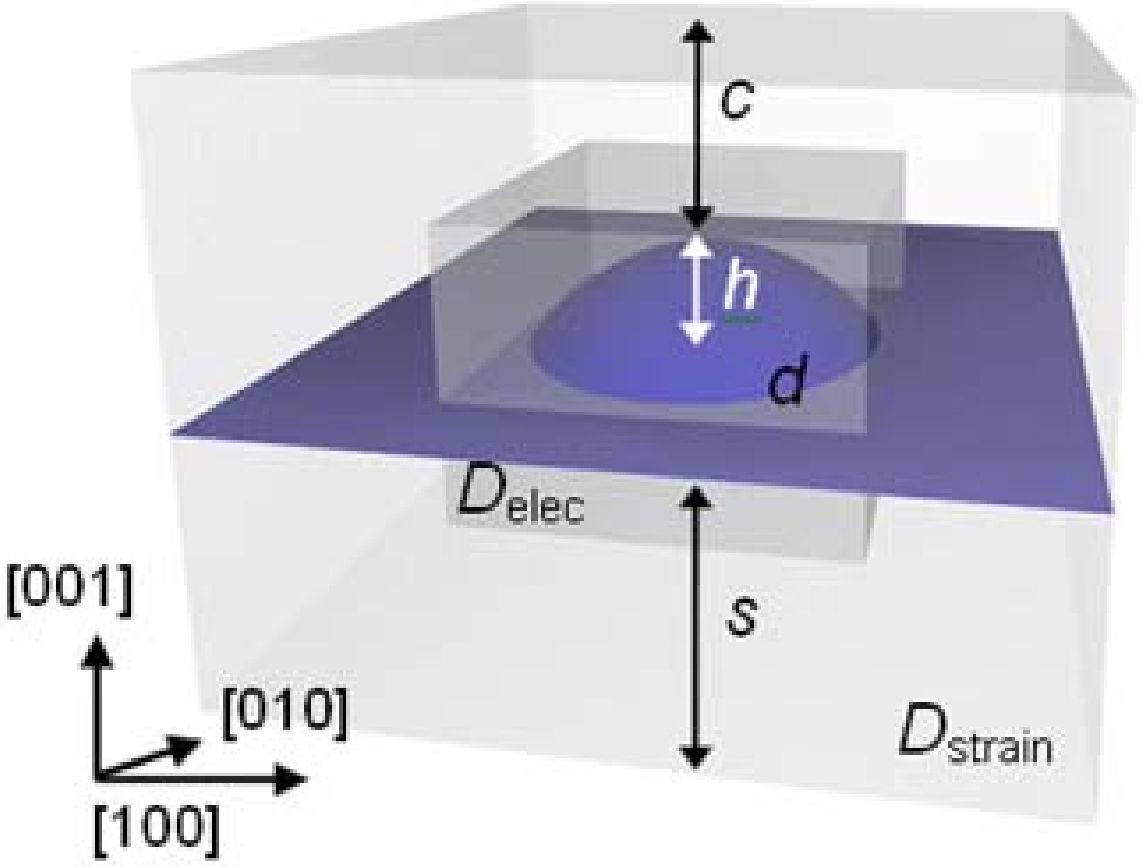


[2] http://purdue.academia.edu/GerhardKlimeck/Papers/1238240/Quantum_and_semi-classical_transport_in_NEMO_1-D

Multi-Physics approach

Multi-scale and Multi-Physics approaches

- Severa ach.



[13] M. Usman et al., "Moving Toward Nano-TCAD Through Multimillion-Atom Quantum-Dot Simulations Matching Experimental Data", IEEE Transactions on Nanotechnology, Vol. 8, No. 3, May 2009.

Multi-scale and Multi-Physics approaches

- Strain experienced by an InAs dot inside a GaAs structure.
- Wavefunctions inside a InAs dot or in a small area surrounding the InAs dot.

What are the models implemented in NEMO5?

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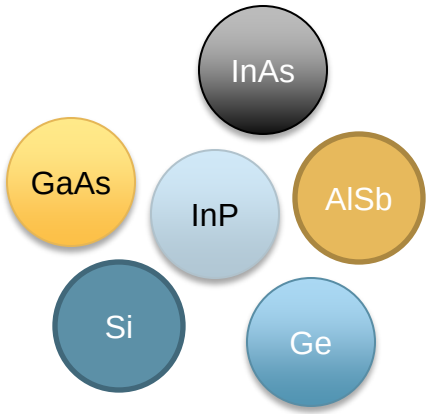
Note:

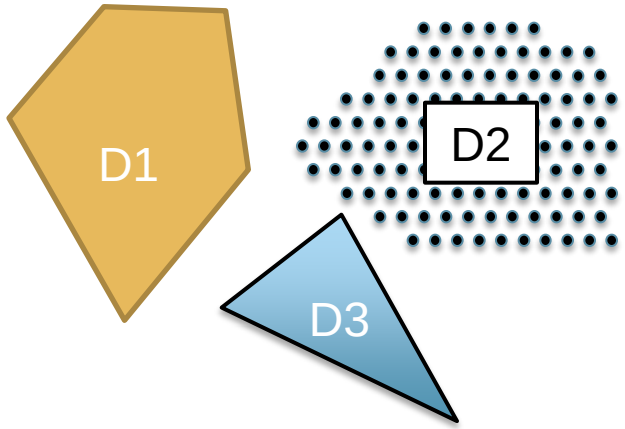
- NEMO5 can be seen as a general framework so it can virtually contain any number of model (solver).

- The real question to ask is:

  What are the model implemented so far..

What are the models implemented in NEMO5?





1. Strain
2. Schroedinger
3. Poisson
4. NEGF

`Materials` definition

Domains consist of regions
Every region has a material

`Domain` definition

Domains go to solvers

`Simulation`

Solvers interaction

Definition of solver input/output

What are the models implemented in NEMO5?

- The models/methods so far implemented in NEMO5 are divided in categories:

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  Phonons

  Electronic Structure

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  Strain models

  Phonons

  Electronic Structure

  Transport

Strain Models

Strain Models

- What is a strain?
  A crystal experiences strain when it undergoes some stress which raises its internal energy in comparison to its strain-free reference compound.

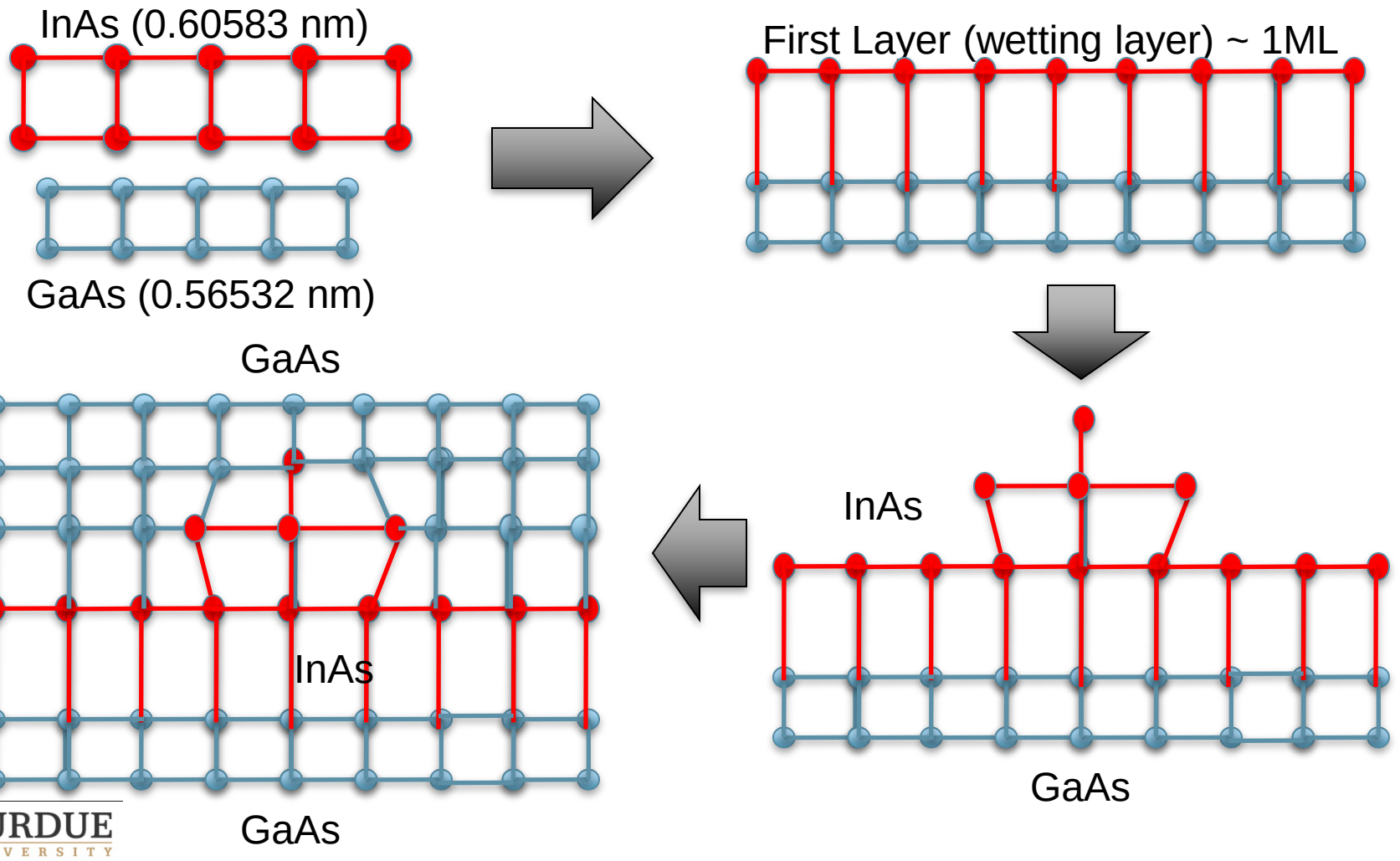
Strain Models

- What is a strain?
  A crystal experiences strain when it undergoes some stress which raises its internal energy in comparison to its strain-free reference compound.

