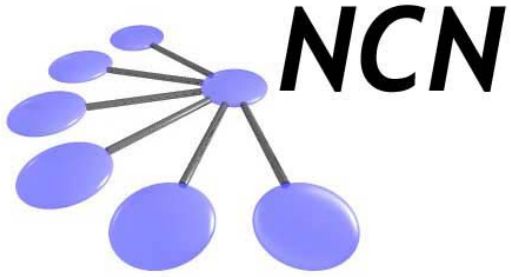
Tutorial 2: Input & output in NEMO5



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Michael Povolotskyi, Tillmann Kubis, James Fonseca,
Jean Michel Sellier, Daniel Mejia

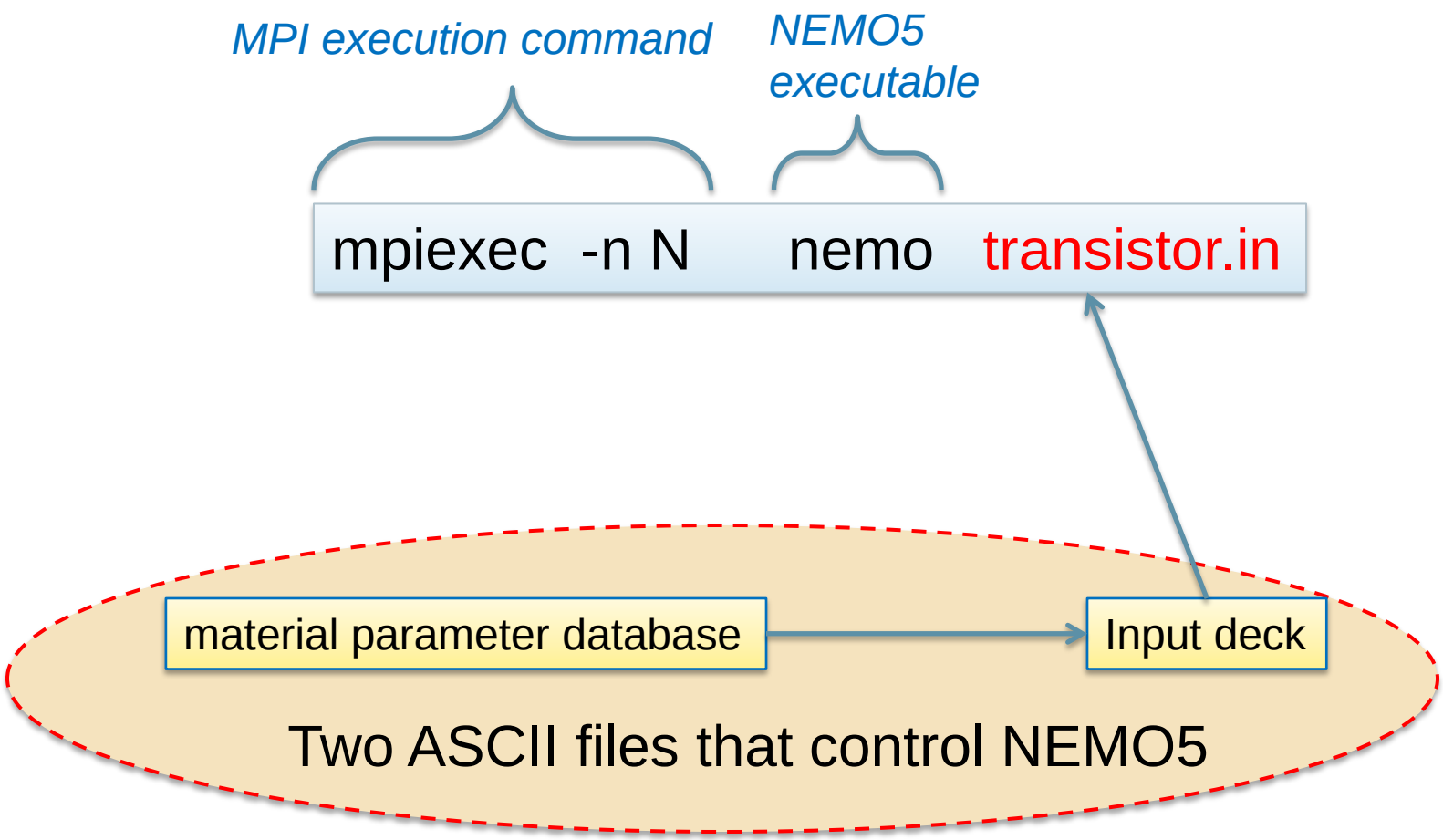
Network for Computational Nanotechnology (NCN)
Purdue University, West Lafayette IN

Synopsis

1. How to control the simulator?
2. The NEMO5 input deck.
3. Creation of atomic structures.
4. Visualization of the atomistic output (structure).
5. Creation of Finite element mesh.
6. Visualization of finite element data (electric potential).

