Tutorial 5B
Strain

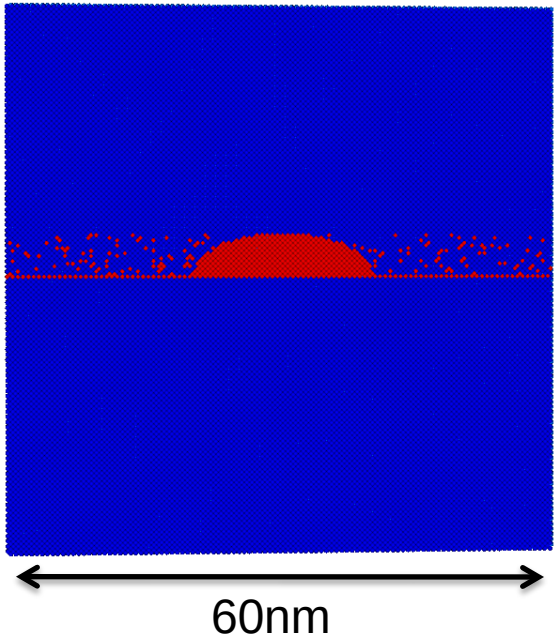
Hesameddin Ilatikhameneh
Yuling Hsueh, Jean Michel Sellier
Jim Fonseca, Tillmann Kubis
Michael Povolotskyi
Prof. Gerhard Klimeck

Strain solver

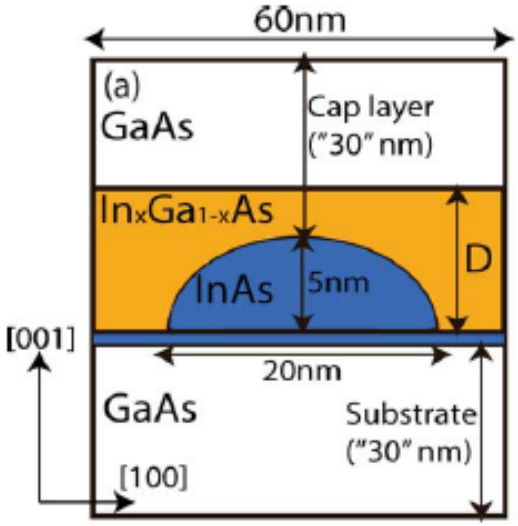
Objective: Find relaxed positions of atoms

Example: Quantum dot (10M Atoms, 100s CPUs, hours)

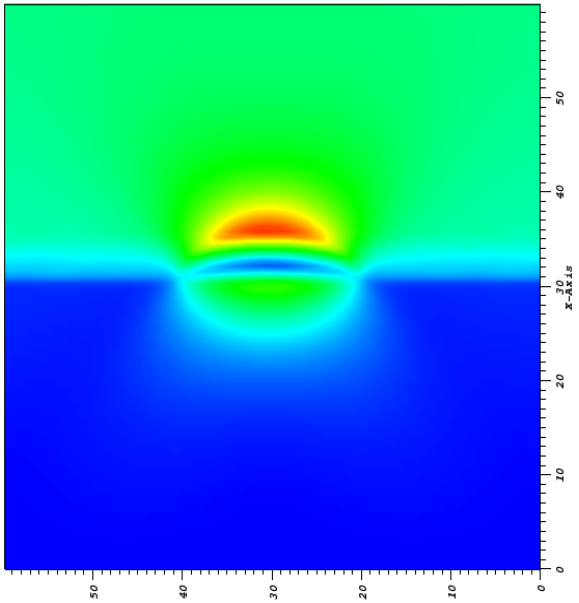
Initial positions



Strain Solver



Displacement magnitude



M. Usman et al., IEEE Transactions on Nanotechnology, Vol. 8, No. 3, May 2009.

Let's run the input-deck (it will take several minutes)

```
cd ~
cd public_examples/NCN_summer_school_2012/Quantum_Dot_Hesam
!ln
```

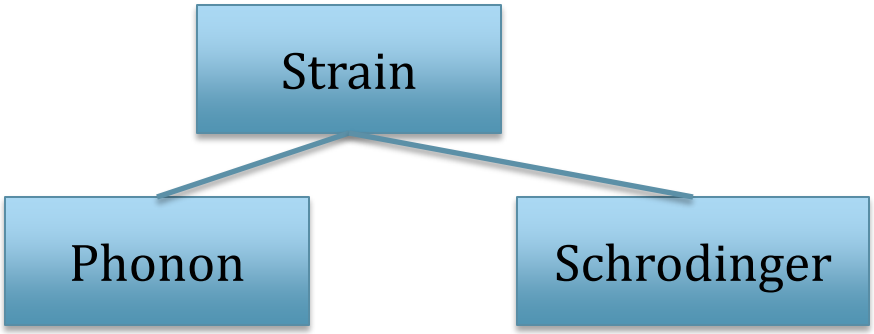
Don't Forget Exclamation Sign !

```
ln -s /apps/share64/nemo/examples/current/materials/all.mat
```

```
submit -v ncn-hub@coates -i ./all.mat -n 8 nemo-r8028 a_QD_10nm_Usman.in
```

Outline

Why do we need relaxed positions?



Strain Examples:

1. Quantum Dot with Open Boundaries
   - » Input deck ⟺ Flow chart
2. Quantum Dot with all types of boundary conditions
   - » How to apply different boundary conditions
3. Quantum well

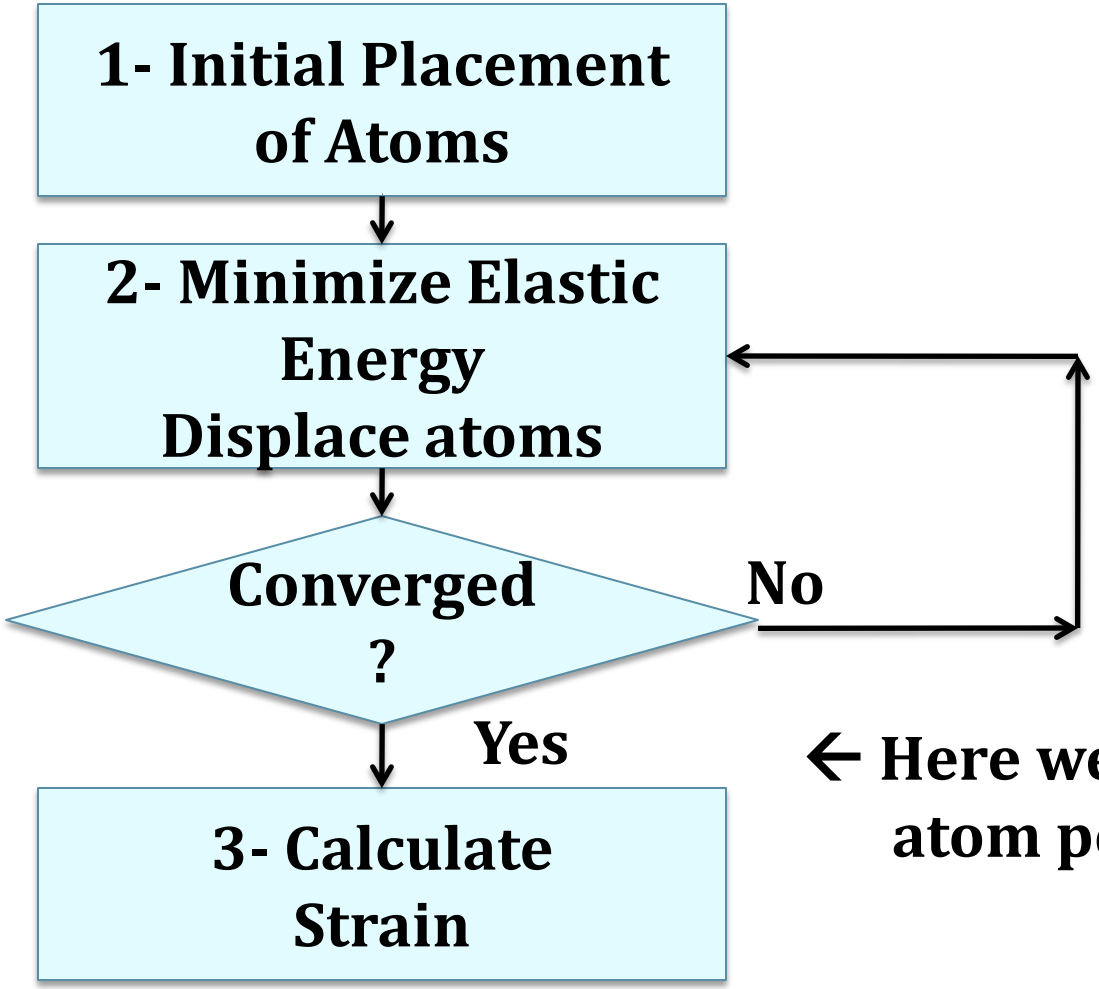
"Stand up to a Computer"

S. Fergusson, Eng. In Mind's Eye, MIT Press

Understand how simulation software works

Flow chart of Strain Simulation

How to obtain the Atoms positions and Strain?