- When does a crystal experience it?
  Nanostructures composed of materials with different lattice constants always exhibit strain.

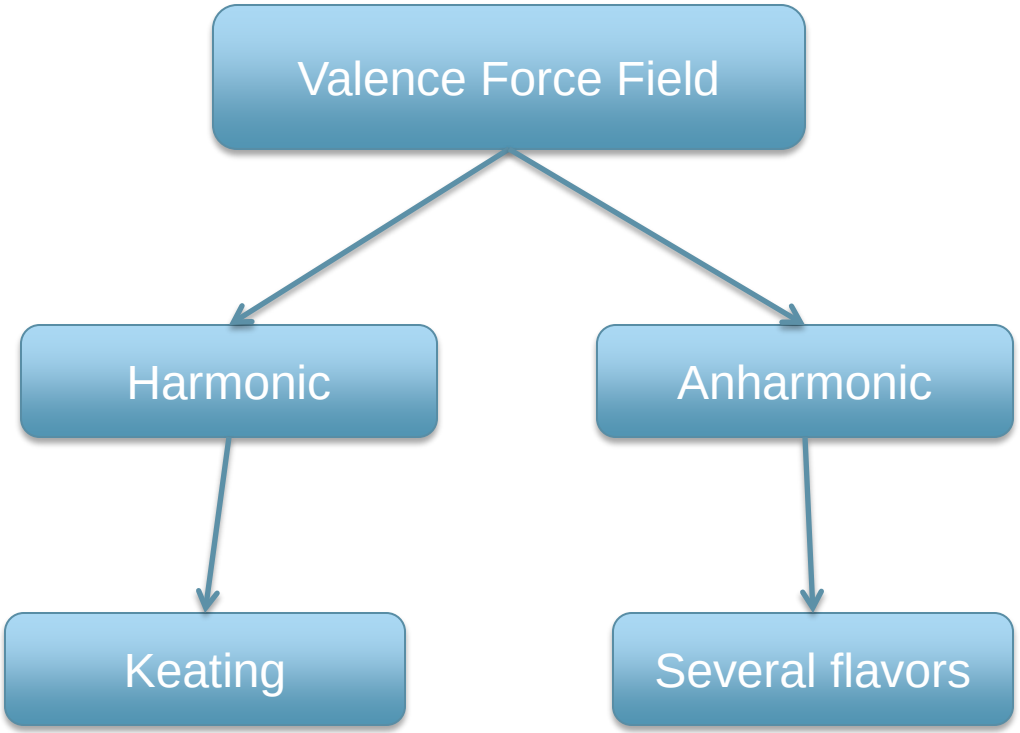
Stranski-Krastanow Growth

Self-Assembly Process ➔ InAs deposition on GaAs substrate



Strain Models

$$E_{tot} = f\left(x_1, x_2, \ldots, x_N\right)$$



Strain Models

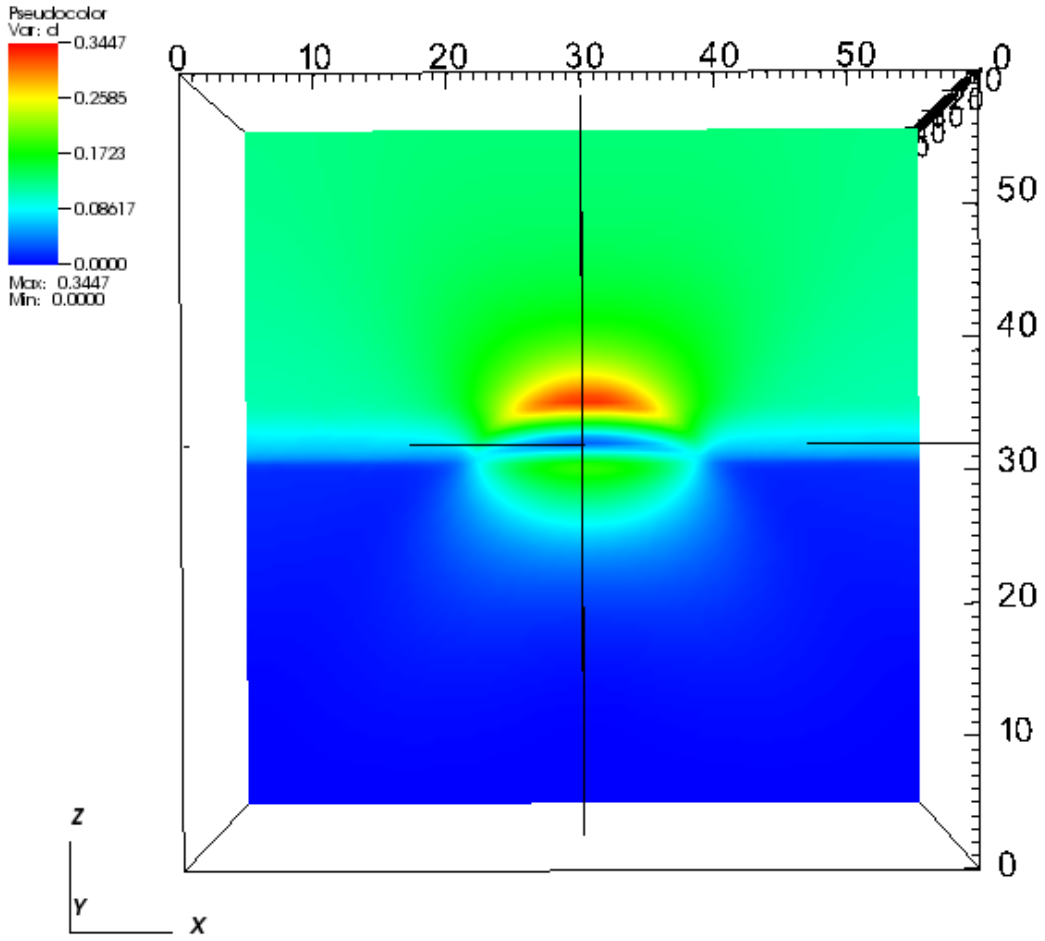
Strategy:
We calculate the total energy of the crystal and find the atoms position that minimize the total energy.

Strain Models

Strategy:
We calculate the total energy of the crystal and find the atoms position that minimize the total energy.

Method:
The minimization is done by means of a Newton optimization method that is based on the calculation of the Jacobian and the Hessian of the total elastic energy.

Strain Models



Strain Solver Options

```
name           = strain
type           = KeatingStrain
domain         = atomic_structure
active_regions = (1,2,3)
models         = harmonic
```

Strain Solver Options

```
// Newton-Raphson parameters
linsolver_max_iters = 30000
linear_solver       = bcgsl
preconditioner      = jacobi
max_num_iters       = 20000
absolute_tol        = 1e-8
relative_tol        = 1e-8
linsolver_monitor   = true
```

Strain Solver Options

- A list that may contain the following: `harmonic` or `anharmonic_Lazarenkova` or `anharmonic_Areshkin` or `anharmonic_Sui`; `stretch-bend`; `cross-stretch`; `coplanar-2ndNN`; `coulomb`.

- Which linear solver is employed in the Newton iteration. See the PETSc manual for possible choices - `gmres` is preferred.

- Which preconditioner is employed in the Newton iteration. See the PETSc manual for possible choices - `asm` is preferred. `lu` does not work for simulations with grid-parallelization.

Strain Solver Options

- Maximum number of Newton iterations.
- Absolute tolerance convergence criterion of the Newton iteration.
- Relative tolerance convergence criterion of the Newton iteration.

Strain Solver Options

- More options in the manual…

Electronic Structure

Electronic Structure

- Electronic structure of a device can be studied by means of Schroedinger-Poisson systems in tight-binding formalism.

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- Electronic structure of a device can be studied by means of Schroedinger-Poisson systems in tight-binding formalism.

Schroedinger equation - tight-binding.

Poisson equation - Finite Element Mesh (FEM).

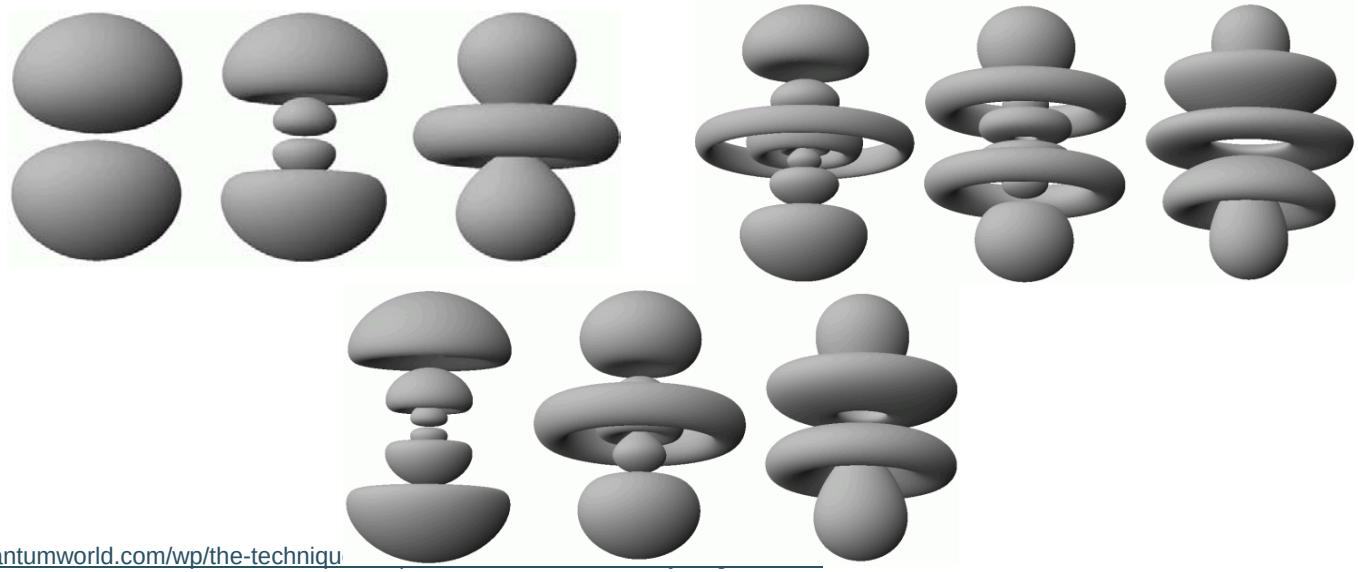
$$[H]\{\Psi\} = E\{\Psi\}$$

Tight-Binding Method

- The underlying ideas of the tight-binding approach are:

  electrons are considered to be tight binded to the potential core.

  selection of a basis consisting of atomic orbitals (such as *s*, *p*, *d*, *f*, and *s**) centered on each atom.