How to control the simulator? (I)

If you have NEMO5 installed in your system:



How to run the code? (III)

User editable files

» Simulations are controlled by input deck

```
163 Solvers
164 {
165 »   solver
166 »   {
167 »   »   name           = quantum_electron
168 »   »   type           = Schroedinger
169 »   »   domain         = atomic_structure
170 »   »   active_regions = (1)
171 »
172 »   »   job_list = (electron_density, derivative_electr
173 »   »   output   = (electron_density, electron_density_
174
175 »   »   eigen_values_solver   = krylovschur
176 »   »   number_of_eigenvalues = 100
177 »   »   max_number_iterations = 5000
```

» Material parameters are stored in a database file

```
5067
5068 group GaSb {
5069 »   group Bands {
5070 »   »   group TB {
5071 »   »   »   group sp3d5sstar_SO {
5072 »   »   »   »   group param_Hegde  {
5073 »   »   »   »   »   VBO        = 0.77;
5074 »   »   »   »   »   VBO_ref    = "Vurgaftman 2001";
5075 »   »   »   »   »   # VBO          = 0.0;
5076 »   »   »   »   »   E_S_Ga       = -0.505375 + VBO;
5077 »   »   »   »   »   E_Px_Ga      = 7.15106 + VBO;
5078 »   »   »   »   »   E_Py_Ga      = 7.15106 + VBO;
5079 »   »   »   »   »   E_Pz_Ga      = 7.15106 + VBO;
5080 »   »   »   »   »   E_Sstar_Ga   = 20.6223 + VBO;
5081 »   »   »   »   »   E_Dxy_Ga     = 9.31722 + VBO;
```

- The input deck files are created by a user.
- The input deck files are written in “NEMO5 input language” or in Python.
  Now we learn the “NEMO5 input language” which is sufficient for any simulation.
- The database file is provided, but can be changed by an experienced user.

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The NEMO5 input deck (I)

- Input deck is an ASCII file – can be opened by any text editor…
- Input deck consists of **blocks** surrounded by "**{**" and "**}**"
- a block contains other blocks and/or **options**
- options are assignments like:
  voltage = 1.0
  k_vector = (0.0, 0.5, 0.5)
- C++ style comments are supported

block name

```
Solvers
{
  solver
  {//solver for the electron density
     name            = quantum_electron
     type            = Schroedinger
     domain          = atomic_structure
     active_regions = (1,2,3)

     job_list = (electron_density)

     eigen_values_solver   = krylovschur
     number_of_eigenvalues = 10
     max_number_iterations = 3000
     convergence_limit     = 1e-12
  }
}
```

Input deck fragment

The NEMO5 input deck. (II)

There are 3 blocks in the input deck:

```
Structure
{

}
```

defines material and simulation domains

```
Solvers
{

}
```

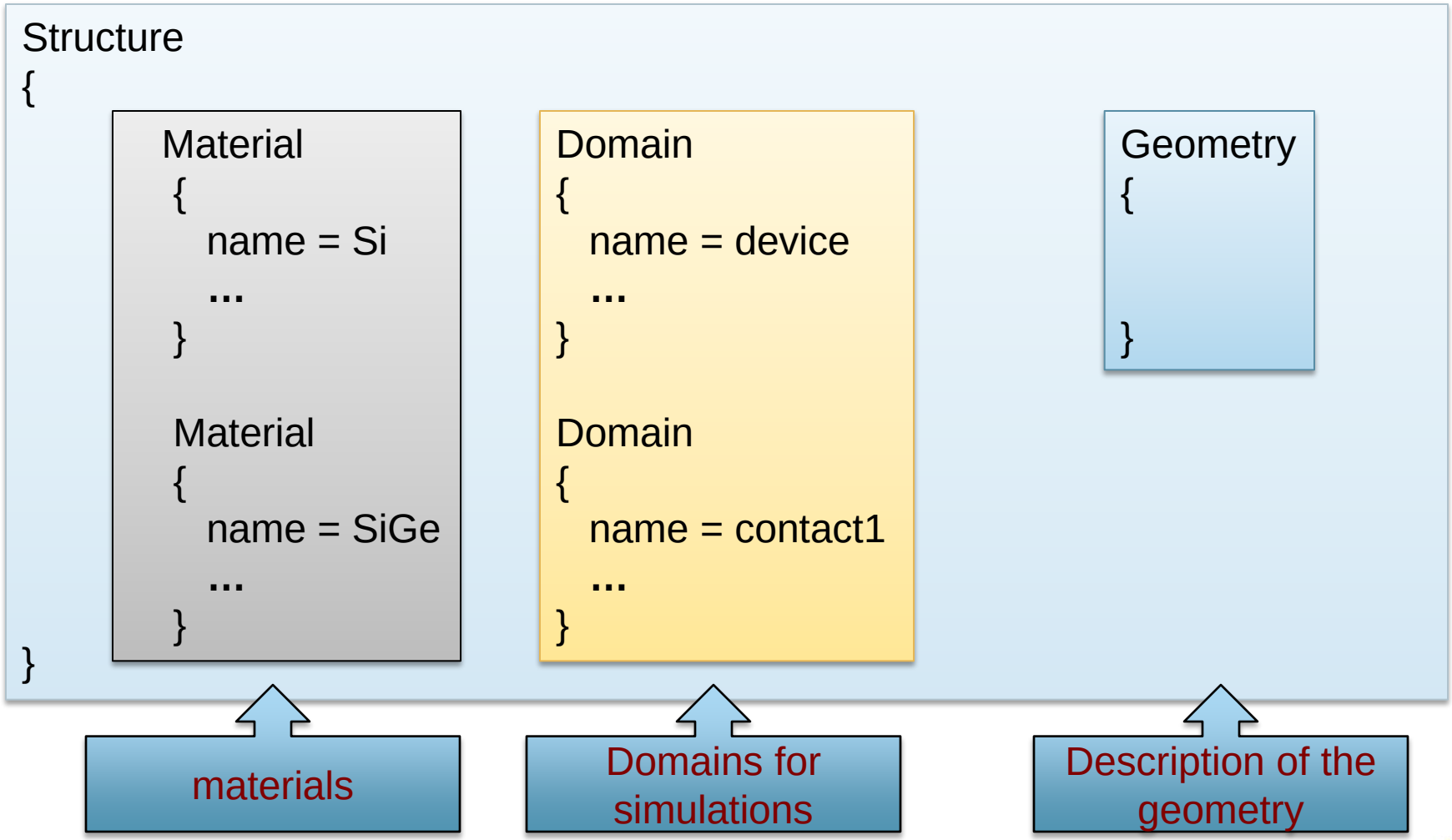
defines simulations that has to be solved, e.g. equations, boundary conditions,iteration processes, output, numerical options, etc

```
Global
{

}
```

