Extending Nemo 5 using Python scripting (PythonSolver)

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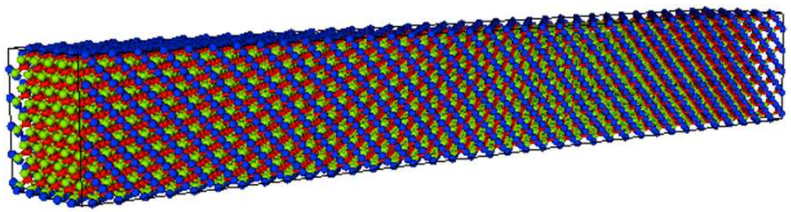
Electrical and Computer Engineering

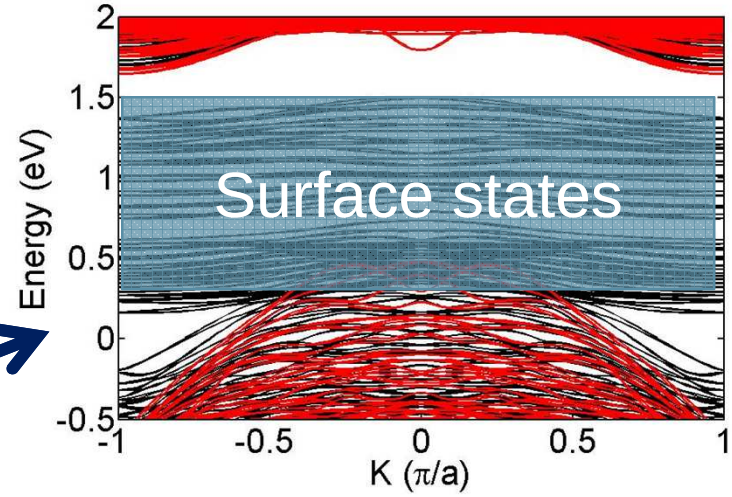
Surface Passivation

- Unpassivated surfaces contain dangling bonds and introduce undesired eigenstates within the bandgap

GaSb nanowire



Nanowire bandstructure
Red: with passivation
Black: without passivation



The goal of passivation : remove surface state from bandgap

- There is not good parameters for passivation
- How determine passivation parameters?

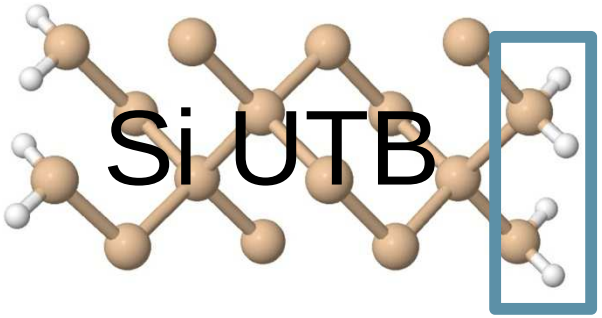
Surface Passivation

Example : optimizing Si passivation parameter.

- Determine the passivation parameter for Si-UTB to match DFT results.

Method:

Calculate E(k) using Nemo5 with different V_S_S_Sigma_H_Si and V_S_P_Sigma_H_Si.
Compare TB bands to reference bands(DFT)



Coupling parameters of H-Si bond are needed.

input deck

```
Material{
    name = Si
    tag = substrate
    crystal_structure = diamond
    regions = (1)
    Bands:TB:sp3d5sstar:param_set = param_Boykin
    Bands:TB:sp3d5sstar:param_Boykin:V_S_S_Sigma_H_Si = -4.0
    Bands:TB:sp3d5sstar:param_Boykin:V_S_P_Sigma_H_Si = 0.3
}
```

Define Material structure specifying a parameter set

```
solver {
    name = Si
    type = Schroedinger
    domain  = structure1
    active_regions = (1)
    job_list  = (…,calculate_band_structure)
    output = (energies, k-points)
    tb_basis = sp3d5sstar
    k_space_basis   = reciprocal
    k_points = [(0.5,0.0),(0,0),(0.5,0.5)]
    number_of_nodes = (10,10)
}
```

Calculate band structure by Nemo5

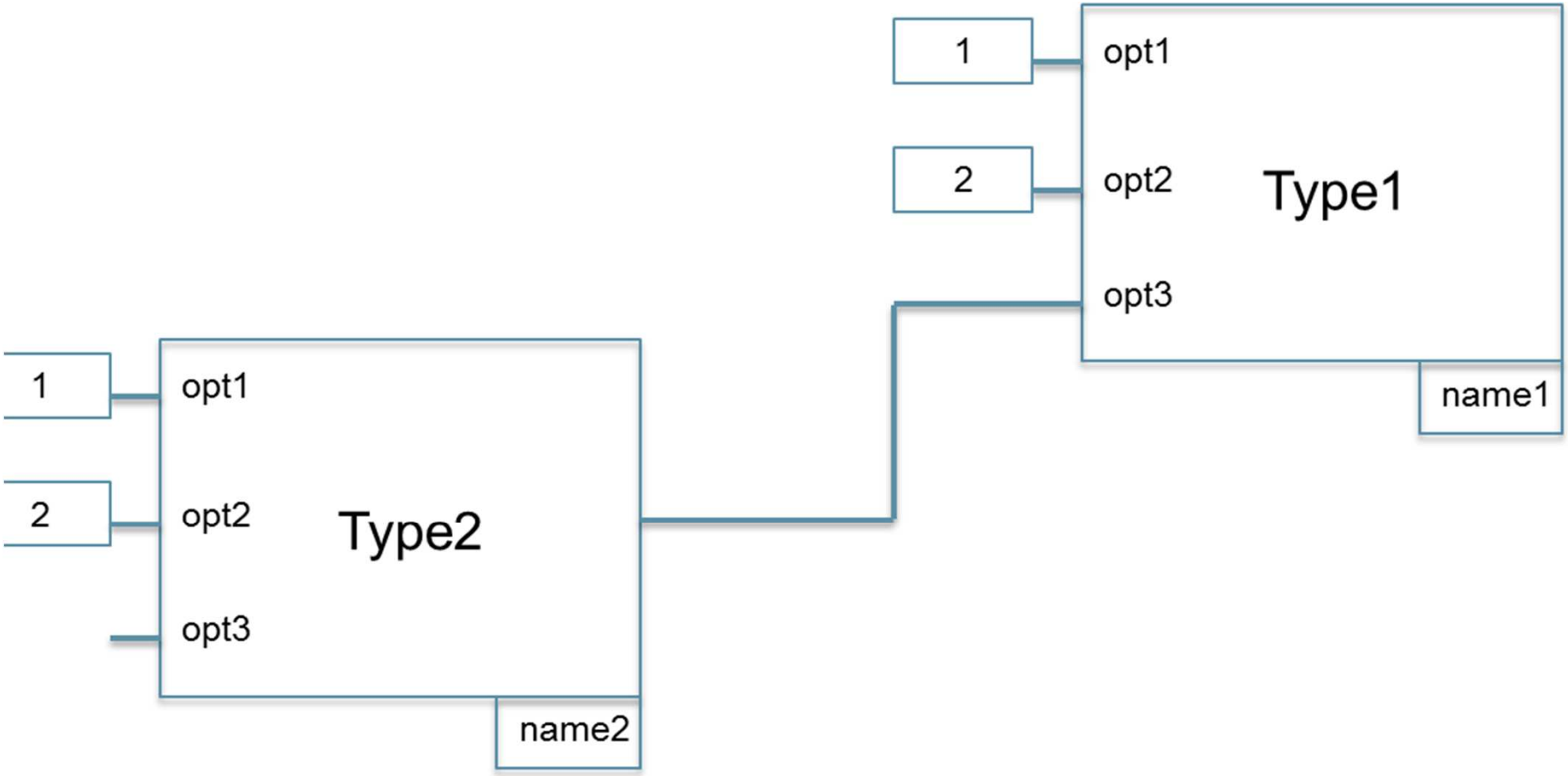
A possible Solution!!!