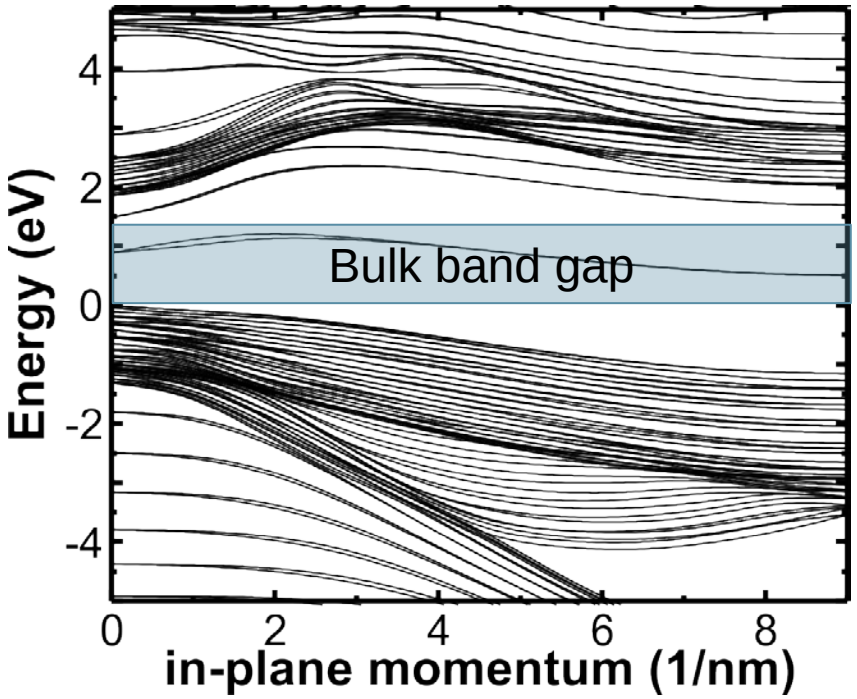


[12] http://thisquantumworld.com/wp/the-techniqu

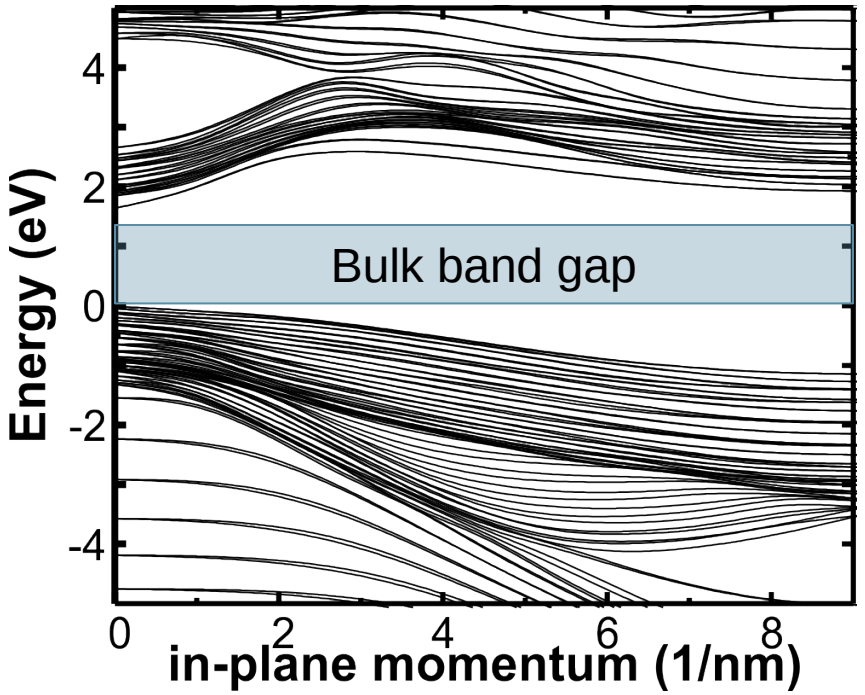
A few words on passivation

In-plane quantum well bandstructure

Bare surfaces

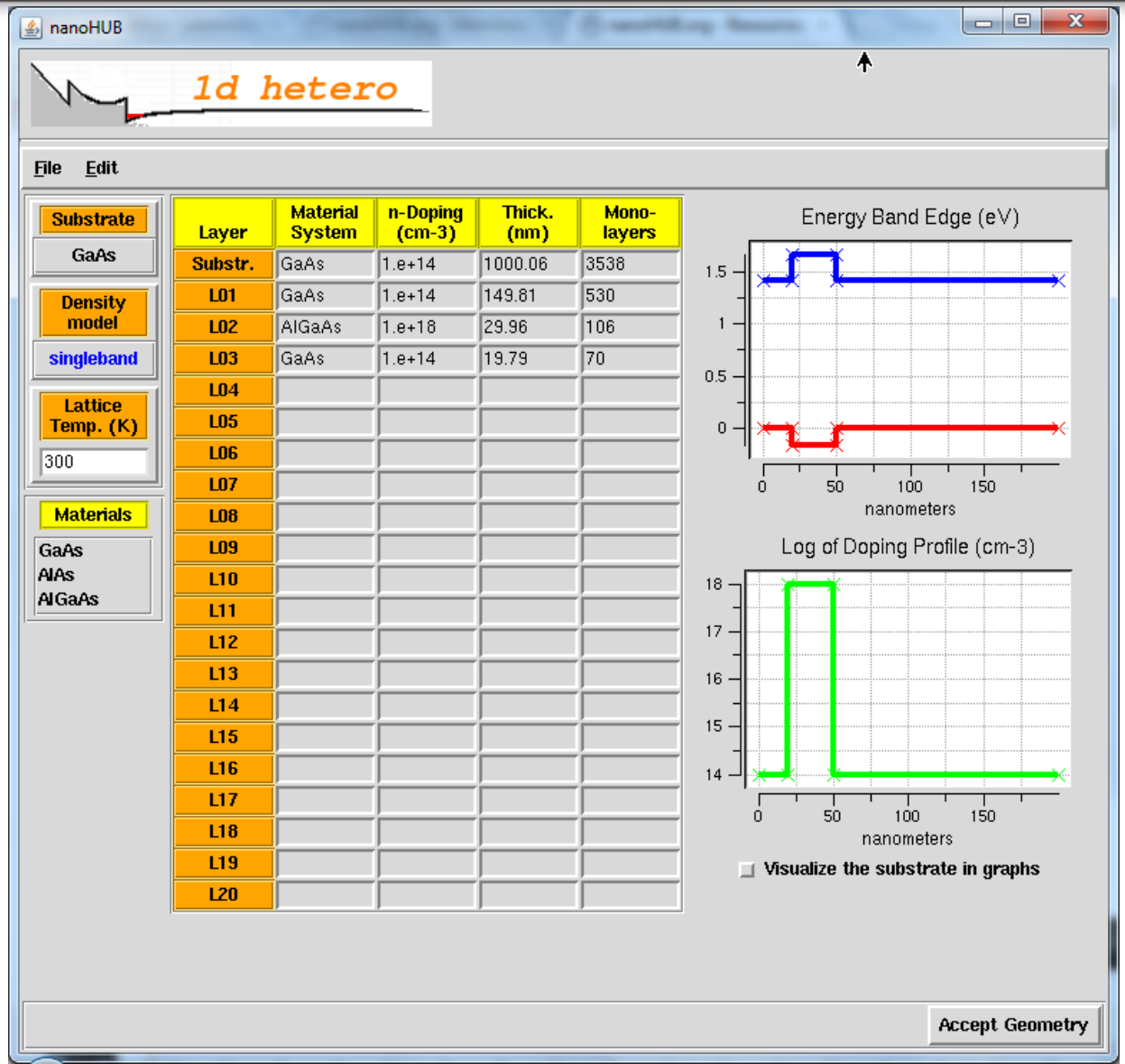


Passivated surfaces



Result:
Surface states successfully shifted to high energies

Example: 1Dhetero



Poisson Solver Options

```
name                = poisson
type                = Poisson
domain              = continuum
active_regions = (1,2,3)

// outputs
fem_output                  = (potential)
atomistic_output            = (potential)

density_solver = ()
```

Poisson Solver Options

```
ksp_type         = gmres
pc_type          = ilu
charge_model     = electron_hole
rel_tolerance    = 1e-6
```

Poisson Solver Options

```
boundary_condition
{
 type                = ElectrostaticContact
 name                = source
 boundary_regions    = (1)
 voltage             = 0.0                  // in Volt
}
boundary_condition
{
 type                = ElectrostaticContact
 name                = drain
 boundary_regions    = (2)
 voltage             = 0.1                  // in Volt
}
```

Poisson Solver Options

- Save atom-based quantities to file. The list can contain the entries `potential`, `charge`, `charge_cm-3`, `free_charge`, `free_charge_cm-3`, `doping`, `doping_cm-3`, `conduction_band` and `valence_band`. For simulations without grid parallelization VTK is used as output format, otherwise Silo.

Poisson Solver Options

- If `true`, then the potential is written to (sim-name)_nodal_potential.dat.

Poisson Solver Options

- Interpolates atom-based quantities onto an axis and generates 1D ASCII output compatible with 1D Matlab-plots. The list can contain the entries `potential`, `free_charge_cm-3`, `doping_cm-3`, `conduction_band` and `valence_band`.

Poisson Solver Options

- If `true` then unit cells are used for the 1D discretization along some direction and some averaging is done within the cells. If `false` then the orthogonal projection of the atomic position serves as the 1D discretization.

Poisson Solver Options

- Linear solver type. See the PETSc documentation for possible choices. Recommended are e.g. `gmres` or `bcgs`.