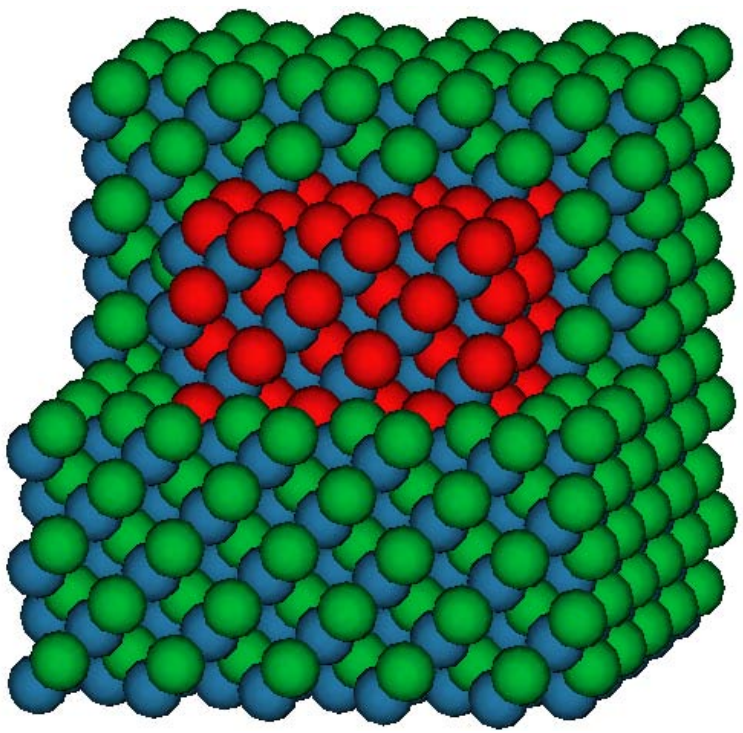


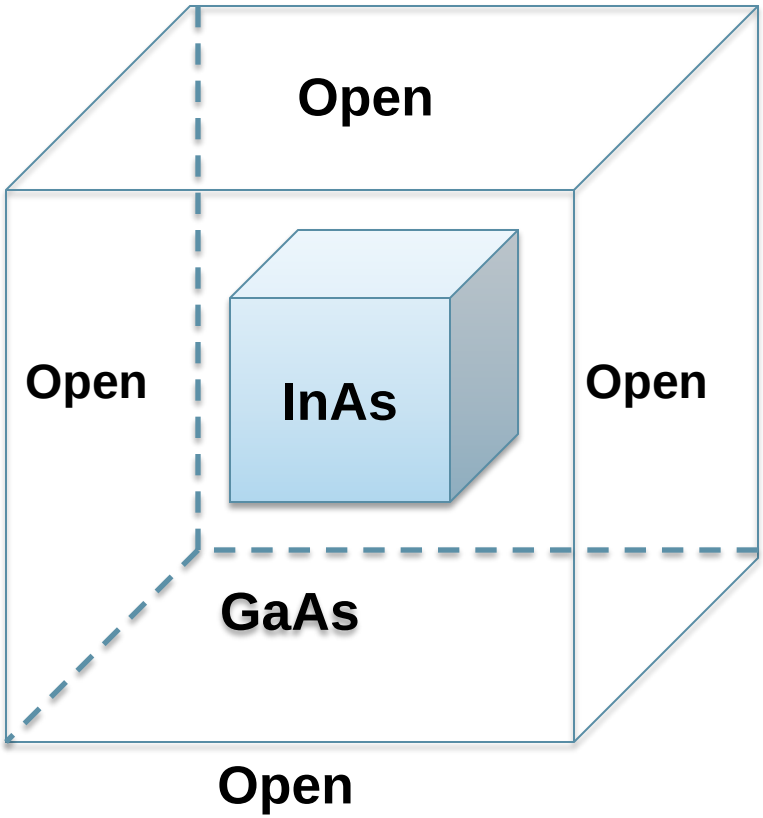
← Here we have final atom positions

Geometry Definition for Strain

Example1: Quantum Dot with Open Boundary

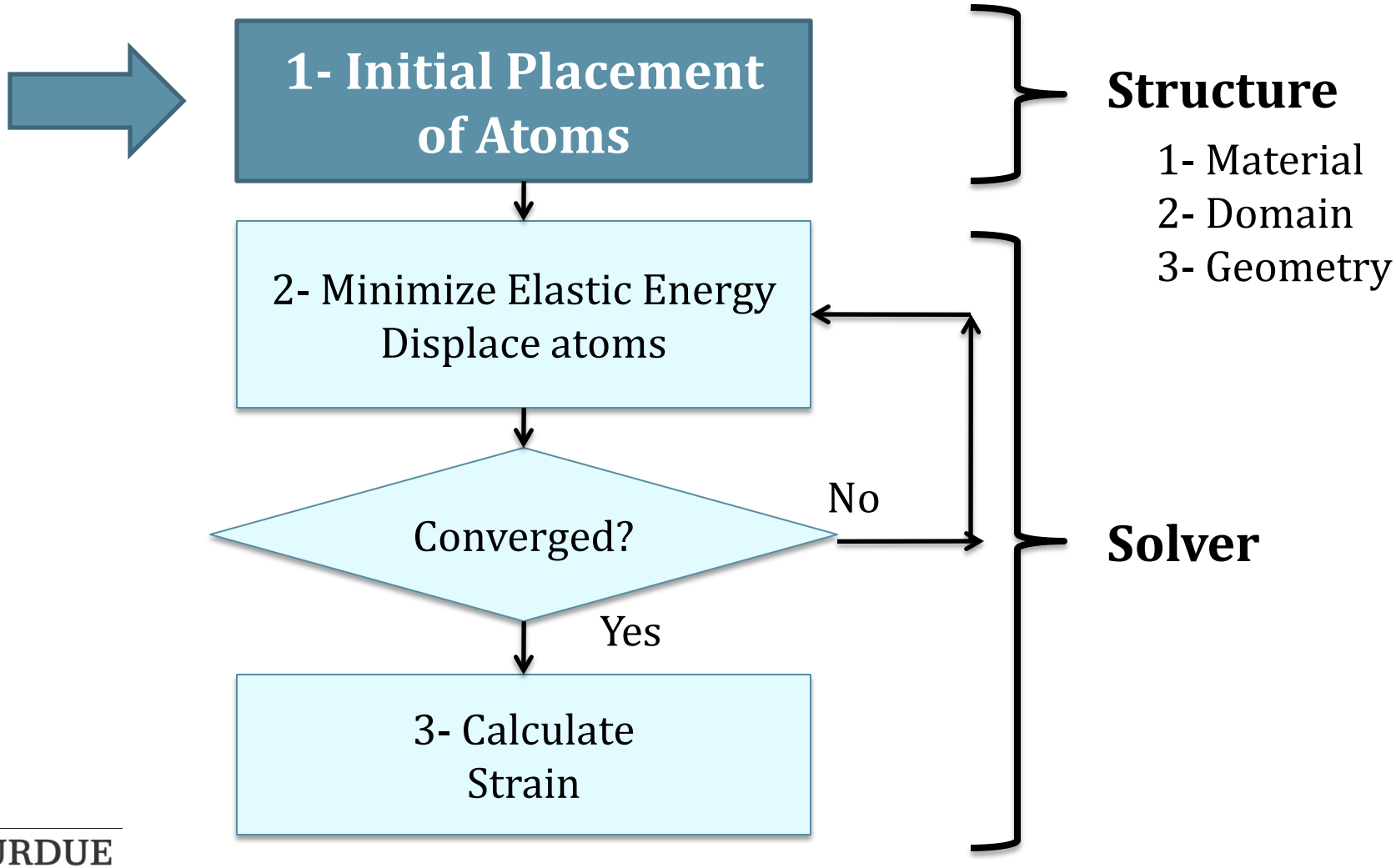
Input deck ⟺ Flow chart





Flow chart of Strain Simulation

1st Step: How to setup initial positions in input-deck?