- Create a set of input decks with different options
- Consolidate all results
- Use an external tool (such as Matlab), post-processing files
- OR use a Python-Solver

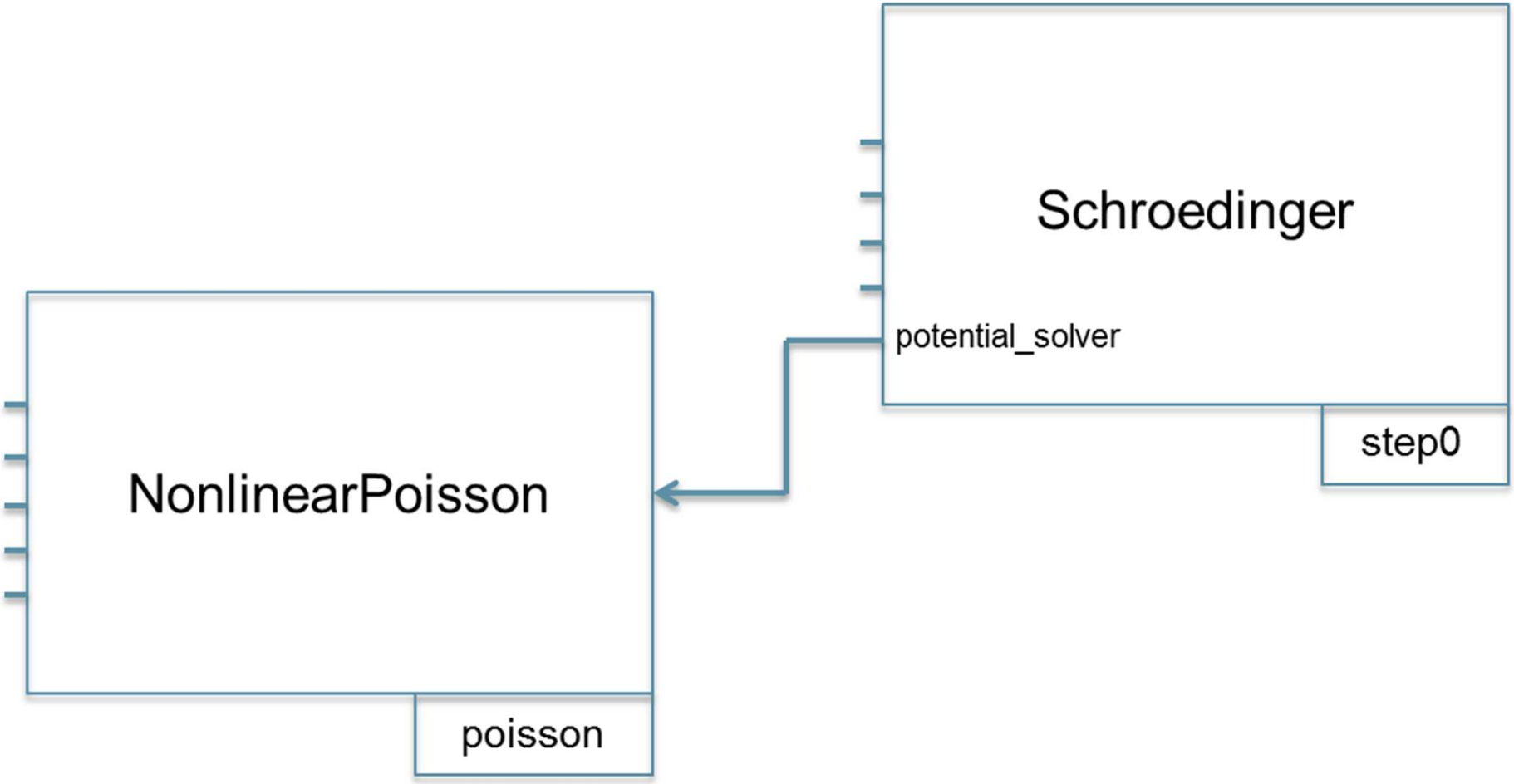
Solver

```
solver  {
        name = solver_name
        type = solver_type
        domain = solver_domain
        input_option_1  = input_1
        input_option_2  = input_2
        input_option_3  = input_3
        input_option_4  = input_4
        …
}
```