defines global variables such as temperature, which database file to use, diagnostic output, etc.

The NEMO5 input deck – the first block “Structure”



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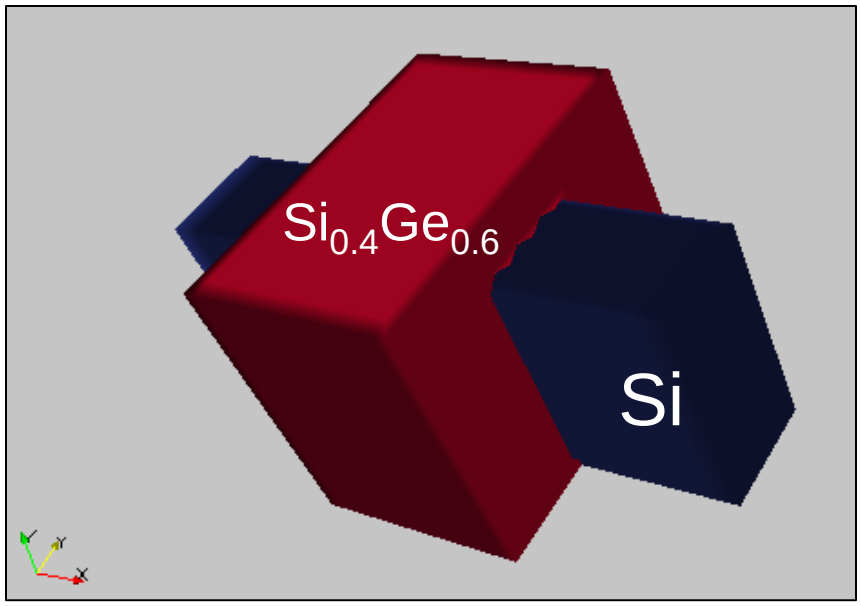
Creation of atomic structures (I)

```
Structure
{
    Material
    {
       name = Si
       ...
    }

    Material
    {
       name = SiGe
       ...
    }

    Domain
    {
       name = device
       ...
    }

    Domain
    {
       name = contact1
       ...
    }

    Geometry
    {

    }
}
```

User's steps		Input deck sections
• Design the device	⇒	Geometry block
• Chose material and crystal structures	⇒	Material and domain blocks
• Define where each equation is solved	⇒	Solver and domain blocks

Example1: Si/SiGe quantum wire

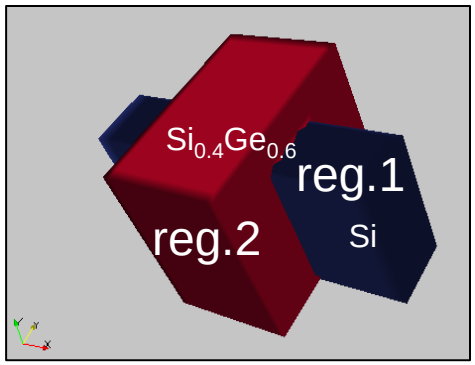
Goal: create Si wire surrounded by a $Si_{0.4}Ge_{0.6}$ layer



Additional requirements:

- [100] transport direction
- SiGe alloy is represented as a disordered system

Example1. Si/SiGe wire: definition of materials.