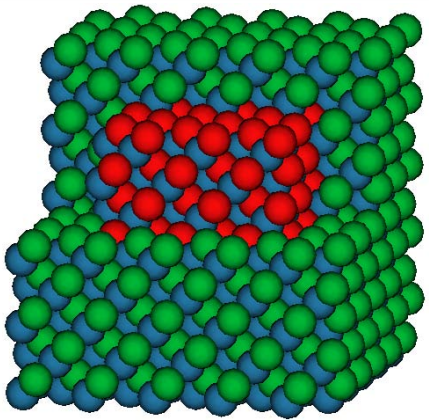
Initial positions of Atoms

```
Structure
{
        Material
        {
                name              = GaAs
                tag               = substrate
                crystal_structure = zincblende
                regions           = (1)
        }

        Material
        {
                name              = InAs
                tag               = dot
                crystal_structure = zincblende
                regions           = (2)
        }
```

1-a) Materials

- GaAs and InAs
- We can change material properties here
- The regions will be determined in Geometry

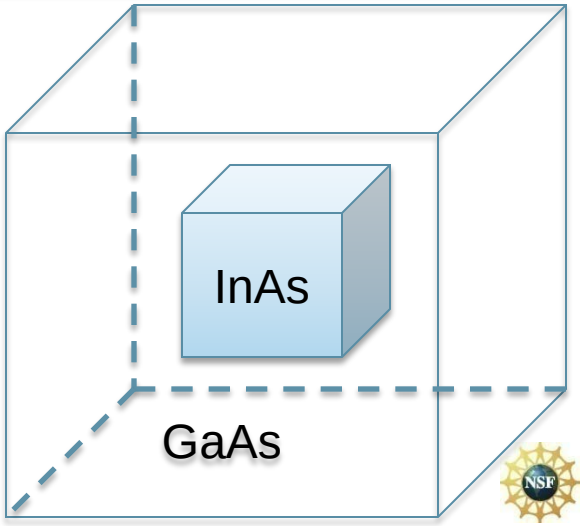


Initial positions of Atoms

```
Geometry
{
                        //---   GaAs Substrate   ---\\
        Region
        {
                shape          = cuboid
                region_number = 1
                priority       = 1
                min            = (-0.1,-0.1,-0.1)
                max            = (3.5,3.5,3.5)
        }
                        //---   InAs Dot         ---\\
        Region
        {
                shape          = cuboid
                region_number = 2
                priority       = 2
                min            = (1.13,1.13,1.13)
                max            = (2.26,2.26,2.26)
        }
```

1-b) Geometry

- dimensions are in nm
- The region numbers are what we specified in material section



Initial positions of Atoms

```
Domain
{
        name           = atomic_structure
        type           = pseudomorphic
        base_material  = substrate
        dimension      = (6,6,6)
        periodic       = (false,false,false)

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

        space_orientation_dir1 = (1, 0, 0)
        space_orientation_dir2 = (0, 1, 0)
        passivate = false
        origin  = (0,0,0)
        output  = (xyz,coupling)
        regions = (1,2)
}
```

1-c) Domain

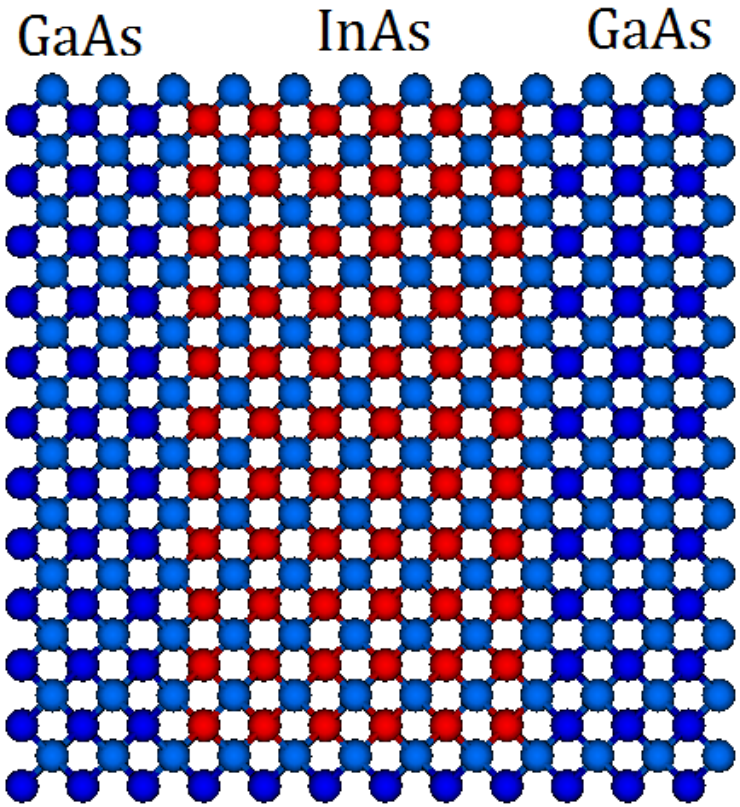
- **Base material** is very important in Strain simulation
- It determines the building block of the structure and initial positions of atoms
- The boundary condition will be applied to these initial positions

Strain Solver Parameters

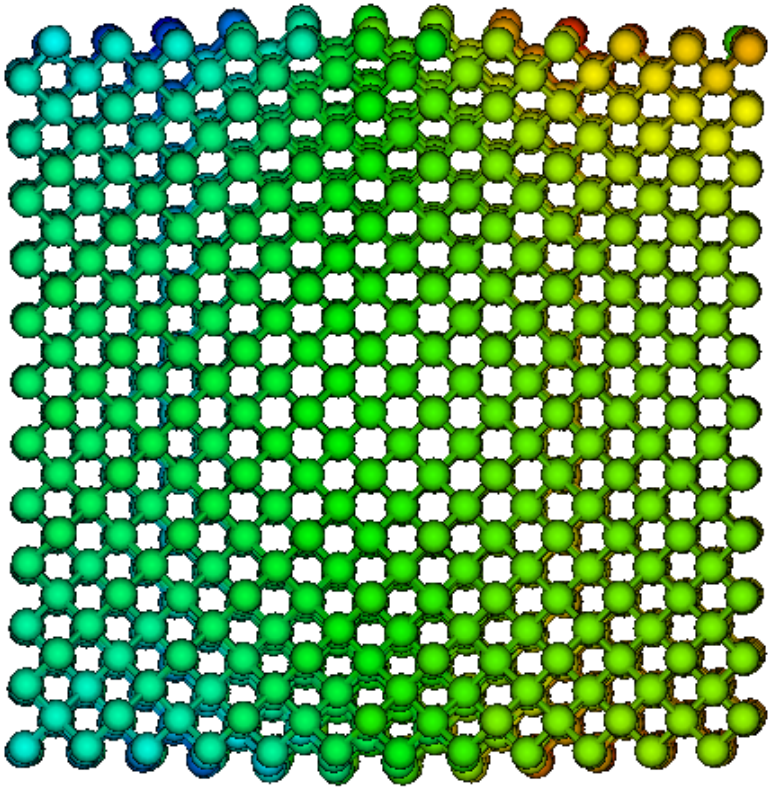
Base Material:

Initially GaAs and InAs have same lattice constant

Initial position

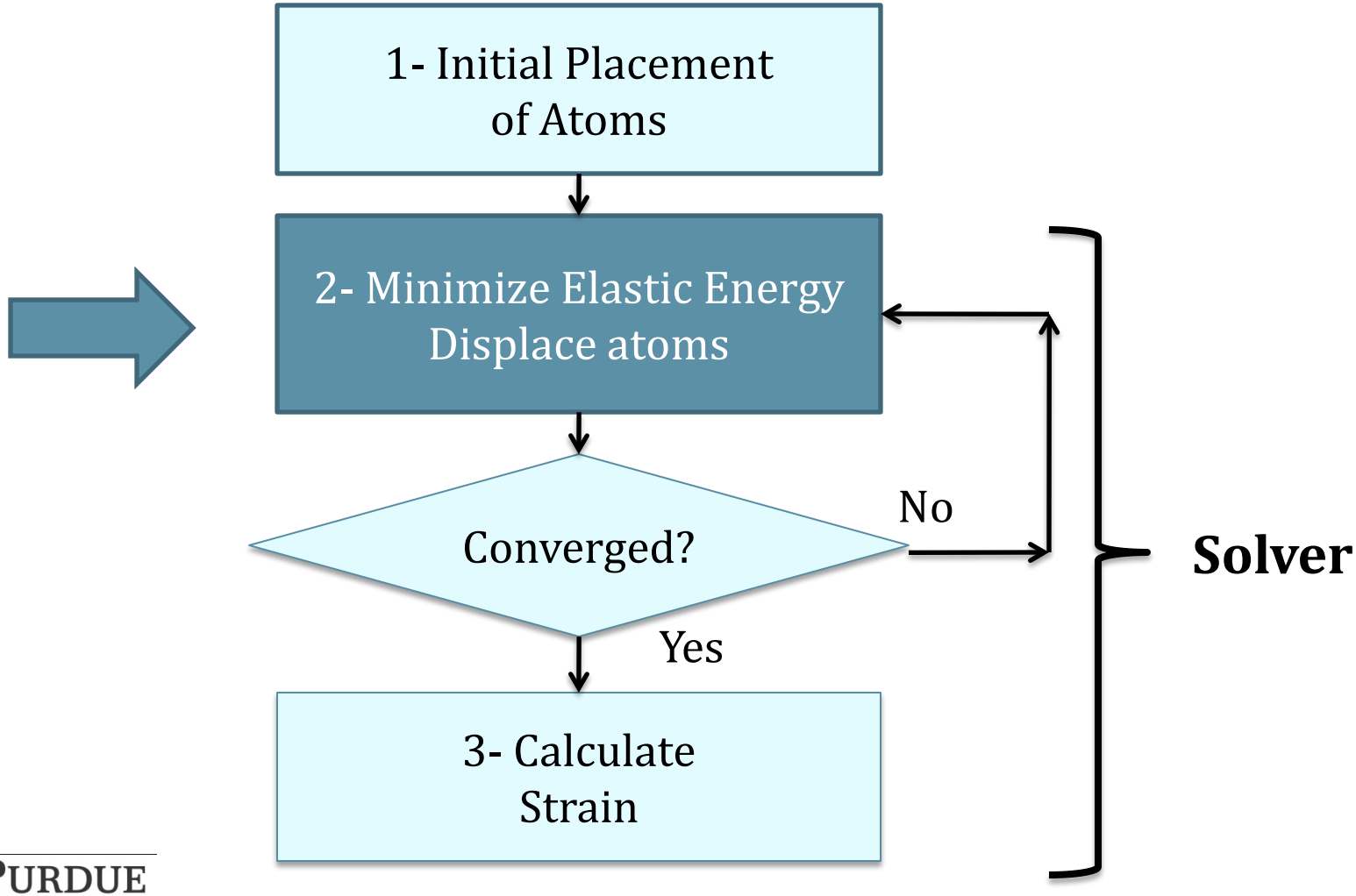


After strain solver



Flow chart of Strain Simulation

2nd Step: How to setup Strain solver in input-deck?



Strain Solver Parameters

```
solver
{
        name           = keating
        type           = KeatingStrain
        domain         = atomic_structure
        active_regions = (1,2)
// Models
        models                 = harmonic
```

2) Strain Solver

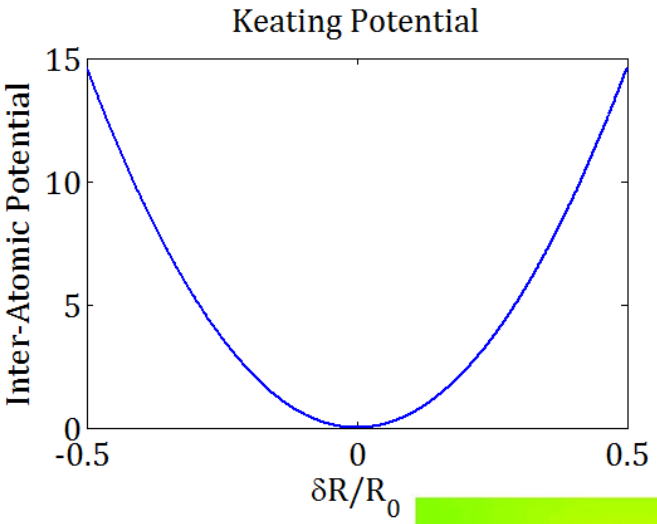
- **type** determines the solver. For strain solver type should be "KeatingStrain" or "VFFStrain".

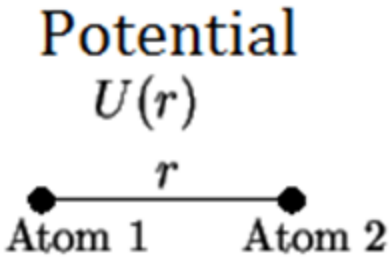
- **models** determine the interatomic potential function

Standard Keating: harmonic
Lazarenkova :anharmonic_Areshkin
Modified VFF: cross-stretch, stretch-bend, …