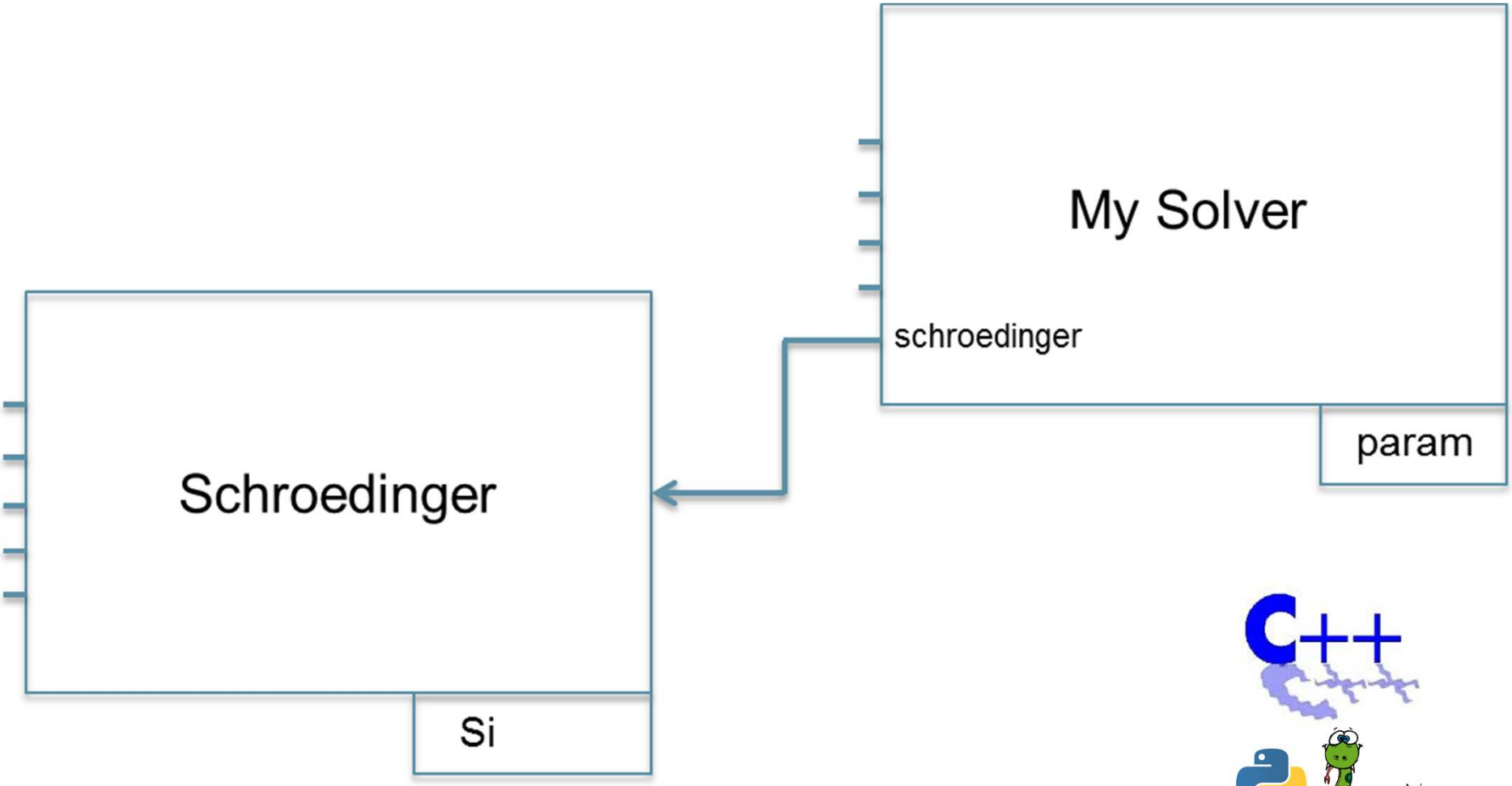
Solvers Interaction



Solvers Interaction



New Solver



Example: Nemo5 input deck

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

Define the structure without specifying the parameter set; (parameters with be specified in the python script)

```
    Domain
    {
        dimension = (1,1,2)
        periodic = (true, true, 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)
        regions = (1)
        passivate= true
        geometry_description = simple_shapes
    }
```

A silicon UTB along 001 direction is define.
The thickness is 2 unit cell, 8 Si mono-layers, with hydrogen passivated

Nemo5 input deck

```
Solvers {
    solver {
        name = Si
        type = Schroedinger
        …
    }
    solver {
        name = d1
        type = PythonSolver
        schroedinger = Si
        python_solver = ./input_python/input_python.py
    }
}
Global {
  solve = (d1)
  database = ./materials/all.mat
}
```

Specify the python solver

schroedinger: name of the solver that calculate Bandstructures.

python_solver: path to the python script

Solve the PythonSolver (d1)

Python script

./input_python/input_python.py

1) Import Libraries

↓

2) write auxiliary methods/ functions

↓

3) Overwrite Nemo5 methods

↓

4) Bind methods to Nemo5 Python Interface

Python script

./input_python/input_python.py

import numpy as np

1) Import Libraries

def do_solve (self):

3) Overwrite Nemo5 methods

```
if self.check_option( "schroedinger" ):
  solver_schroedinger_str = self.get_option( "schroedinger" )
  solver_schroedinger = self.find_simulation( solver_schroedinger_str )

  if solver_schroedinger is not None :
    Num = 10;
    Fitness = np.zeros(shape=(Num,Num))
    list_valuesi = range(Num)
    list_valuesj = range(Num)
    for i in list_valuesi :
      for j in list_valuesj :

        materials = solver_schroedinger.get_materials()

        for m in materials:
          m.set_option('Bands:TB:sp3d5s*star:param_set', 'param_Boykin')
          m.set_option('Bands:TB:sp3d5s*star:param_Boykin:V_S_S_Sigma_H_Si', str(-20+i*2))
          m.set_option('Bands:TB:sp3d5s*star:param_Boykin:V_S_P_Sigma_H_Si', str(0+j*3))

        solver_schroedinger.set_option('

        solver_schroedinger.reinit()
        solver_schroedinger.reinit_materials()
        solver_schroedinger.solve()
        solver_schroedinger.output()
        # post process
        energy = np.loadtxt('Si_' + str(i)+ '_' + str(j)+'_energies.dat','float')
        Ref_energy = [-1,-0.7,-0.5,0]
        TB_energy = energy[[25,26,27,28]]
        Dif = TB_energy-Ref_energy
        Fitness[i,j] = np.dot(Dif,Dif)
  else :
    raise NameError('solver_schroedinger doesnt exists')
  print Fitness
  np.savetxt('Fitness.dat',Fitness)
else :
  raise NameError('schroedinger parameter required')
```

spaces for indentation matter in python

do_solve
do_init
do_reinit
do_output
get_data_...

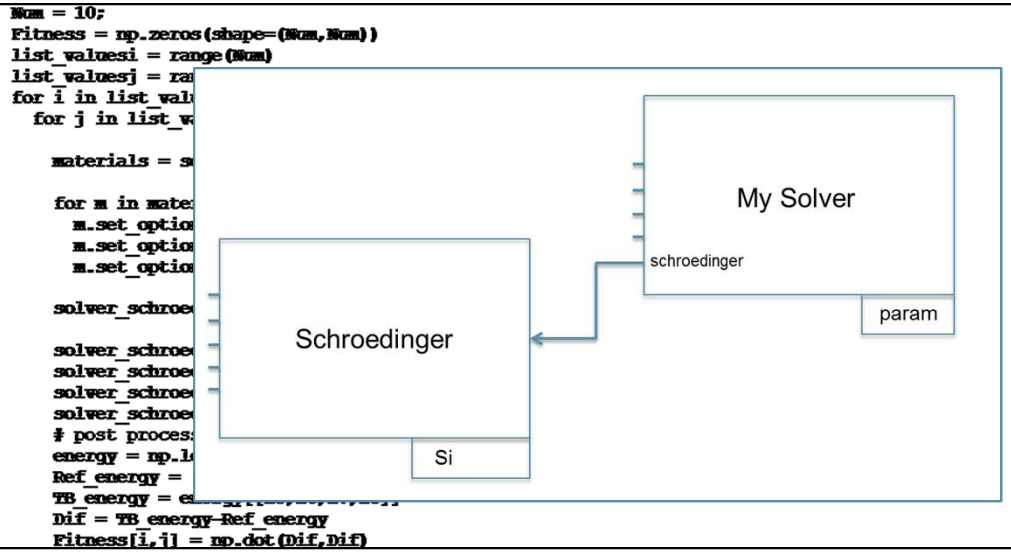
PythonSolverInterface.do_solve = do_solve