Poisson Solver Options

- Preconditioner type. See the PETSc documentation for possible choices. Recommended are e.g. `asm` for distributed-grid simulations, `lu` for small systems or `jacobi`.

Poisson Solver Options

- In case of an iterative linear solver, this is the maximum number of iterations to solve the linear system.

Poisson Solver Options

- Maximum number of Newton iterations (default: 100).
- Not sure what the difference to the previous option is.
- Maximum number of Newton right-hand-side evaluations (default: 1000).
- Relative residual tolerance of the Newton solver (default: 1e-6).

Poisson Solver Options

- Absolute step tolerance of the Newton solver (default: 1e-10).

- Relative step tolerance of the Newton solver (default: 1e-10).

Poisson Solver Options

- More options in the manual…

Schroedinger Solver Options

```
// eigensolver options
// ====================
eigen_values_solver          = krylovschur
max_number_iterations        = 8000
convergence_limit            = 1e-9
monitor_convergence          = true
preconditioner               = mumps
ncv                          = 42
shift                        = 1.10
solver_transformation_type = sinvert
eps_orthog_refinement        = never
```

Schroedinger Solver Options

```
// number of eigenvalues
// ======================
number_of_eigenvalues = 7

// specify the tight-binding model
// ================================
tb_basis = sp3d5sstar_SO

job_list  =  (passivate_H,calculate_band_structure)
output    = (energies,eigenfunctions_Point3D,eigenfunctions_Silo)


potential_solver = poisson

k_space_basis    = cartesian
k_points         = [(0,0,0)]
number_of_nodes = (1)
```

Schroedinger Solver Options

- sp3sstar, sp3sstar_SO, sp3d5sstar, sp3d5sstar_SO

- A list that deterimes what is done. Choose from assemble_H, passivate_H, include_strain_H, include_shear_strain_H, calculate_band_structure, electron_density, derivative_electron_density_over_potential, hole_density, derivative_hole_density_over_potential, spin, DOS. assemble_H is activated by any other option automatically.

Schroedinger Solver Options

- Which eigenvalue solver to use. Setting `lapack` always computes all eigenvalues and is feasible only for very small systems. Recommended choices are `krylovschur` and `arpack`. Other choices are `arnoldi`, `jd`, `gd`.

Schroedinger Solver Options

- Which eigenvalue solver to use. Setting `lapack` always computes all eigenvalues and is feasible only for very small systems. Recommended choices are `krylovschur` and `arpack`. Other choices are `arnoldi`, `jd`, `gd`.

Lanczos Solver

Schroedinger Solver Options

- Choose from `Hamiltonian`, `energies`, `k-points`, `DOS`, `electron_density`, `electron_density_VTK`, `hole_density`, `hole_density_VTK`, `ion_density`, `eigenfunctions`, `eigenfunctions_k0`, `eigenfunctions_VTK`, `eigenfunctions_VTK_k0`, `eigenfunctions_Silo`, `eigenfunctions_Silo_k0`, `spin`.

- Accuracy of saved eigenvalues within output file.

Schroedinger Solver Options

- The (optional) name of the simulation object where the electrostatic potential is drawn from.

- Only relevant for `calculate_band_structure`. This parameter is a list of points in k-space along which the band structure is calculated.

- This list gives the uniform discretization of each segment set by the `k_points` parameter (note that specifying N points means $N-1$ segments). For density calculations, setting this parameter to 0 leads to computation of $k = 0$ only and application of an analytical formula that assumes parabolic subbands.

Schroedinger Solver Options

- Linear solver employed in the shift-and-invert operation. This should be preferable a direct linear solver since the LU factorization can be reused during the Krylov iterations.

- (default: `lu`) Preconditioner employed in the shift-and-invert operation.

- Eigensolver shift. Not sure when this is relevant, but only in few cases.

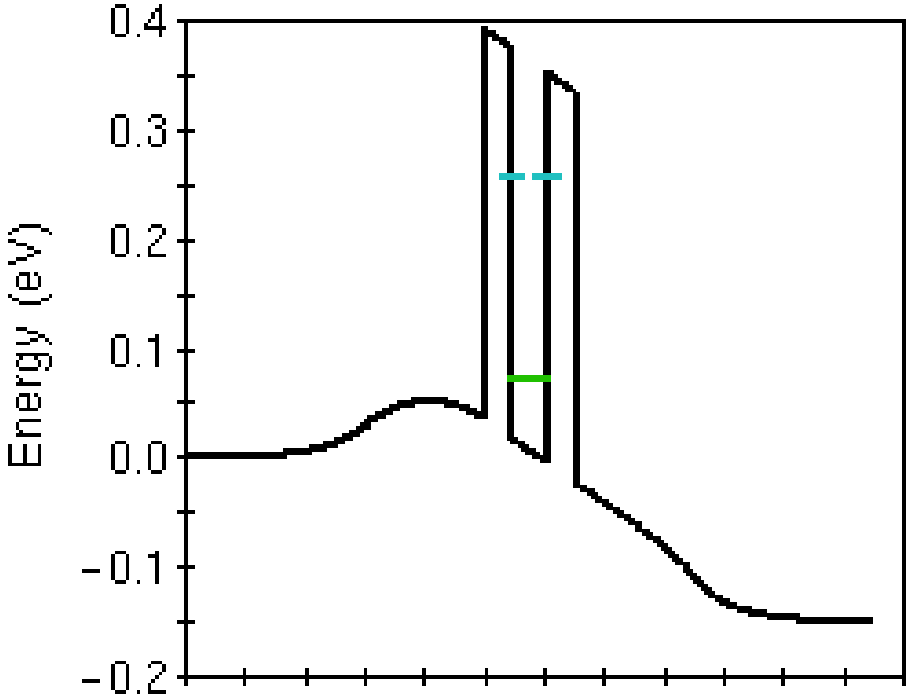
- When set to `true`, terminal output related to the Krylov iteration is generated.

Schroedinger Solver Options

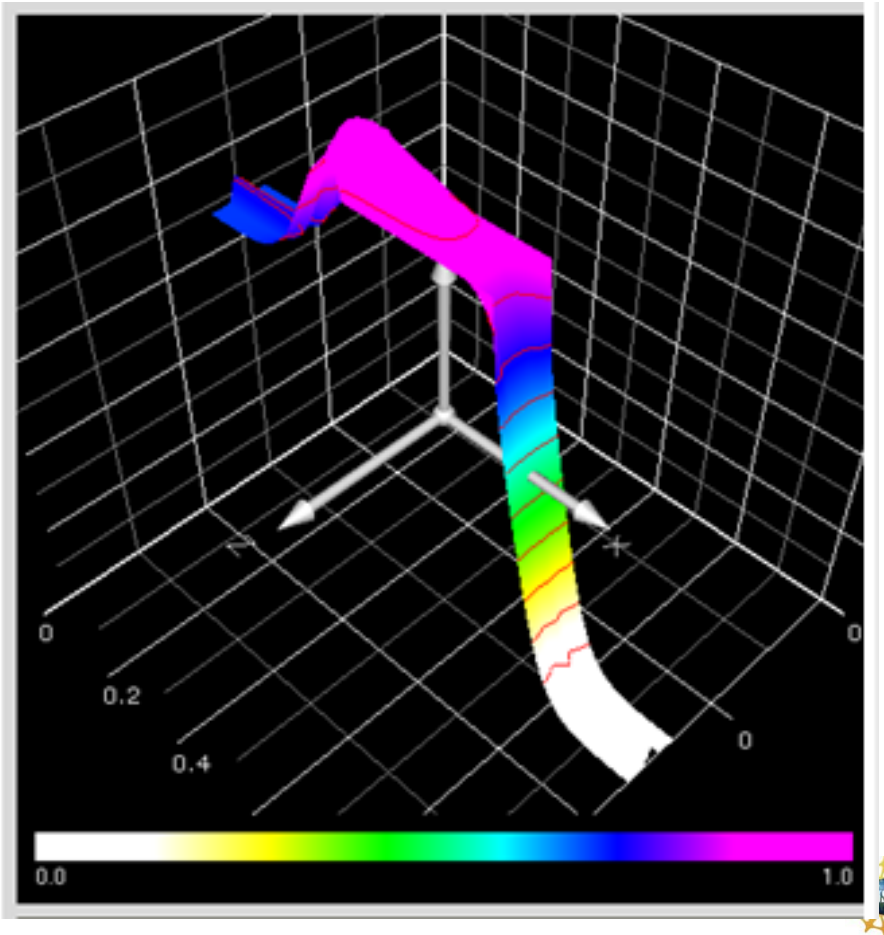
- More options in the manual…

Transport

Transport



[15] https://engineering.purdue.edu/gekcogrp/software-projects/nemo1D/



Transport

- Non-equilibrium Green functions (NEGF) formalism is a very powerful way for the simulation of charge transport from a quantum perspective. It easily includes:

Transport

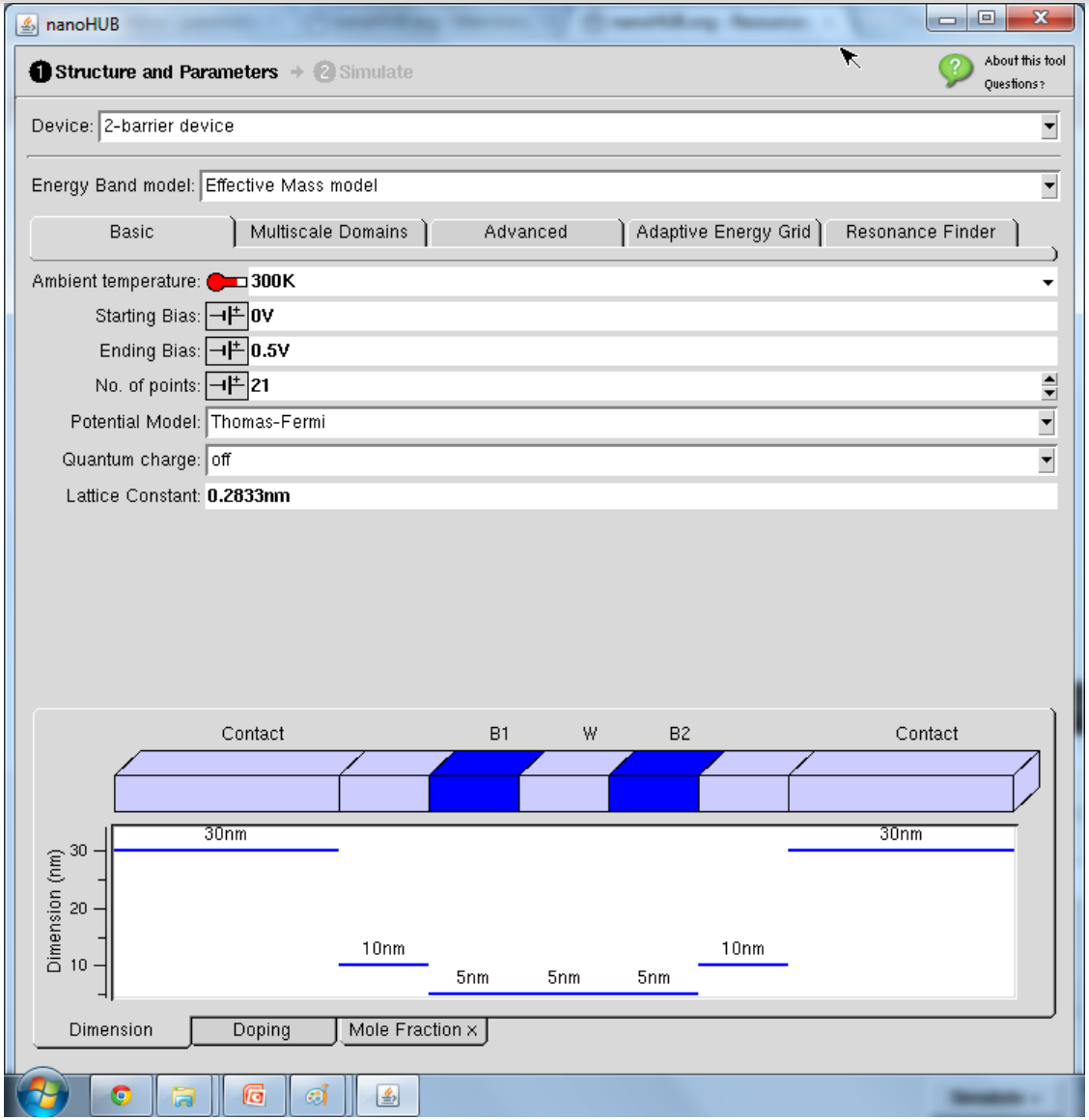
- Non-equilibrium Green functions (NEGF) formalism is a very powerful way for the simulation of charge transport from a quantum perspective. It easily includes:

  Fully quantum transport (not just quantum corrections)

  Open boundary conditions (contacts)

  Inclusion of realistic scattering

Example: RTDNEGF



Transport

- Semiclassical density calculations

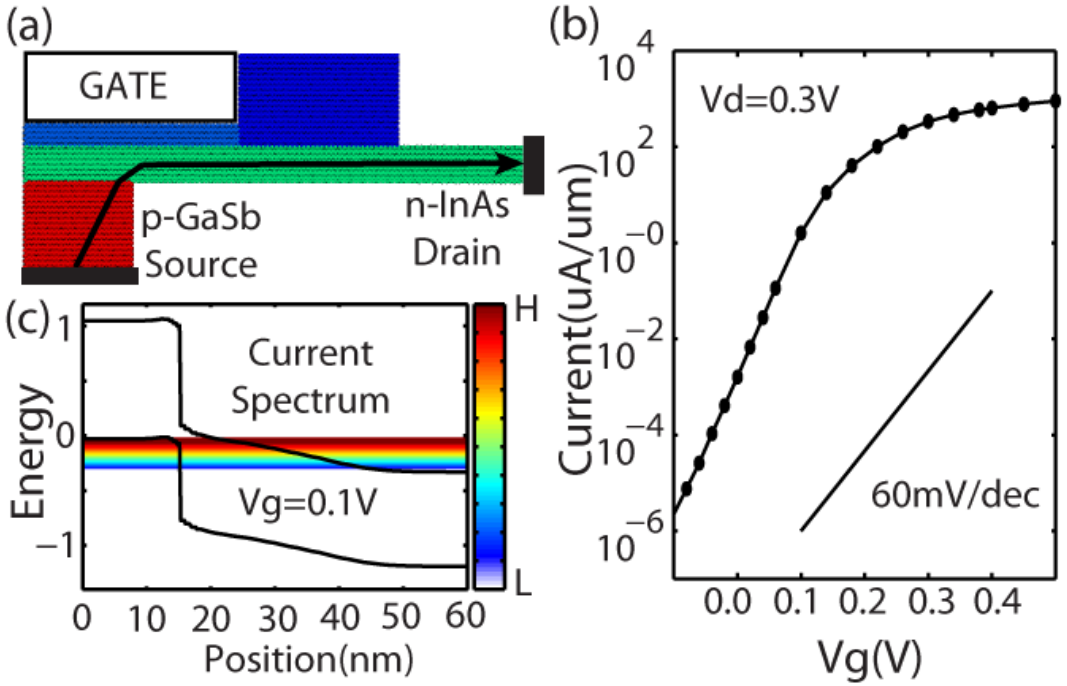
$$n = N_C F_{1/2}(\eta_F)$$

- Continuum
- Effective mass
- Parabolic band

Fermi-Dirac Integral

Poisson Equation

faster NEGF calculations!



[17] Z. Jiang, et al., "Quantum Transport in GaSb/InAs nanowire TFET with semiclassical charge density", Poster at IWCE 2012.

Semi-classical Solver Options

```
potential_solver = my_potential_solver
fermilevel_solver = my_density_solver
equilibrium_contacts = (source_contact, drain_contact, gate)
equilibrium_regions = [(1, 6), (2), (3, 4, 5)]
```

```
Ef_approximation = average
fermilevel  = 0.0
temperature = 300
```

Semi-classical Solver Options

- The name of the simulation where the electrostatic potential is computed.
- (default: false) This boolean determines whether a selfconsistent iteration with the potential solver is done.
- Atom-based output to be generated in the end. Can be `transmission`, `potential`, `free_charge`, `free_charge_cm-3`, `current`, `electron_energy` (average electron energy $\frac{\int dE\ En(x,E)}{\int dE\ n(x,E)}$) and `hole_energy`.

Semi-classical Solver Options

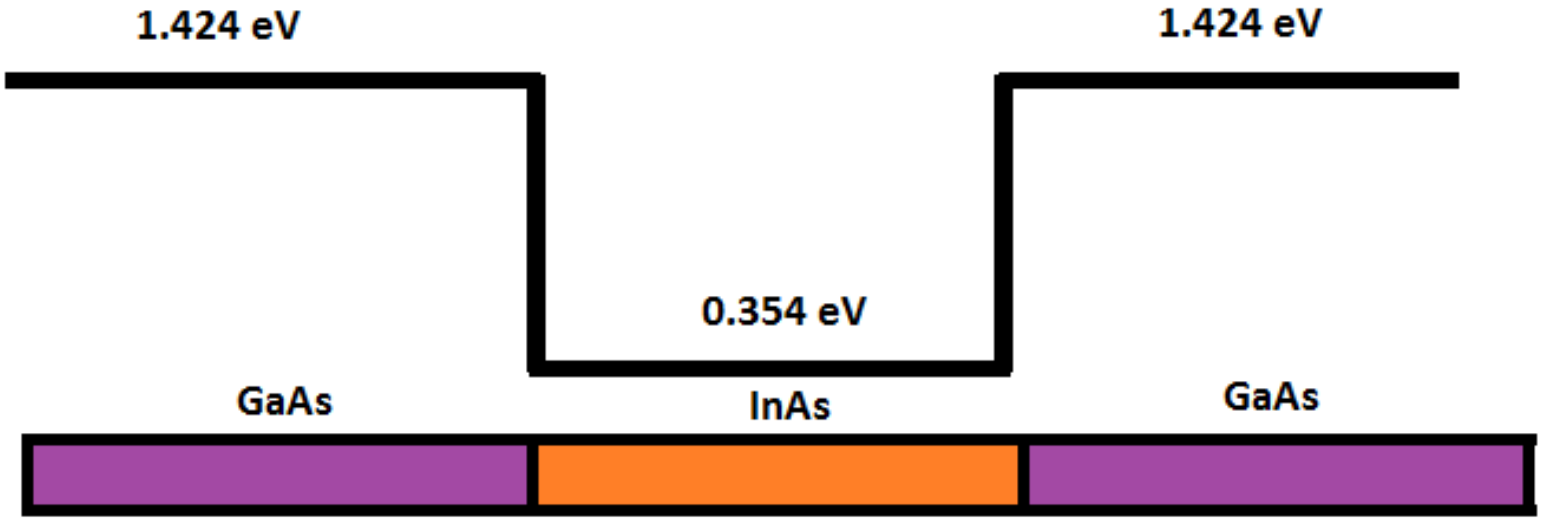
- More options in the manual…

Example and Exercises

Example and Exercises

- Let us see a simple example:

  calculate the wavefunctions of a very small quantum well GaAs-InAs-GaAs with strain and applied potential.