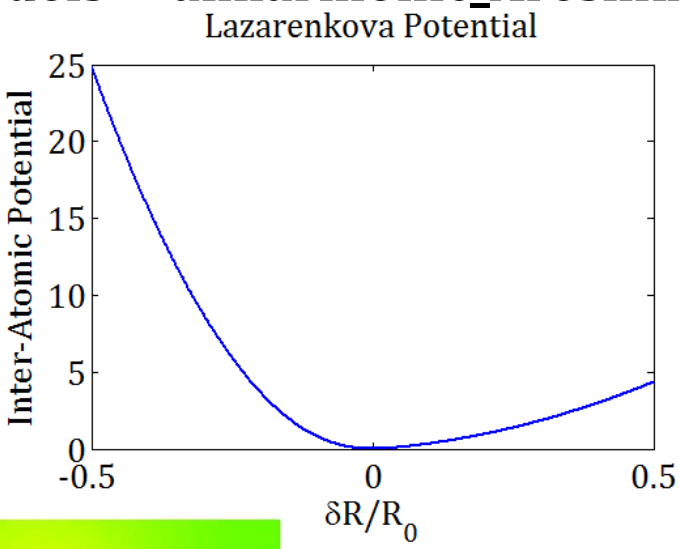
Strain Solver Parameters

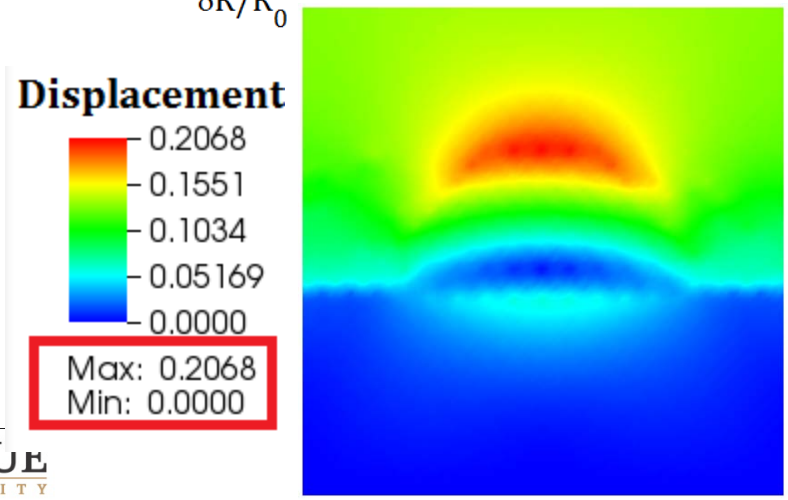
Keating
Models = harmonic

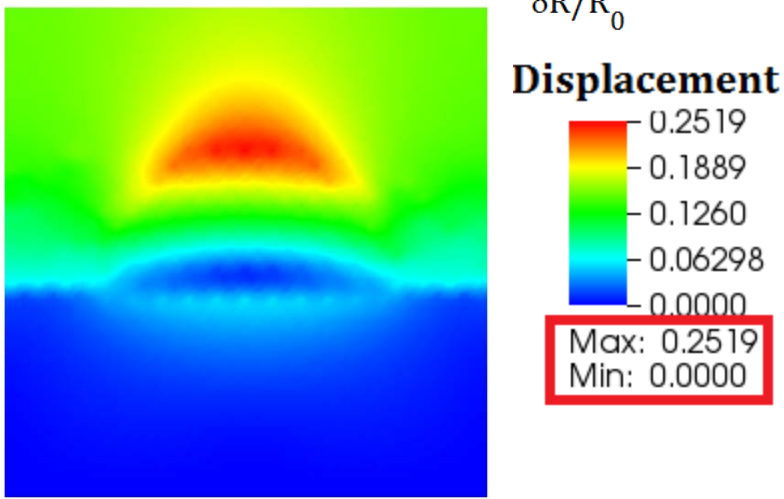




Lazarenkova
Models = anharmonic_Areshkin

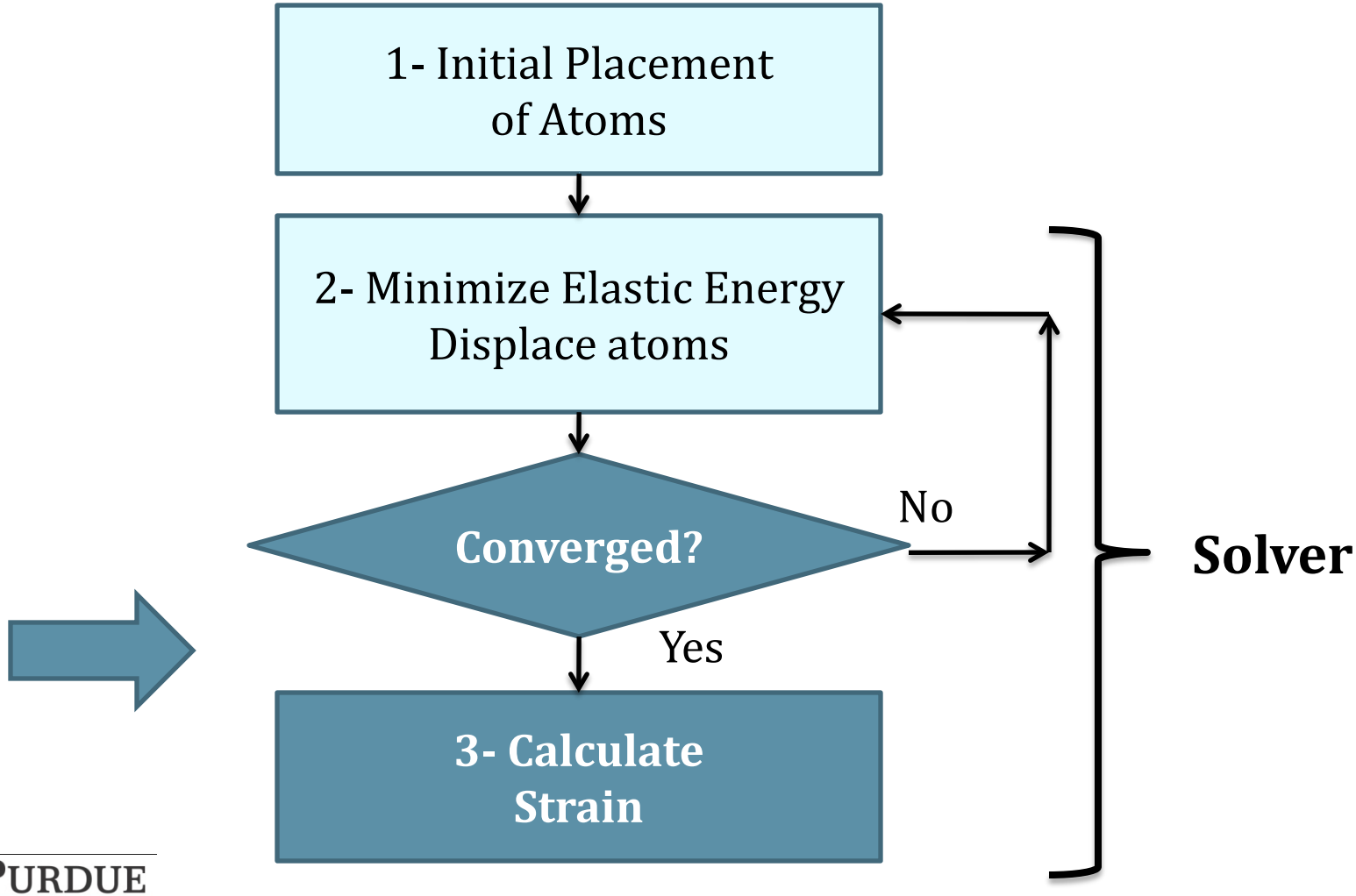






Flow chart of Strain Simulation

3rd Step: Convergence criteria and outputs in input-deck



Strain Solver Parameters

```
solver
{
        ...

// Outputs
   calculate_piezo            = true
   calculate_epsilon          = true
   silo_file                  = Graphic_Output.silo
   xyz_file                   = Text_Output.xyz
   xy_file                    = Text_Output_Strain.xy
   calculate_bond_stats       = Bond_Lengths.bonds

// Petsc options
    linsolver_max_iters        = 30000
    linear_solver              = bcgsl
    preconditioner             = jacobi
    max_num_iters              = 20000
    absolute_tol               = 1e-8
    relative_tol               = 1e-8
    linsolver_monitor          = true
 }
```

2) Strain Solver

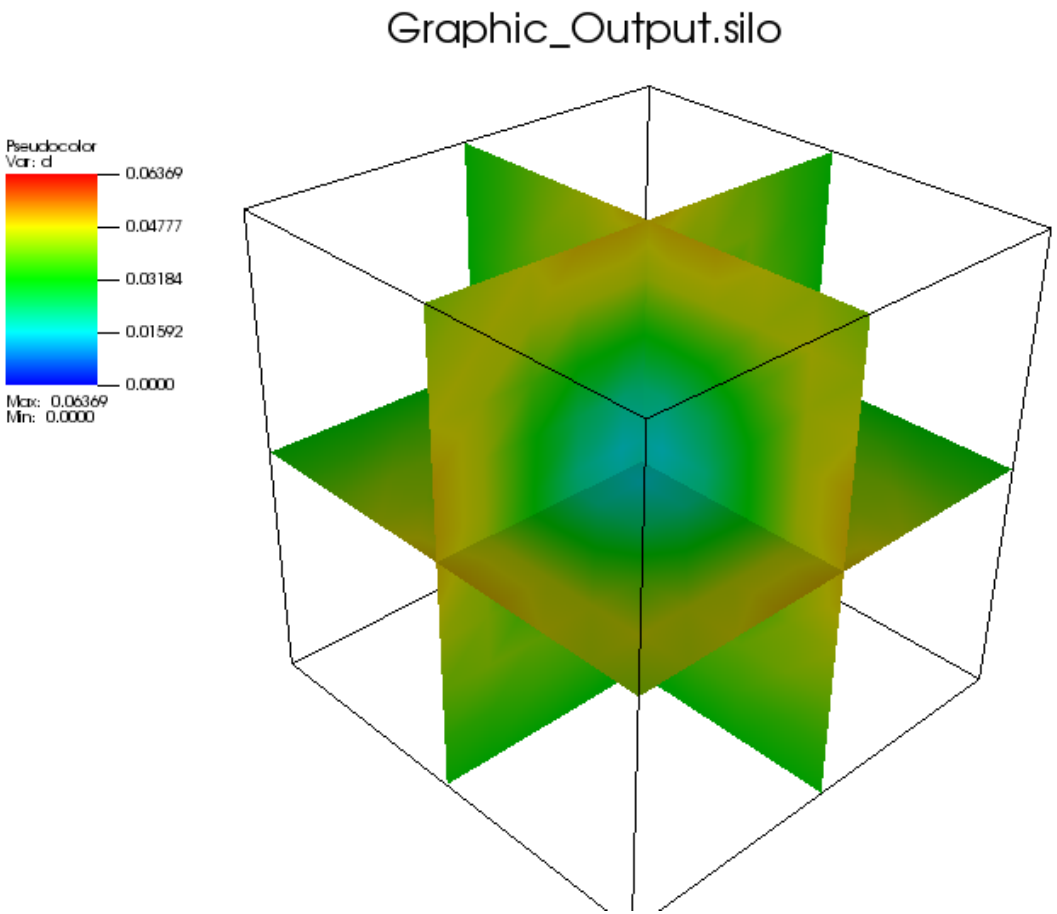
- **calculate_epsilon**
  Enables the strain calculation