4) Bind methods to Nemo5 Python Interface

do_solve

./input_python/input_python.py

```
if self.check_option( "schroedinger" ):
    solver_schroedinger_str = self.get_option( "schroedinger" )
    solver_schroedinger = self.find_simulation( solver_schroedinger_str )
    if solver_schroedinger is not one :
```



In the nemo5 input.in :

```
solver
  {
    name = d1
    type = PythonSolver
    schroedinger = Si
    …
  }
```

```
    else :
        raise NameError('solver_schroedinger doesn't exists')
else:
    raise NameError('schroedinger parameter required')
```

do_solve

./input_python/input_python.py

```
if self.check_option( "schroedinger"
  solver_schroedinger_str = self.get_
  solver_schroedinger = self.find_si

  if solver_schroedinger is not None
```

100 samples

Reconfigure Schroedinger solver

```
for i in range(10) :
  for j in range(10) :
    materials = solver_schroedinger.get_materials()
    for m in materials:
      m.set_option('Bands:TB:sp3d5sstar:param_set', 'param_Boykin‘)
      m.set_option('Bands:TB:sp3d5sstar:param_Boykin:V_S_S_Sigma_H_Si', \
      str(-20+i*0.2))
      m.set_option('Bands:TB:sp3d5sstar:param_Boykin:V_S_P_Sigma_H_Si', \
      str(0+j*0.3))
    solver_schroedinger.set_option('output_file_suffix', '_' + str(i)+ '_' + str(j))
```

Set parameters for each material

```
        solver_schroedinger.reinit()
        solver_schroedinger.reinit_material_properties()
        solver_schroedinger.solve()
        solver_schroedinger.output()
        # post process
        energy = np.loadtxt('Si_' + str(i)+ '_' + str(j)+'_energies.dat','float')
        Ref_energy = [-1,-0.7,-0.5,0]
        TB_energy = energy[[25,26,27,28]]
        Dif = TB_energy-Ref_energy
        Fitness[i,j] = np.dot(Dif,Dif)
    else :
      raise NameError('solver_schroedinger doesnt exists')
    print Fitness
    np.savetxt('Fitness.dat',Fitness)
  else :
    raise NameError('schroedinger parameter required')
```

Specify the name of output file for each set of parameters

do_solve

./input_python/input_python.py

Re-initialize Schroedinger solver

```
if self.check_option( "schroedinger" ):
  solver_schroedinger_str = self.get_option( "schroedinger" )
  solver_schroedinger = self.find_simulation( solver_schroedinger_str )

  if solver_schroedinger is not None :
    Num = 10;
    Fitness = np.zeros(shape=(Num,Num))
    list_valuesi = range(Num)
    list_valuesj = range(Num)
    for i in list_valuesi :
      for j in list_valuesj :

        materials = solver_schroedinger.get_materials()

        for m in materials:
          m.set_option('Bands:TB:sp3d5sstar:param_set', 'param_Boykin')
          m.set_option('Bands:TB:sp3d5sstar:param_Boykin:V_S_S_Sigma_H_S
          m.set_option('Bands:TB:sp3d5sstar:param_Boykin:V_S_P_Sigma_H_S

        solver_schroedinger.set_option('output_file_suffix', '_' + str(i
```

Re-initialize the options in the solver;
Re-initialize the parameters of the material;

```
solver_schroedinger.reinit()
solver_schroedinger.reinit_material_properties()
solver_schroedinger.solve()
solver_schroedinger.output()
```

```
        energy = np.loadtxt('Si_' + str(i)+ '_' + str(j)+'_energies.dat
        Ref_energy = [-1,-0.7,-0.5,0]
        TB_energy = energy[[25,26,27,28]]
        Dif = TB_energy-Ref_energy
        Fitness[i,j] = np.dot(Dif,Dif)
  else :
    raise NameError('solver_schroedinger doesnt exists')
  print Fitness
  np.savetxt('Fitness.dat',Fitness)
else :
  raise NameError('schroedinger parameter required')
```

Generate outputs

do_solve

```
if self.check_option( "schroedinger" ):
  solver_schroedinger_str = self.get_option( "schroedinger" )
  solver_schroedinger = self.find_simulation( solver_schroedinger_str )

  if solver_schroedinger is not None :
    Num = 10;
    Fitness = np.zeros(shape=(Num,Num))
    list_valnesi = range(Num)
    list_valnesj = range(Num)
    for i in list_valnesi :
      for j in list_valnesj :

        materials = solver_schroedinger.get_materials()

        for m in materials:
          m.set_option('Bands:TB:sp3d5sstar:param_set', 'param_Boykin')
          m.set_option('Bands:TB:sp3d5sstar:param_Boykin:V_S_S_Sigma_H_Si', str(-20+i*2))
          m.set_option('Bands:TB:sp3d5sstar:param_Boykin:V_S_P_Sigma_H_Si', str(0+j*3))

        solver_schroedinger.set_option('output_file_suffix', '_' + str(i)+ '_' + str(j))

        solver_schroedinger.reinit()
        solver_schroedinger.reinit_material_properties()
        solver_schroedinger.solve()
        solver_schroedinger.output()
        # post process
```