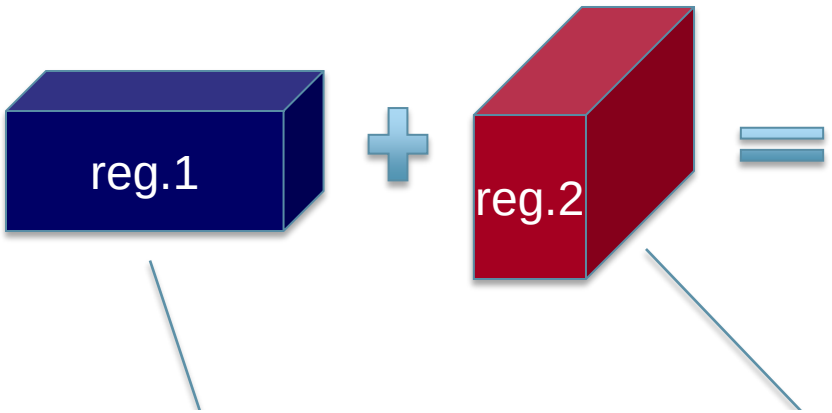


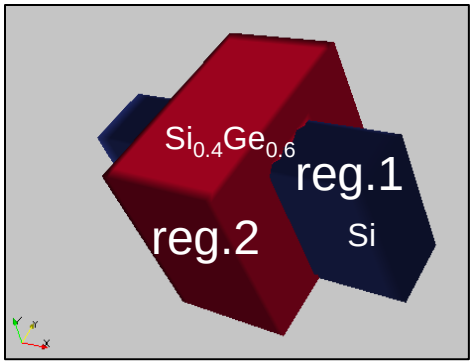
- Each material occupies a region (or regions)
- Material definition requires:
  - name
  - tag
  - crystal_structure

```
Material
{
      name = Si
      tag = core
      crystal_structure = diamond
      regions = (1)
}

Material
{
      name = SiGe
      tag = substrate
      crystal_structure = diamond
      regions = (2)
      mole_fraction = 0.4
      disorder_type = totally_random_alloy
}
```

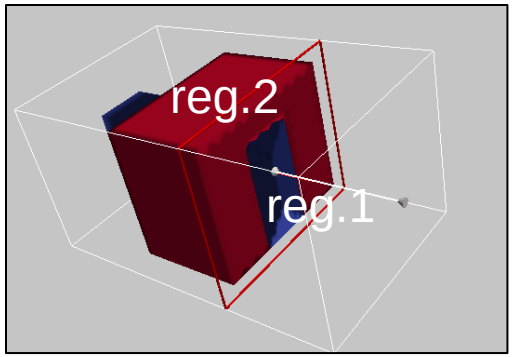
special parameters for an alloy

Example1. Si/SiGe wire: definition of geometry shapes.





Full view



Cross-section view

If two regions overlap, then the biggest priority value wins!

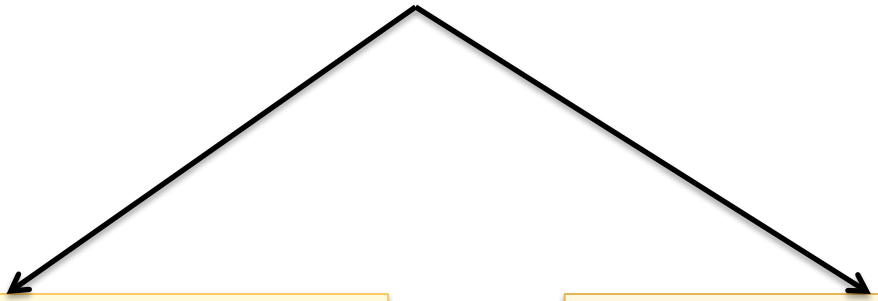
```
Region
   {
     shape          = cuboid
     region_number  = 1
     priority       = 2
     min            = ( 0,2,0)
     max            = ( 10,4,4)
   }
```

```
Region
   {
     shape          = cuboid
     region_number  = 2
     priority       = 1
     min            = (3,0,0)
     max            = (7,6,5)
    }
```

*coordinates are defined in nanometers

Example1. Si/SiGe QWR. Atomistic domain.

Two ways to create an atomistic domain:



Read-in atomic structure
(see discussion forum for details)

- Any structures (crystals, amorphous, bio molecules, etc…) are possible;
- Chemical bonding has to be provided;

Generate atomic structure.
(this tutorial)

- Only pseudomorphic lattice is supported;
- Chemical bonds are calculated by NEMO5;
- Strain relaxation is required for lattice mismatched systems (see tutorial 5)

Example1. Si/SiGe wire: Pseudomorphic domain (I)

Pseudomorphic domain is an ideal lattice that consists of materials with the same crystallographic structure.

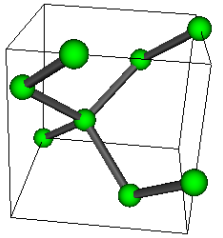
- No defects.
- No different lattices in one domain such as GaN and Si together.

but…

- Different lattice constants are possible.
- Some defects in the lattice may be created by NEMO5 (e.g. single impurities, Lecture 7).

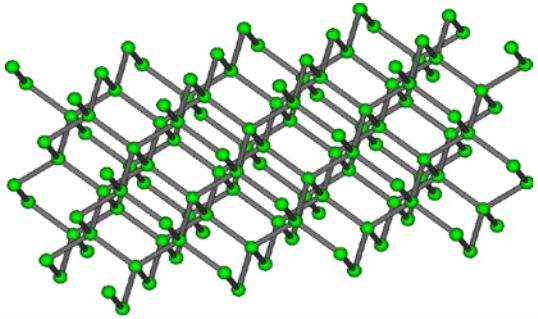
Steps to create a pseudomorphic domain.

Select the base material.



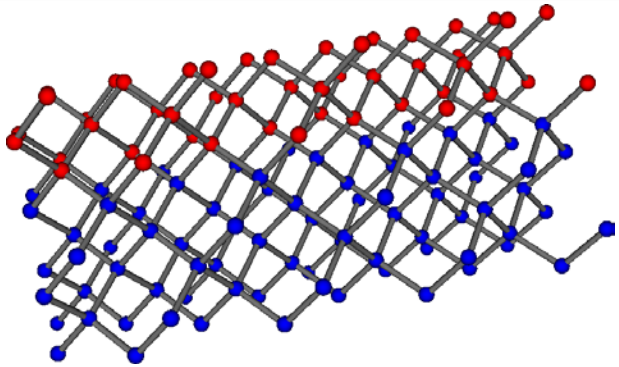
Domain block

Create a big lattice by repeating the base material unit cells.