- **absolute_tol** **and** **relative_tol**
  determine the convergence condition

- There are different matrix solvers and preconditioners which affect convergence speed

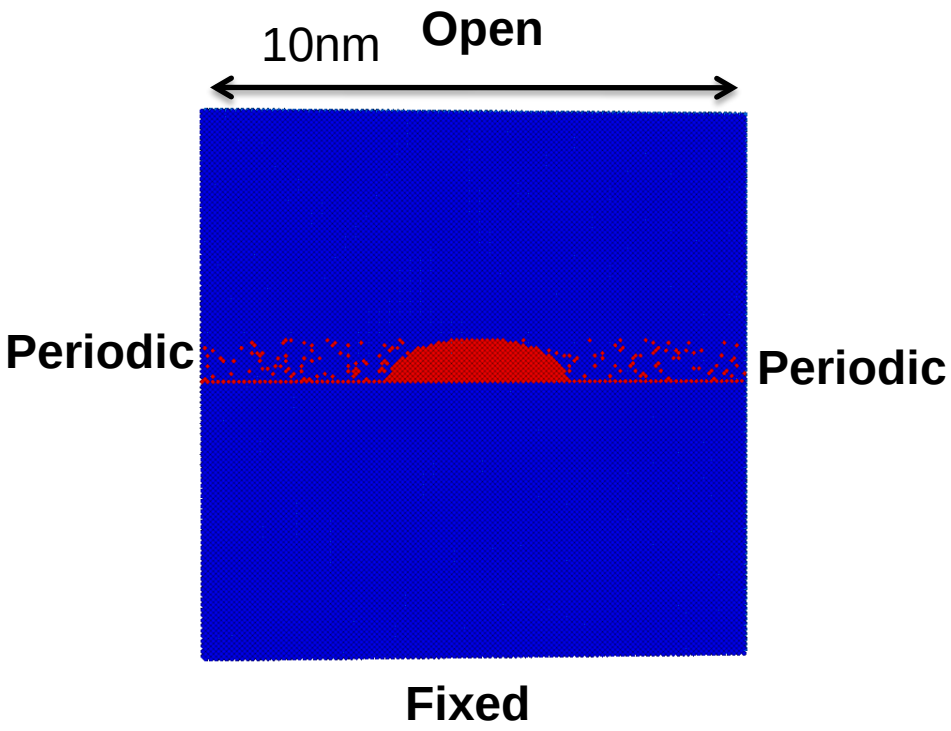
Strain Outputs

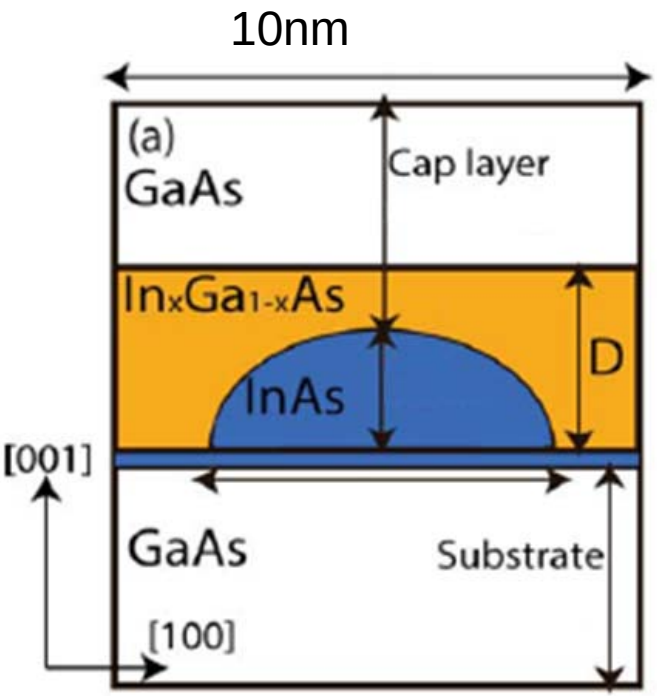
- Graphic Output (Displacement, Strain)