Fitness

Read nemo5 results

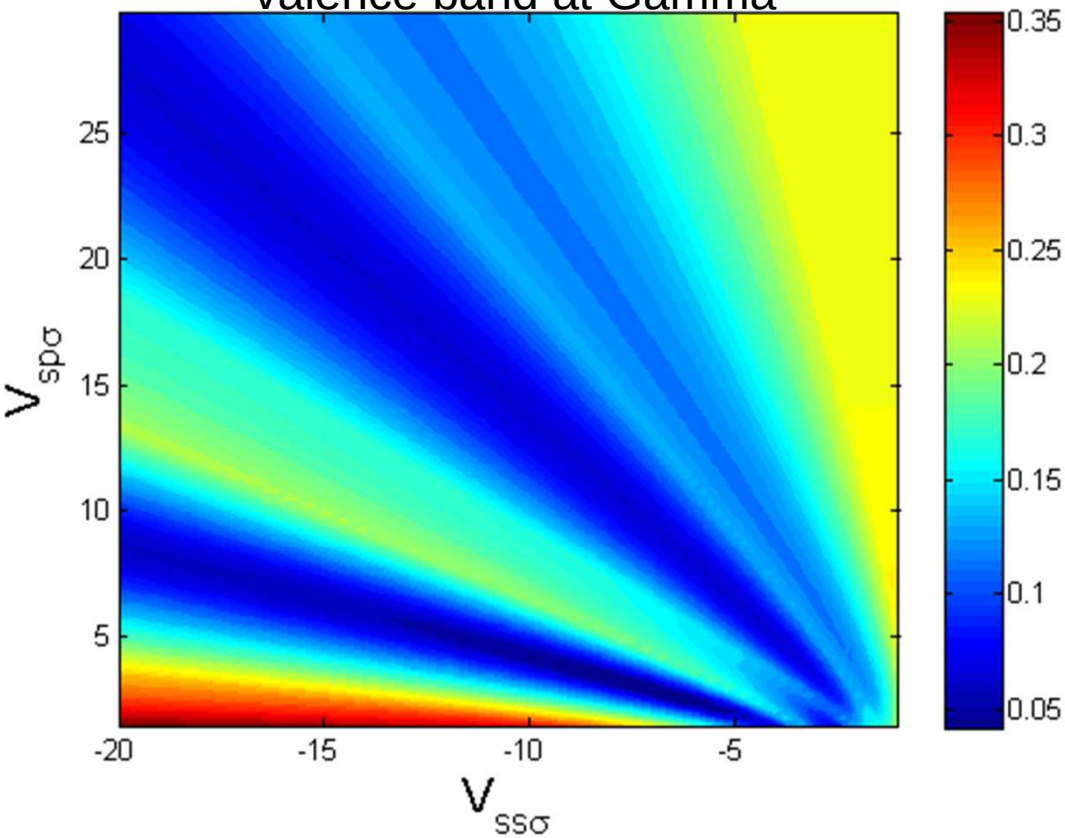
```
energy = np.loadtxt('Si_' + str(i)+ '_' + str(j)+'_energies.dat','float')
Ref_energy = [-1,-0.7,-0.5,0]
TB_energy = energy[[25,26,27,28]]
Dif = TB_energy-Ref_energy
Fitness[i,j] = np.dot(Dif,Dif)
np.savetxt('Fitness.dat',Fitness)
```

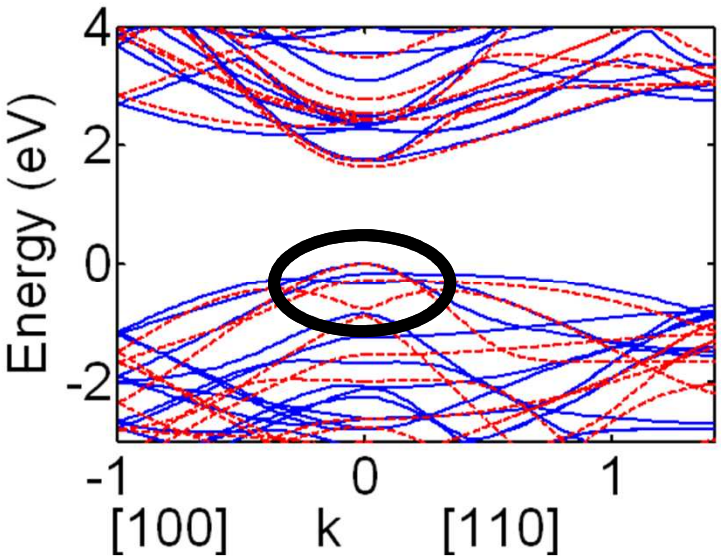
Compare selected bands with reference bands

```
  else :
    raise NameError('solver_schroedinger doesnt exists')
  print Fitness
  np.savetxt('Fitness.dat',Fitness)
else :
  raise NameError('schroedinger parameter required')
```

Results of Example

Average error of the highest 4 valence band at Gamma





Band structure of Si UTB:
Blue lines: DFT results
Red lines: nemo5 results

100 different values for Vspσ_H_Si and Vssσ_H_Si →10000 samples
DFT result is generated by ABINIT

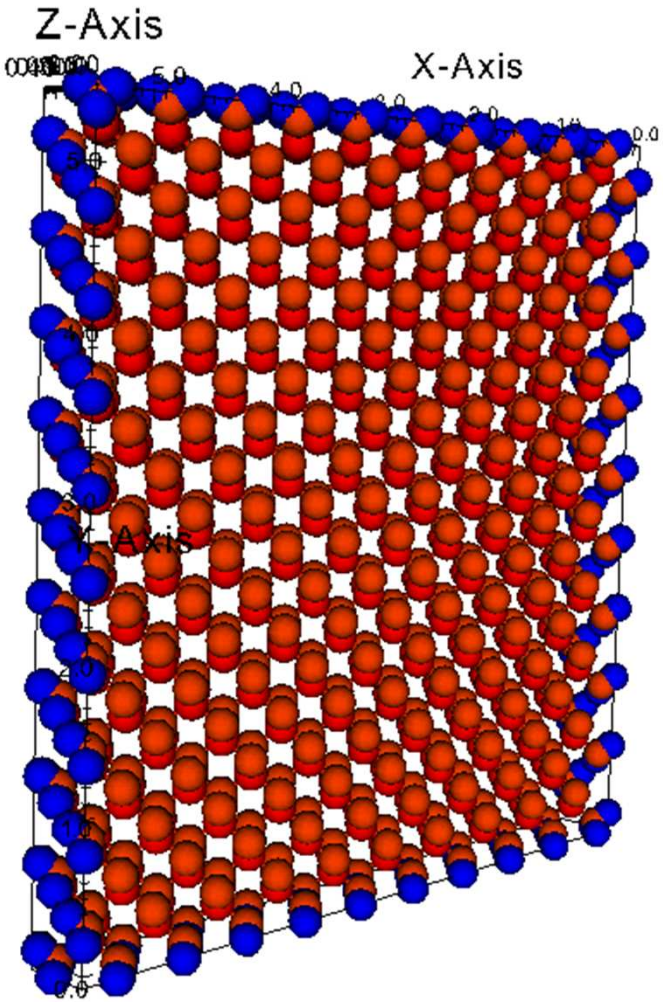
step0.in

~/public_samples/Python_solver/Python_tutorial/step0.in

- GaAs Nanowire

- Solvers:
  - NonlinearPoisson
  - Schroedinger
  - Structure

```
Region{
        shape = cuboid
        region_number = 1
        priority = 1
        min = (-1.5,-1.5,-1.5)
        max = (5.5,5.5,2.5)
}
```