Domain block

Substitute the base material atoms by the actual material atoms.
Remove unnecessary atoms if needed.



Geometry block

Relax the structure (will be shown in tutorial 5)

Example1. Si/SiGe wire: Pseudomorphic domain (II)

```
Domain{
  name = wire_atomistic
  type = pseudomorphic

  base_material = core
  crystal_direction1 = (1,0,0)
  crystal_direction2 = (0,1,0)
  crystal_direction3 = (0,0,1)
  space_orientation_dir1 =(1.0,0.0,0.0)
  space_orientation_dir2 =(0.0,1.0,0.0)


  dimension = (30,20,20)
  periodic = (false, false, false)

  regions = (1,2)
  geometry_description = simple_shapes

  passivate = true
  random_alloy = true
}
```

Base material cell definition

Bravais vectors of the cell (miller indexes)

Orientation of the crystal directions in the laboratory Cartesian system

Repetition of the unit cell.

Shaping of the domain

Post-processing of the domain

Synopsis

1. How to control the simulator? *Done*
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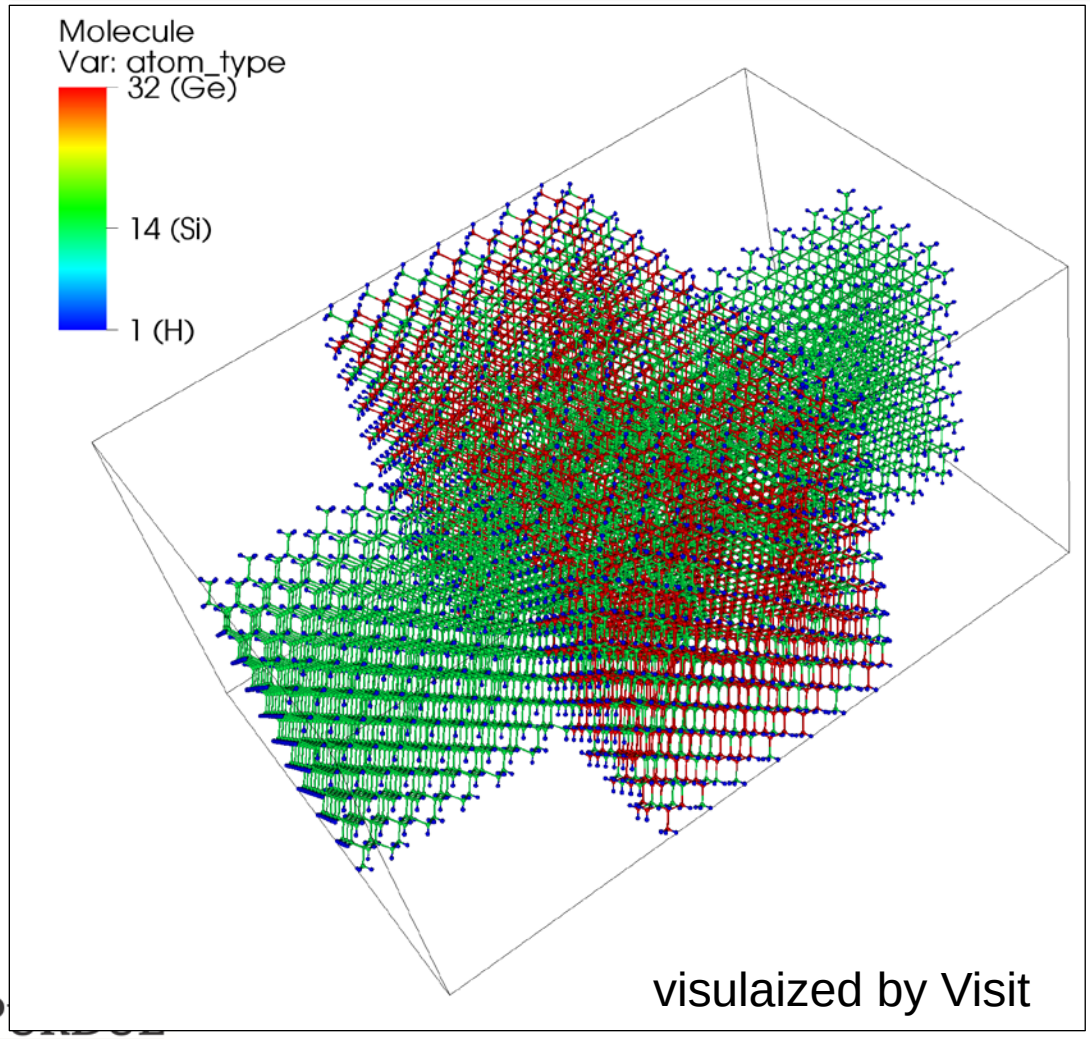
3. Creation of atomic structures. *Done*
4. Visualization of the atomistic output (structure solver).
5. Creation of Finite element mesh.
6. Visualization of finite element data (electric potential of the Poisson solver).

Visualization of atomic structures in NEMO5

Task: visualize atomic structure of our Si/SiGe wire.