Example and Exercises

- The solver needed for this exercise will be:

  1) Strain solver

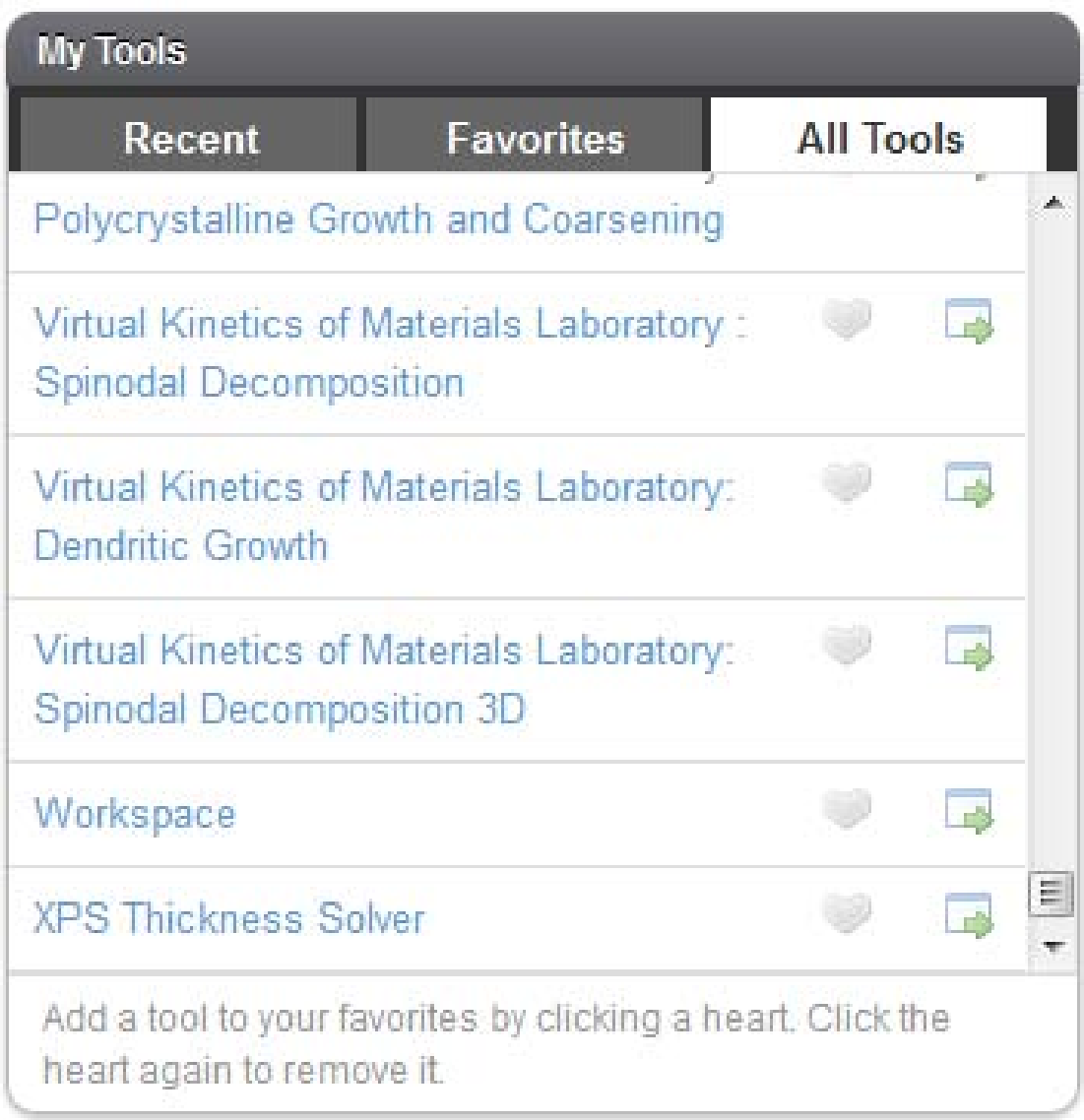
  2) Poisson solver

  3) Schroedinger solver

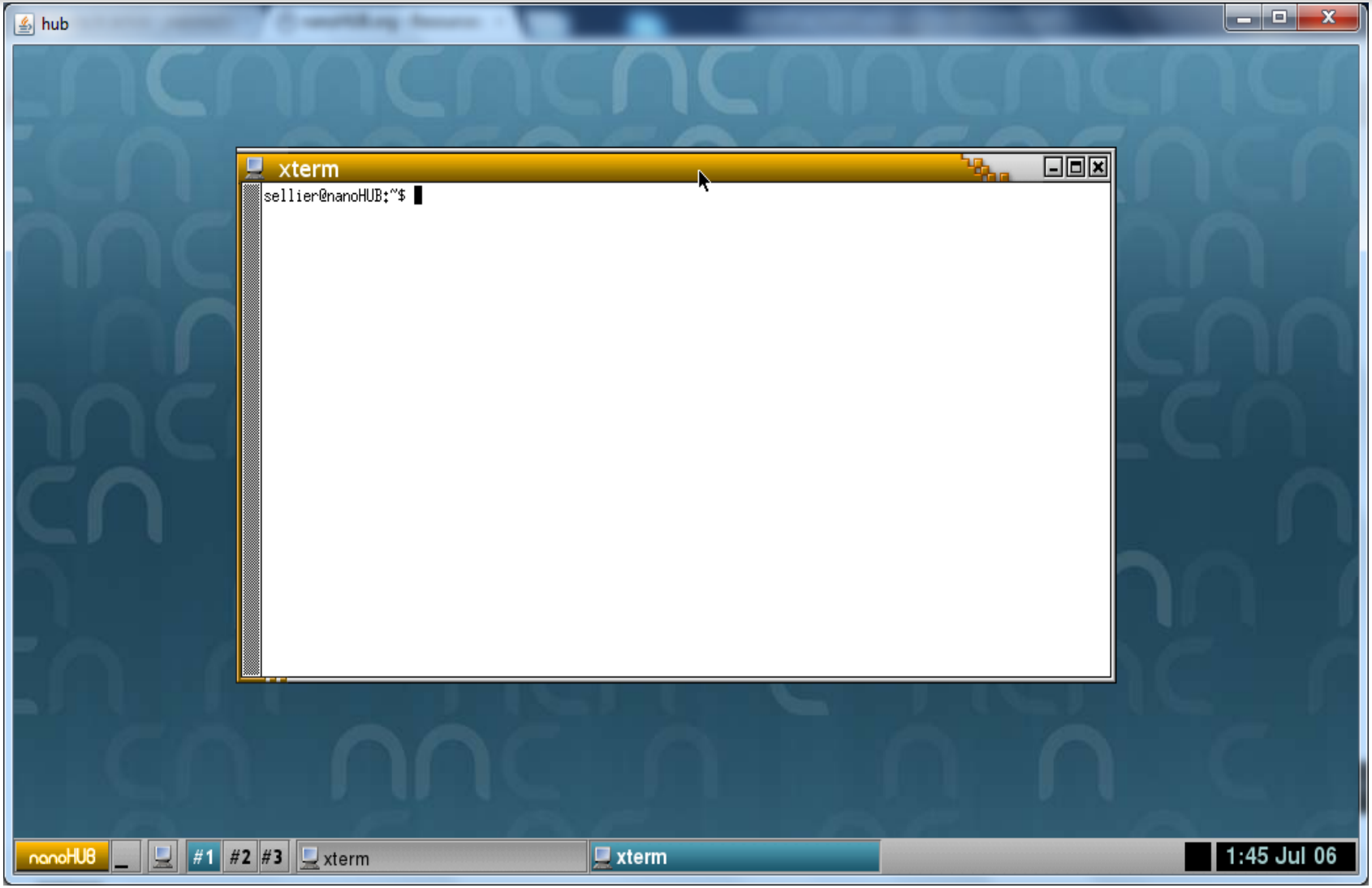
Example and Exercises

- www.nanohub.org
- Login in
- Click on “MyHUB”

Example and Exercises



Example and Exercises

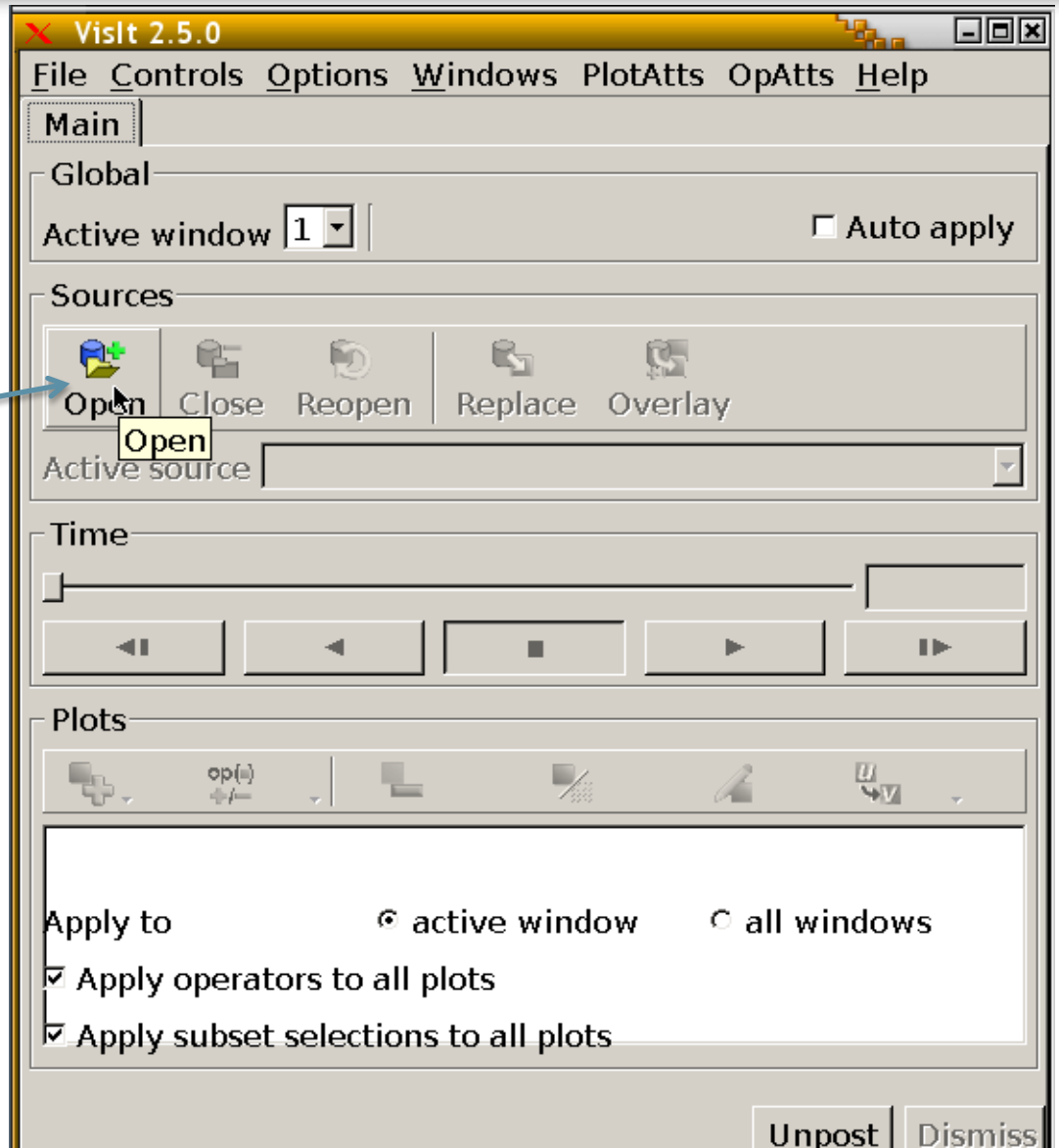


Run the simulation

- The command is (in a shell)