step0.in

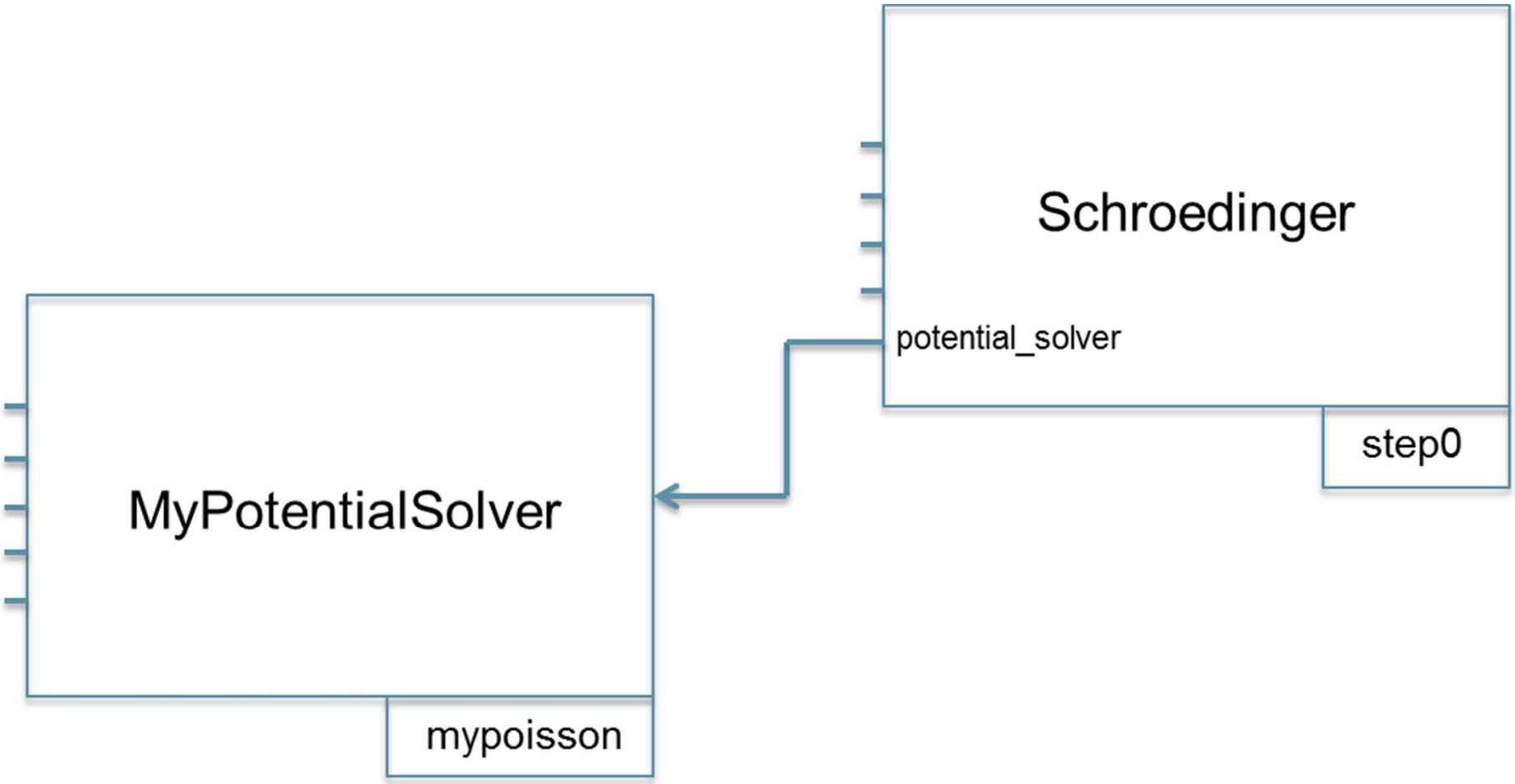
~/public_samples/Python_solver/Python_tutorial/step0.in

```
…
solver {
    name       = poisson
    type       = NonlinearPoisson
    domain     = continuum
    …
}
solver {
    name           = step0
    type           = Schroedinger
    domain         = atomic_structure
    active_regions = (1)
    job_list = (passivate_H, calculate_band_structure)
    output = (energies,eigenfunctions_Point3D, eigenfunctions_VTK)
    potential_solver = poisson
    …
}
…
```