Solution:

1. Define a solver that outputs the structure in the input deck.
2. Run NEMO5.
3. Use available visualization software.

Solver that dumps out structures

```
solver
{
  name = view_shapes
  type = GeometryVIS
  geometry_volumes_output = true
  geometry_volumes_resolution = 20
  geometry_volumes_filename = regions.vtk
}

solver
{
  name            = view_atoms
  type            = Structure
  domain          = wire_atomistic
  output_format   = vtk
  structure_file = Si_SiGe_wire.vtk
}
```

Outputs user-defined geometry

Outputs an atomistic domain

Let's see example1...

1. Execute tutorial2_1.in input deck

2. Visualize the output using Paraview

3. Modify the input deck: change crystallographic grows directions

```
crystal_direction1 = (1,0,0)
crystal_direction2 = (0,1,0)
crystal_direction3 = (0,0,1)
```

```
crystal_direction1 = (1,1,0)
crystal_direction2 = (-1,1,0)
crystal_direction3 = (0,0,1)
```

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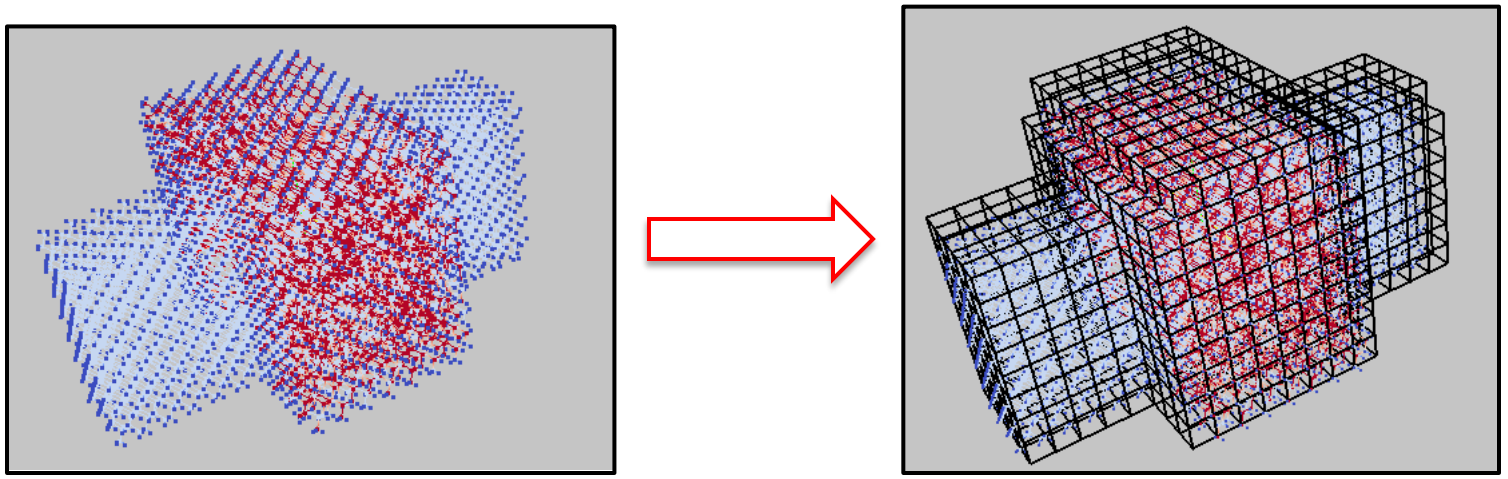
Finite element (FE) domains.

Device simulation requires solution of the Poisson equation: $\nabla(\kappa\nabla\phi) = -\rho$

NEMO5 solves the Poisson equation using the FE method.

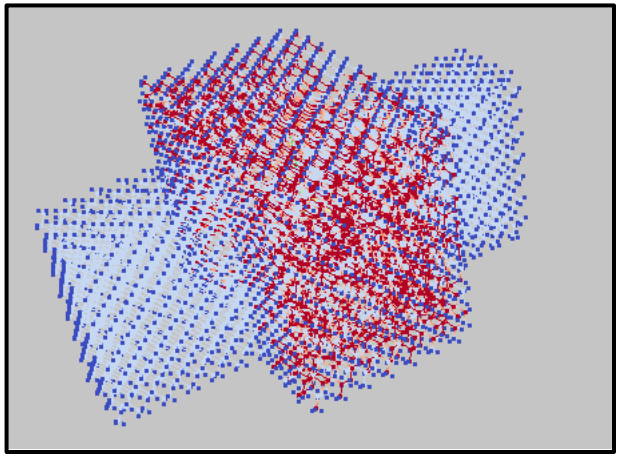
NEMO5 can create the FE mesh automatically:



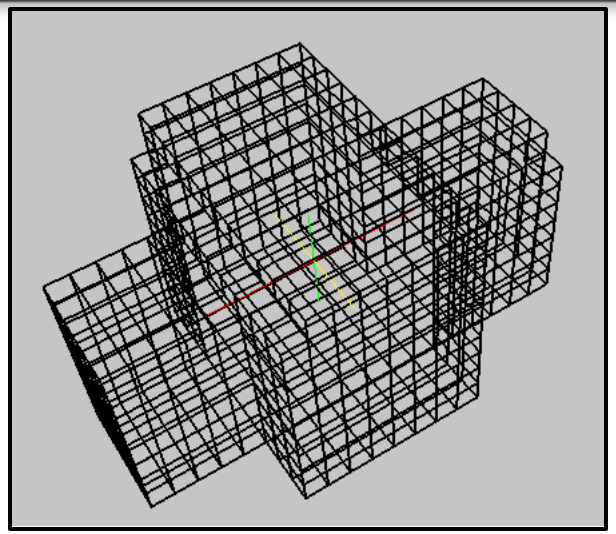
atoms

atoms and mesh

Example 2. Si/SiGe wire: creation of a FE mesh domain



Atomistic domain "wire_atomistic"