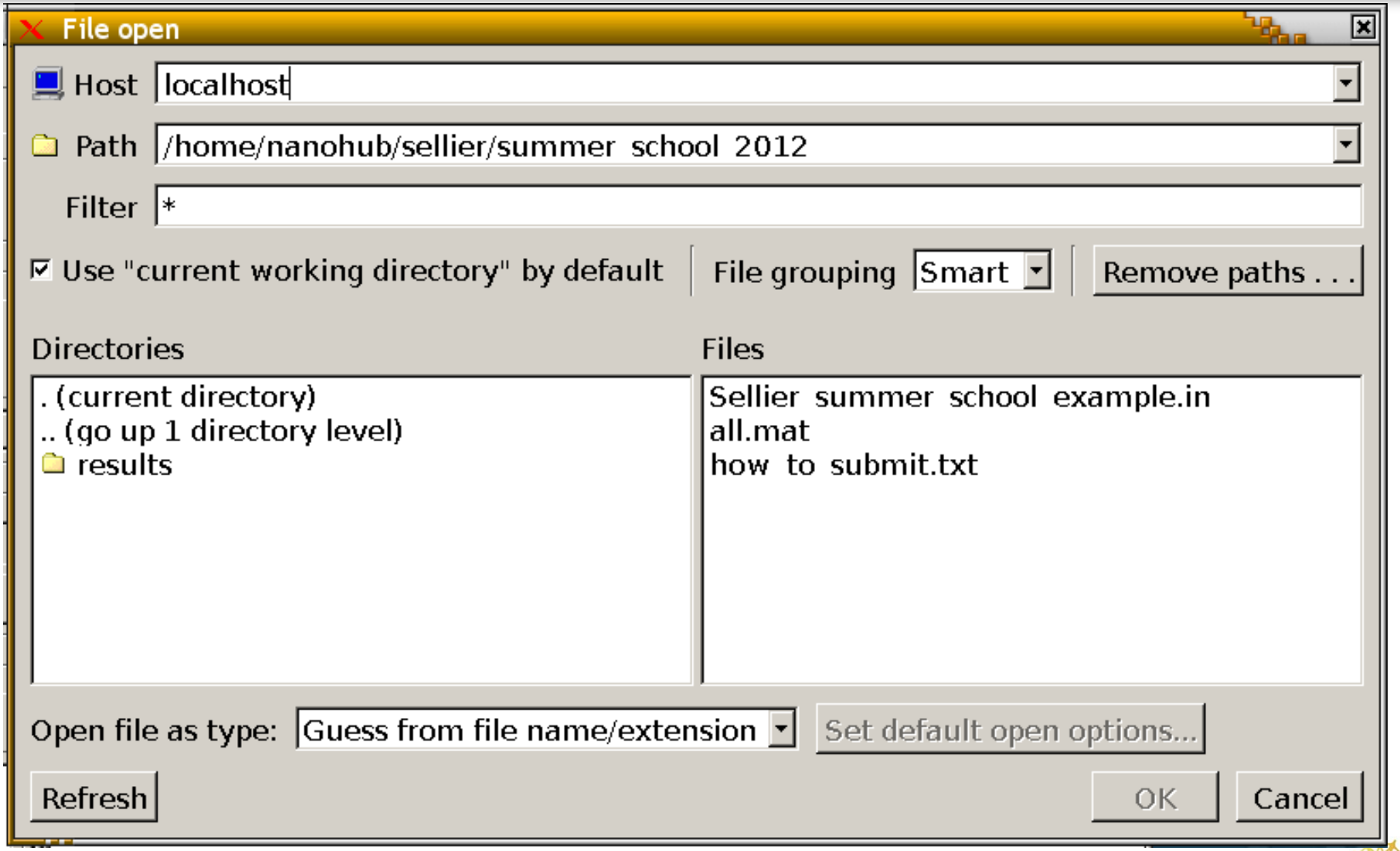
> submit -v coates -i ./all.mat nemo-r7962 Sellier_summer_school_example.in