Exercise: Strain and displacement in Quantum dot

Goal: How to run solver and plot the displacement/strain

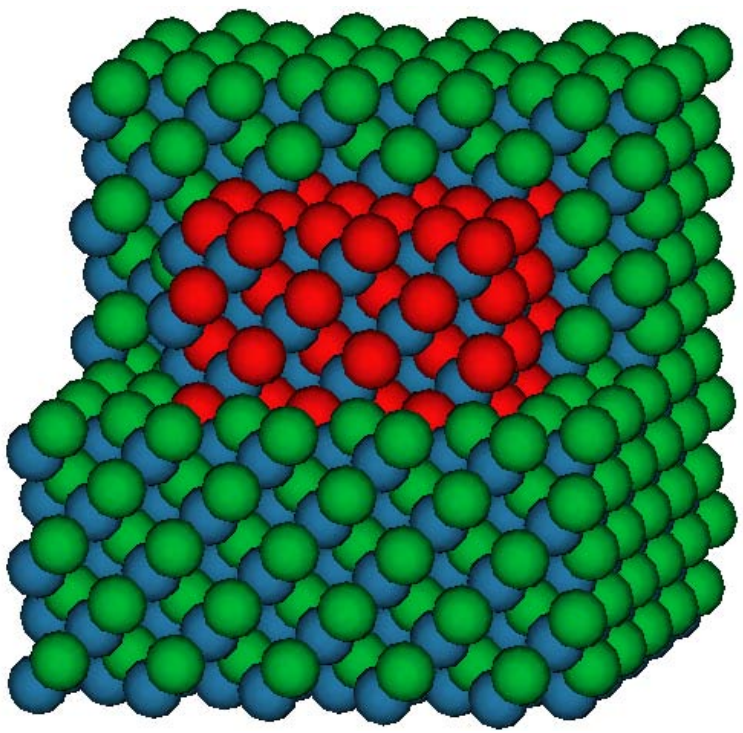


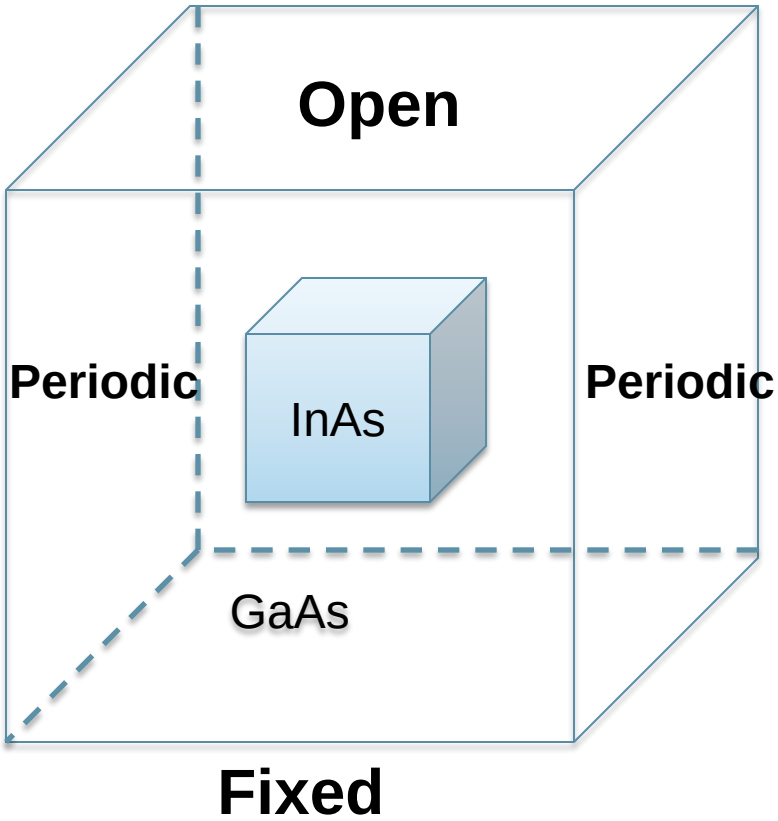


M. Usman et al., IEEE Transactions on Nanotechnology, Vol. 8, No. 3, May 2009.

Geometry Definition for Strain

2. Quantum Dot with all types of boundary conditions
   - » How to apply different boundary conditions





Periodic Boundary Condition

- How to make periodic boundary condition?

```
Domain
{
        name          = atomic_structure
        type          = pseudomorphic
        base_material = substrate
        dimension     = (6,6,6)

        periodic      = (true,true,false)  // <---- Periodic in x and y directions

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

        space_orientation_dir1 = (1, 0, 0)
        space_orientation_dir2 = (0, 1, 0)
        passivate = false
        origin  = (0,0,0)
        output  = (xyz,coupling)
        regions = (1,2)
}
```

Fixed boundary condition

- How to make fixed boundary condition?

```
Geometry
{
        ...
        Boundary_region
        {
                shape          = cuboid
                region_number  = 1
                priority       = 1
                min            = (-0.1,-0.1,-0.1)
                max            = (3.5,3.5,0.1)
        }
}
```

- All atoms in this volume will be fixed

To fix a boundary

➢ **Change in Geometery**
Introduce the boundary region

➢ **Change in strain solver**
Choose the boundary in fixed_boundary = (1,5,6)

Fixed boundary condition

- How to make fixed boundary condition?

```
solver
{
    name  = keating
    type  = KeatingStrain
    ...
// Boundary
    fixed_boundary = (1)
}
```

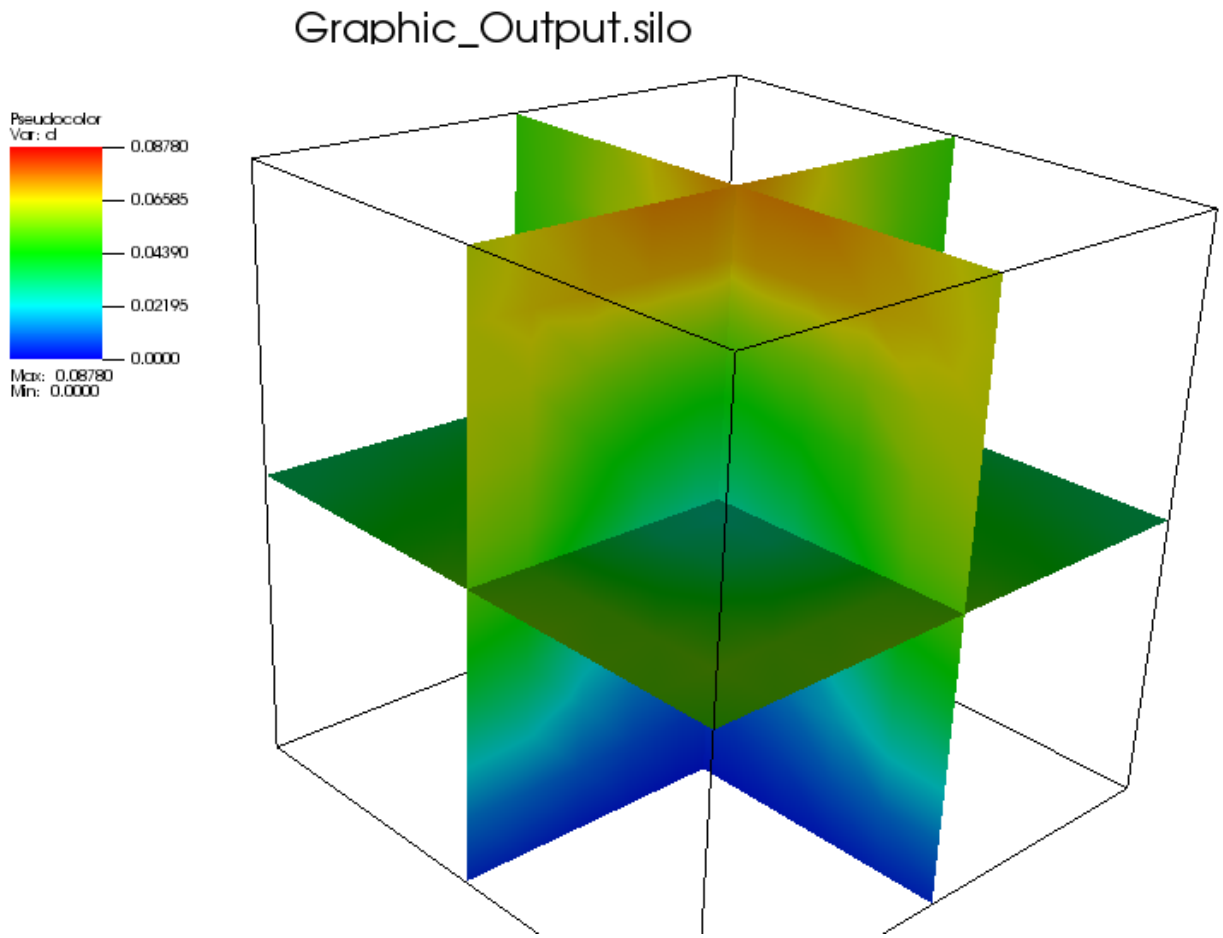
To fix a boundary

➢ **Change in Geometery**
Introduce the boundary region

➢ **Change in strain solver**
Choose the boundary in
fixed_boundary = (1,5,6)