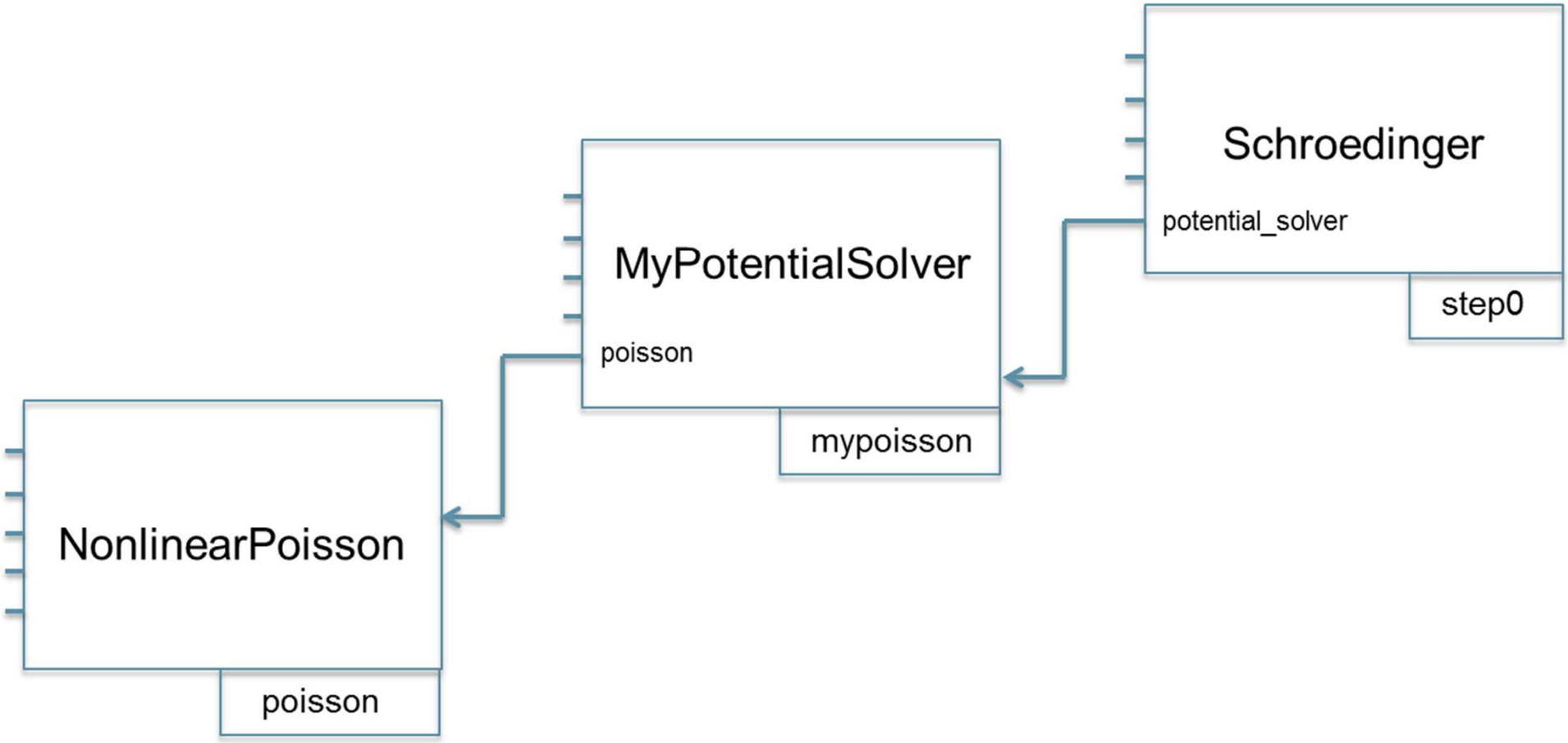
VTK Format

3D Format

Solvers Interaction



Solvers Interaction



step1.in

~/public_samples/Python_solver/Python_tutorial/step1.in

```
solver {
  name = poisson
  type = NonlinearPoisson
  domain = continuum
  …
}
```

```
solver {
  name = pythonpoisson
  type = PythonSolver
  domain = atomic_structure
  poisson = poisson
  python_solver = ./step1.py
}
```

```
solver {
  name = step1
  type = Schroedinger
  domain = atomic_structure
  potential_solver = pythonpoisson
  …
}
```

PythonSolvers Interaction

Data Flow

Call methods:
get_data(…)
get_multidata(…)

step1.py

Rewrite method:
get_..._data_...(…)

~/public_samples/Python_solver/Python_tutorial/step1.py

1) Import Libraries

```
import math
import random
```

- import numpy
- import scipy
- import vtk
- from math import *

- import sys
- sys.path.append('…/my_path/')

~/public_samples/Python_solver/Python_tutorial/step1.py

2) write auxiliary methods/ functions

```
#returns a perturbation [-0.05, 0.05]
def random_perturbation ():
  return (random.random()-0.5)/10

#pot = Atom Id
#ori_pot = Original Potential
#new_pot = Perturbated Potential
def print_potential (pot, ori_pot, new_pot):
  txt = ""
  txt += "Potential[" + str(pot) + "]:" + str(ori_pot)
  txt += " - " + str(new_pot)
  print txt
```

- Functions

```
def name_function(…):
  …
```

- Methods

```
def name_method( self, …):
  …
```

~/public_samples/Python_solver/Python_tutorial/step1.py

3) Overwrite Nemo5 methods

```
def do_init(self):
  self.potentials = {}
  if self.check_option( "poisson" ):
    poisson_str = self.get_option( "poisson" )
    self.poisson = self.find_simulation( poisson_str )
  else:
    self.poisson = None
```

- do_init(self):
- do_reinit(self):
- do_solve(self):
- do_output(self):

- get_..._data_... (self, …)

bool check_option(string opt) -> was ‘opt’ defined in the input deck?
string get_option(string opt) -> returns input option ‘opt’
N5_Solver find_simulation (string solver_name) -> returns a ‘pointer’ to the instance of solver_name

~/public_samples/Python_solver/Python_tutorial/step1.py

3) Overwrite Nemo5 methods

```
void Simulation::get_data(const string& variable,
                const vector<double>& in_data, std::vector<double>&  out_data)
```

```
def get_list_uint_data_list_double ( self, variable, in_data ):
 out_data = []
  if self.poisson is not None:
    self.poisson.get_multidata(params, in_data, result, "list<uint>:list<double>")
    for i, v in enumerate(in_data[0]):
      original_potential = out_data[0][i]
      if v in self.potentials:
        out_data[0][i] = self.potentials[v]
      else :
        out_data[0][i] += random_perturbation()
        self.potentials[v] = result[0][i]
      print_potential(v, original_potential, result[0][i])
  return out_data
```

Given a list of unsigned integer, this returns a list of doubles

step1.py

~/public_samples/Python_solver/Python_tutorial/step1.py

4) Bind methods to Nemo5 Python Interface

```
import math
import random
def do_init(self):
  self.potentials = {}
  if self.check_option( "poisson" ):
    poisson_str = self.get_option( "poisson" )
    self.poisson = self.find_simulation( poisson_str )
  else:
    self.poisson = None

def random_perturbation ():
  return (random.random()-0.5)/100

#pot = Atom Id
#ori_pot = Original Potential
#new_pot = Perturbated Potential
def print_potential (pot, ori_pot, new_pot):
  txt = ""
  txt += "Potential[" + str(pot) + "]:" + str(ori_pot)
```

```
PythonSolverInterface.do_init = do_init
PythonSolverInterface.get_list_uint_data_list_double = get_list_uint_data_list_double
```

```
    self.poisson.get_multidata(params, variables, result, "list<uint>:list<double>")
    for i, v in enumerate(variables[0]):
      original_potential = result[0][i]
      if v in self.potentials:
        result[0][i] = self.potentials[v]
      else :
        result[0][i] += random_perturbation()
        self.potentials[v] = result[0][i]
      print_potential(v, original_potential, result[0][i])
  return result

PythonSolverInterface.do_init = do_init
PythonSolverInterface.get_list_uint_data_list_double = get_list_uint_data_list_double
```