Visualization: VisIt



Click here

Visualization: VisIt



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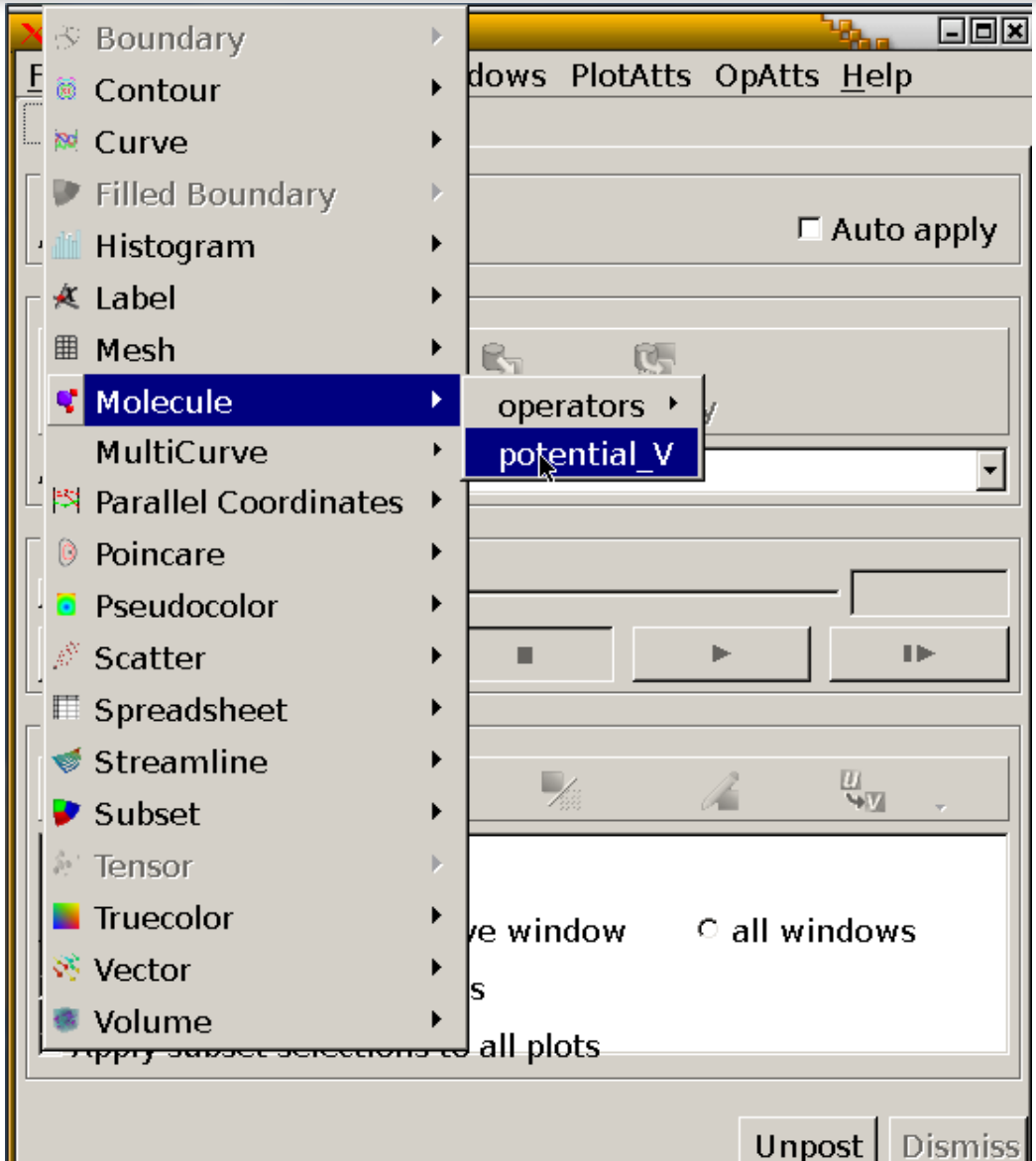
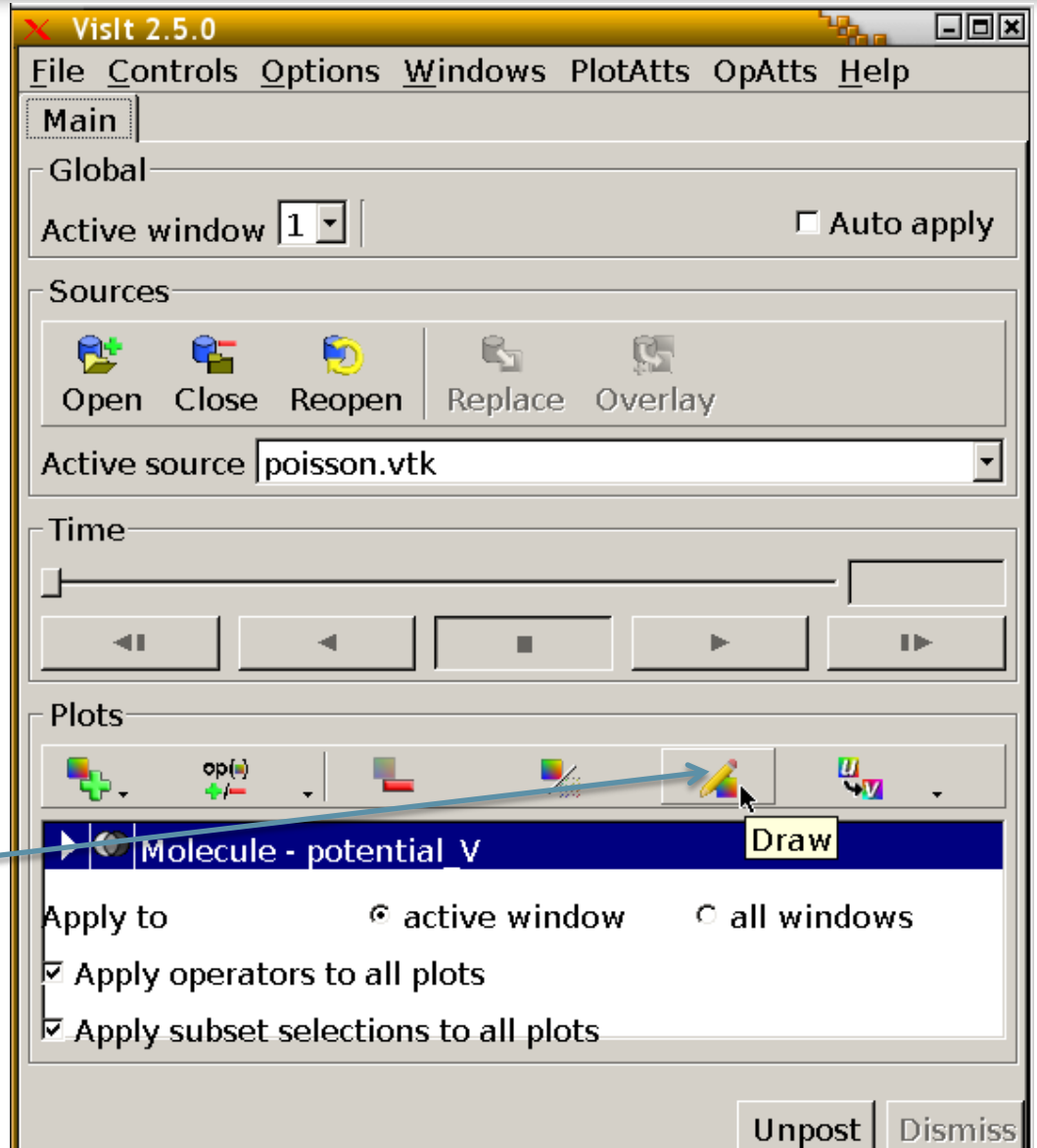
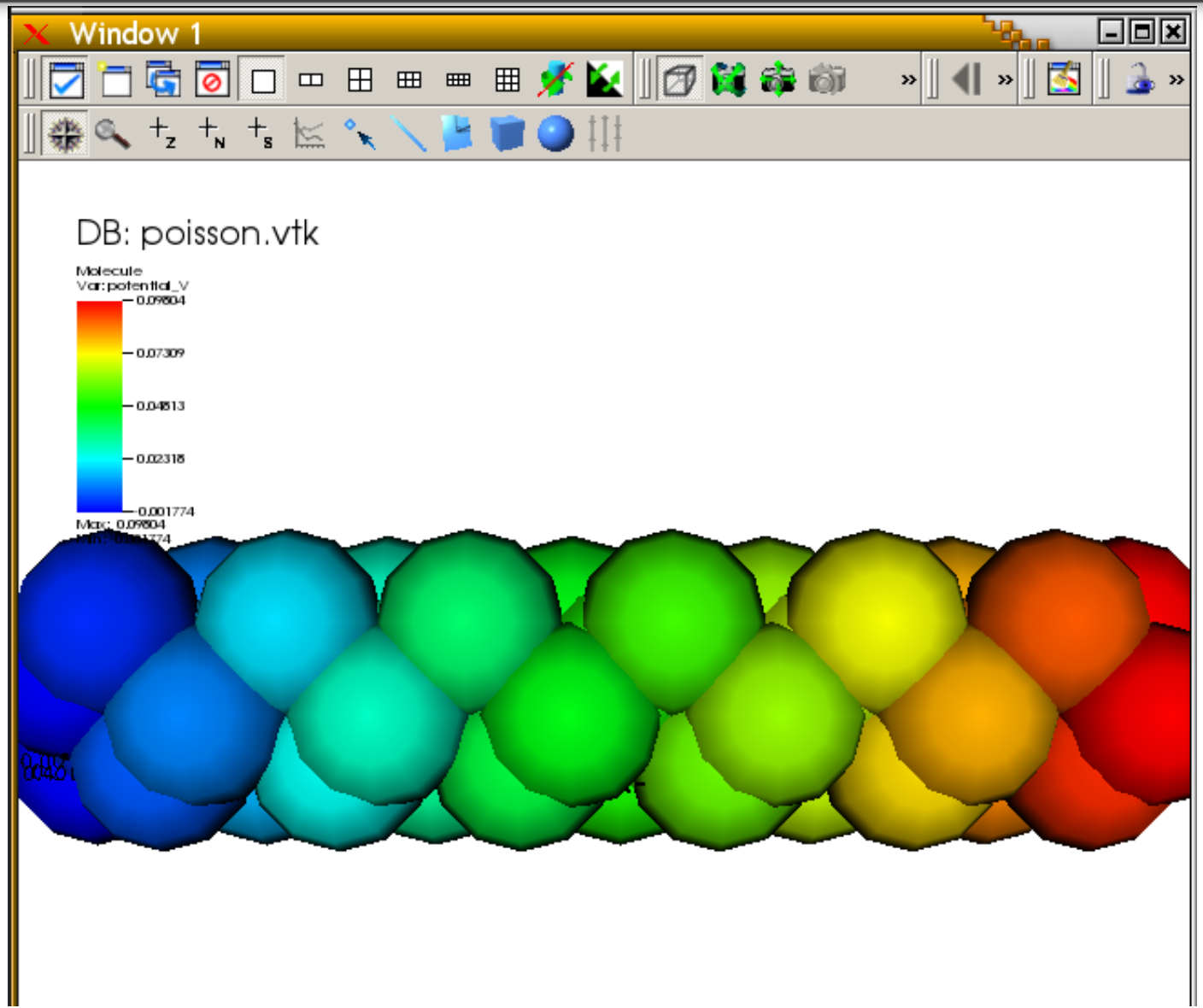


Visualization: VisIt

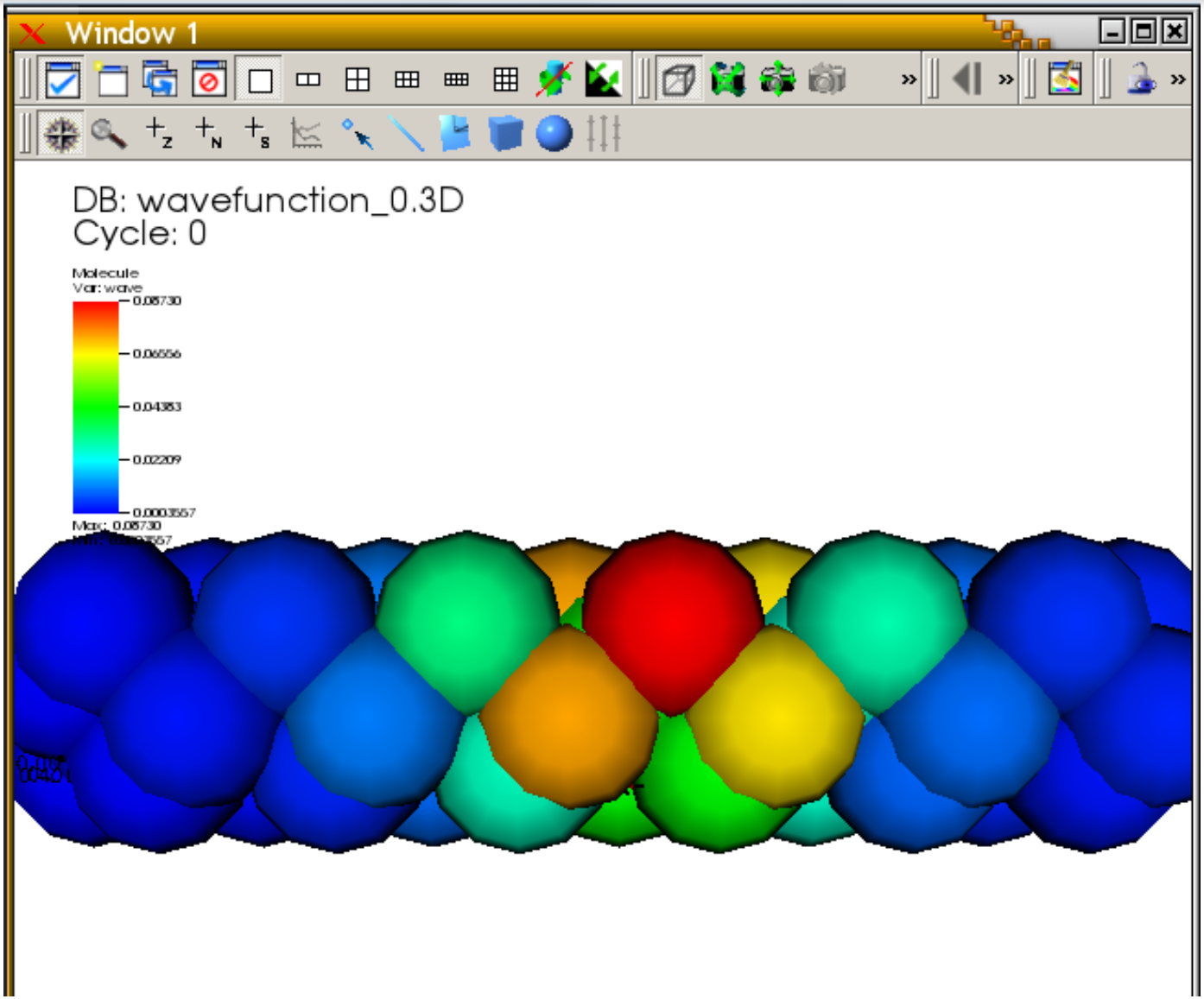


Click here

Visualization: Potential



Visualization: Wavefunctions



Thanks!

THANKS!

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