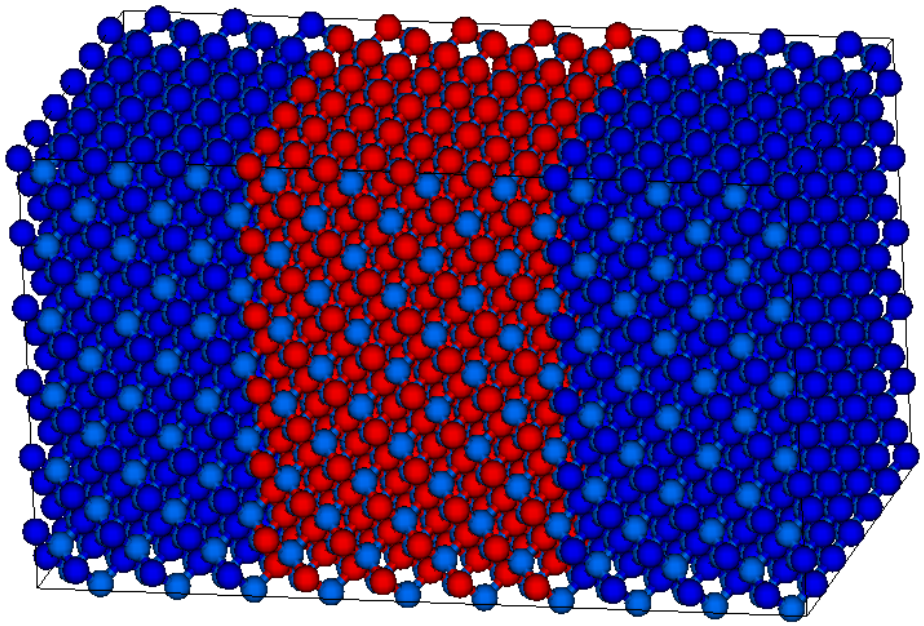
Outputs

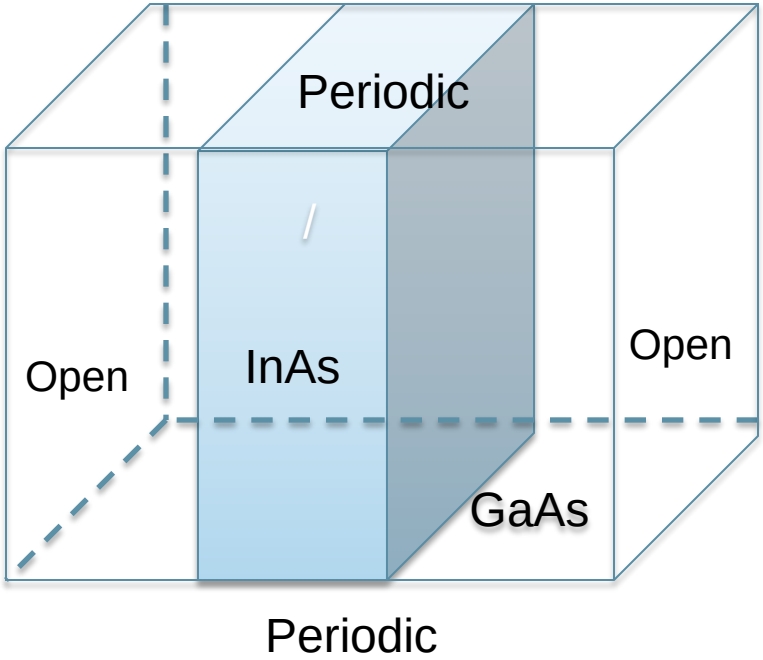
- Displacement output



Example3

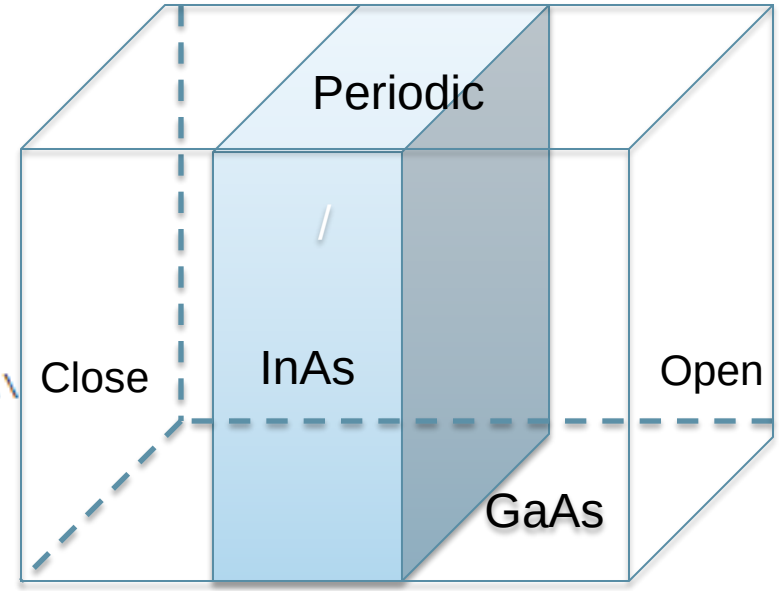
- Example3: Quantum well





Setting the Geometry

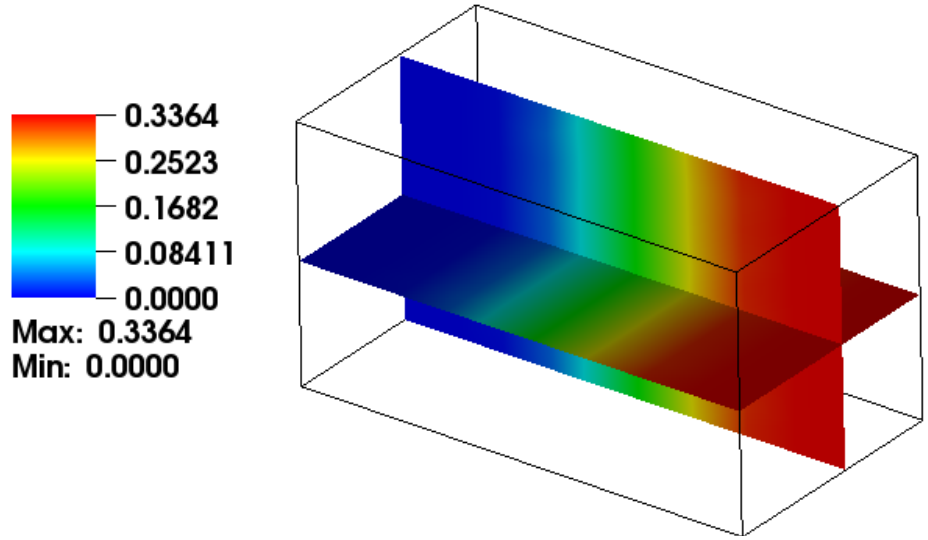
```
Geometry
{
                    //---   GaAs Substrate  ---\\
        Region
        {
                shape         = cuboid
                region_number = 1
                priority      = 1
                min           = (-0.1, -0.1 , -0.1)    // Units: nm
                max           = (4.0 , 5.7  ,  4.0)    // Units: nm
        }
                    //---   InAs Well       ---\\
        Region
        {
                shape         = cuboid
                region_number = 2
                priority      = 2
                min           = (-0.1, 1.6 , -0.1)
                max           = (4.0 , 3.8 ,  4.0)
        }
                    //---   Left Fixed Boundary       ---\\
        Boundary_region
        {
                shape         = cuboid
                region_number = 1
                priority      = 1
                min           = (0,0,0)
                max           = (4.0,0.2,4.0)
        }
```



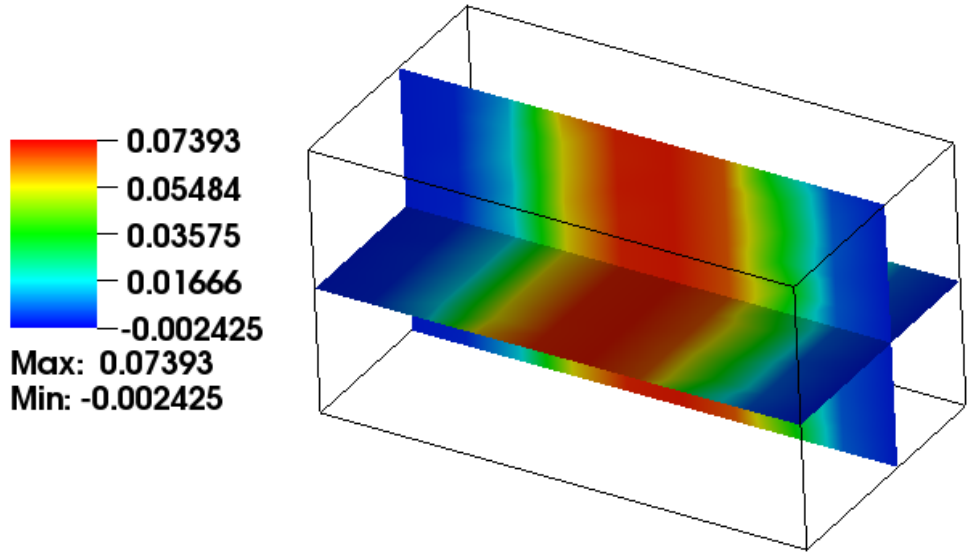
Strain outputs

Outputs

- Displacement



- Strain eyy



Thanks