FE domain "wire_fem"

```
Domain
{
    name = wire_fem
    type = finite_elements
    mesh_from_domain = wire_atomistic
    output = mesh
}
```

Example 2. Si/SiGe wire: electrostatic boundary conditions (I)

Device simulation requires solution of the Poisson equation: $\nabla(\kappa\nabla\phi) = -\rho$

The Poisson equation requires boundary conditions:

1. If no boundary conditions are specified, the Neumann boundary condition is applied : $\nabla\phi = 0$

2. In the input deck one can define **boundary regions** and apply boundary conditions there, e.g. impose a fixed potential value.

Example 2. Si/SiGe wire: electrostatic boundary conditions (II)

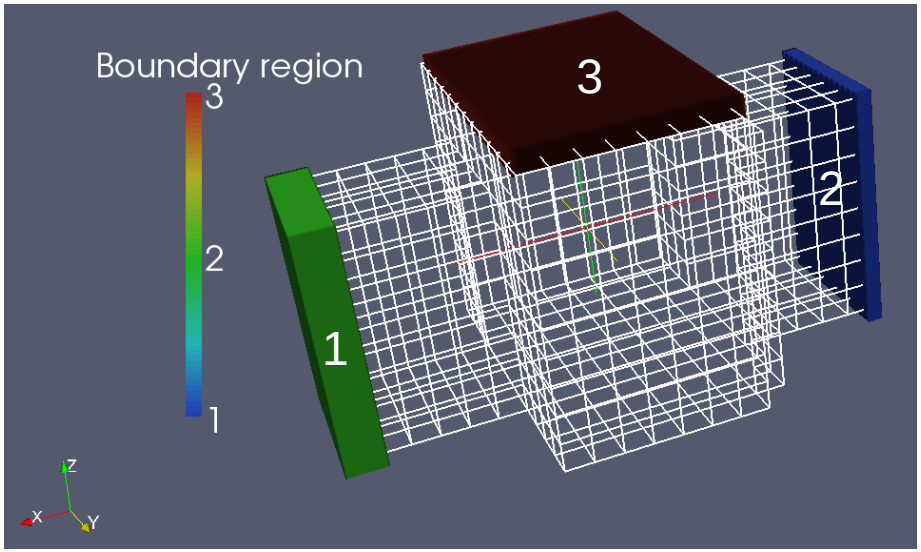
Device simulation requires solution of the Poisson equation: $\nabla(\kappa\nabla\phi) = -\rho$

The Poisson equation solution depends on boundary condition:

1. If no boundary conditions are specified, the Neumann boundary condition is applied.

2. In the input deck one can define **boundary regions** and apply boundary conditions there.

Example 2. Si/SiGe wire: electrostatic boundary conditions (III)



Output of the boundary regions and FE mesh

Boundary conditions are applied to the mesh points that are inside the boundary regions.

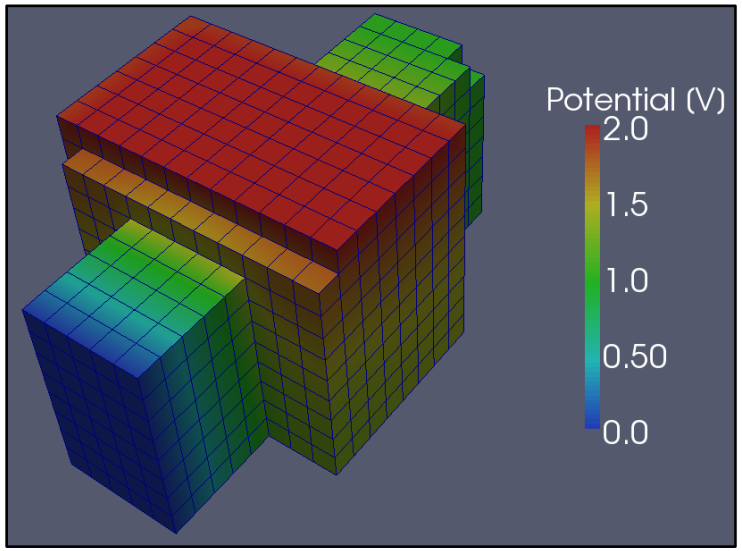
Let's apply 3 boundary conditions.

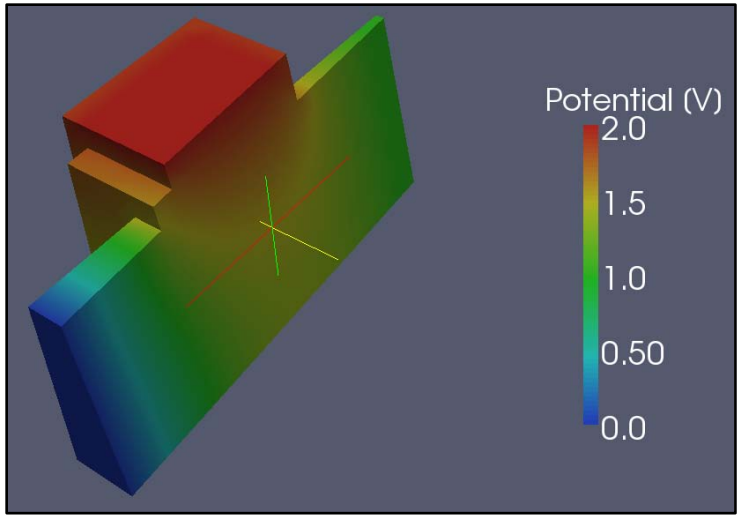
```
Boundary_region {
    shape          = cuboid
    region_number  = 1
    priority       = 1
    min            = ( -0.1,1.5,-0.2)
    max            = (  0.2,4.5, 4.5)
}
Boundary_region  {
    shape          = cuboid
    region_number  = 2
    priority       = 1
    min            = ( 9.7, 1.5,-0.2)
    max            = ( 10.5,4.5, 4.5)
}
Boundary_regionn {
     shape          = cuboid
     region_number  = 3
     priority       = 1
     min            = ( 3, 0, 5.2)
     max            = ( 7, 6, 5.6)
}
```

Example 2. Si/SiGe wire: solving the Poisson equation.

```
solver{
  name = my_poisson
  type = Poisson
  domain = wire_fem
  fem_output = (potential)

  boundary_condition{
    type = ElectrostaticContact
    boundary_regions = (1)
    voltage = 0.0
  }
  boundary_condition{
    type = ElectrostaticContact
    boundary_regions = (2)
    voltage = 1.0
  }
  boundary_condition{
    type = ElectrostaticContact
    boundary_regions = (3)
    voltage = 2.0
  } }
```





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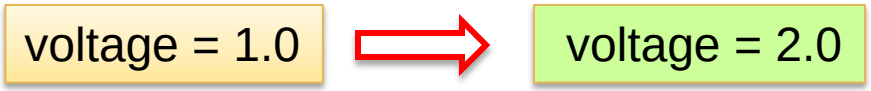
Let's run example 2...

1. Execute tutorial2_2.in input deck

2. Visualize the output using Paraview

3. Modify the input deck: change applied voltage.



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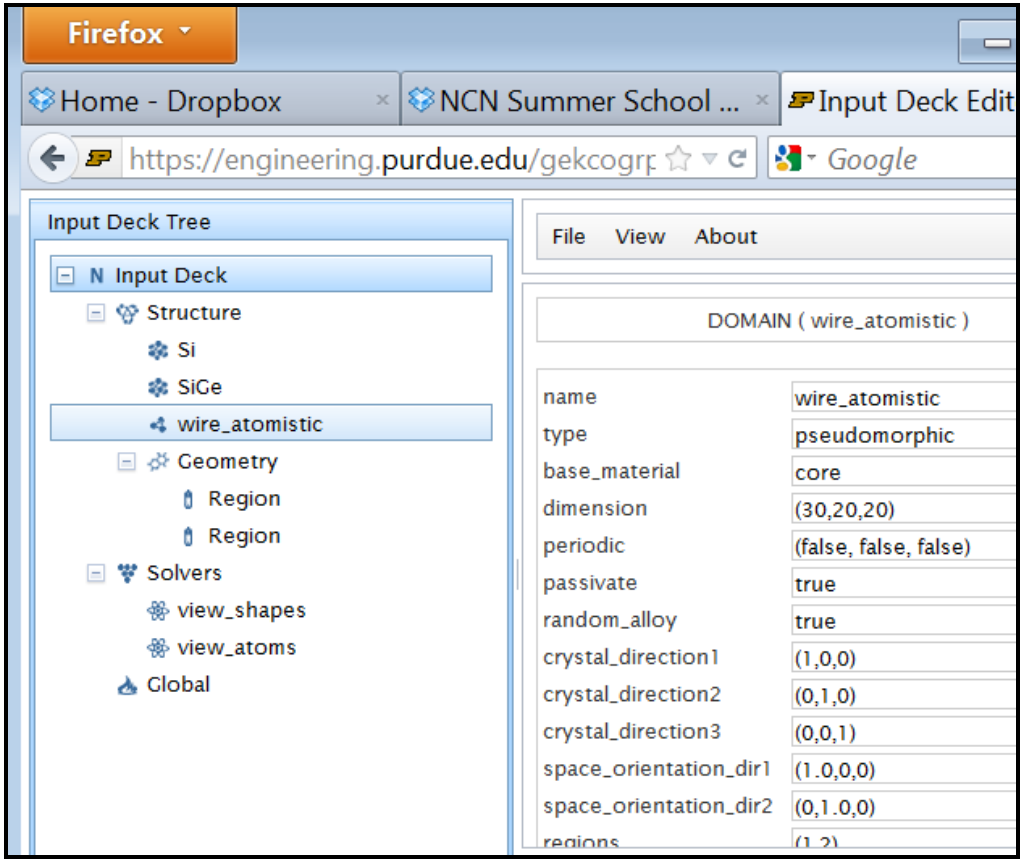
Appendix. Input deck editor and database browser.

https://engineering.purdue.edu/gekcogrp/software-projects/nemo5/InputDeckEditor/



PHP based input deck editor:

- can show input deck/database in a structured form;
- can facilitate input deck edition;
- can automatically translate input deck into Python;