Run step1_small.py

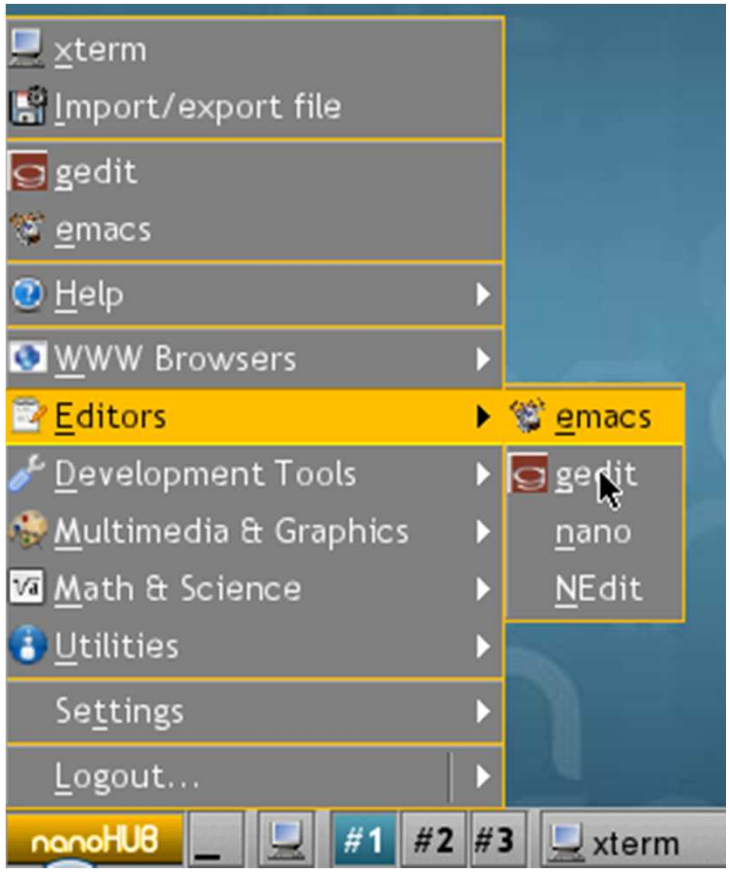
```
submit -v coates \
    -i /apps/share64/nemo/examples/current/materials/all.mat \
    -i ./step1_small.in \
    -i ./step1.py \
    nemo-r7962 step1_small.in
```

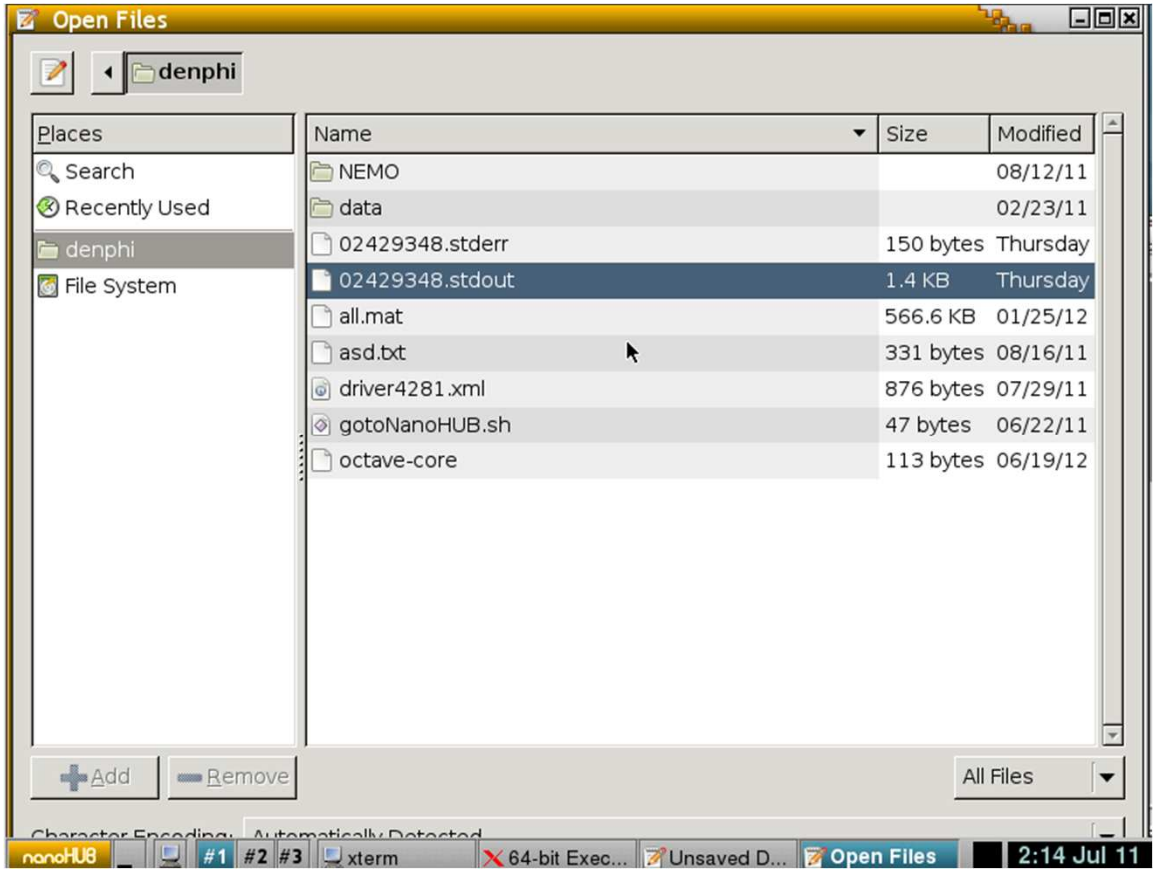
Open file XXXXXX.stdout in a text editor (emacs, vi, gedit, …)

Search line (~320):
“[Schroedinger] band dispersion loop at: 0%, k=(0,0,0)”

step1_small.py

Search line (~320): “[Schroedinger] band dispersion loop at: 0%, k=(0,0,0)”





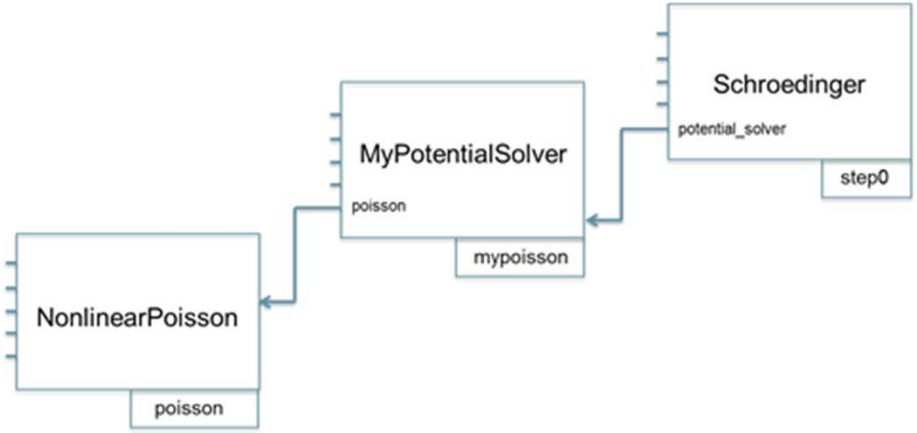
Run step1.py

submit -v coates -i ./all.mat -i ./step1.in -i ./step1.py nemo-rXXXX step1.in

Atom ID

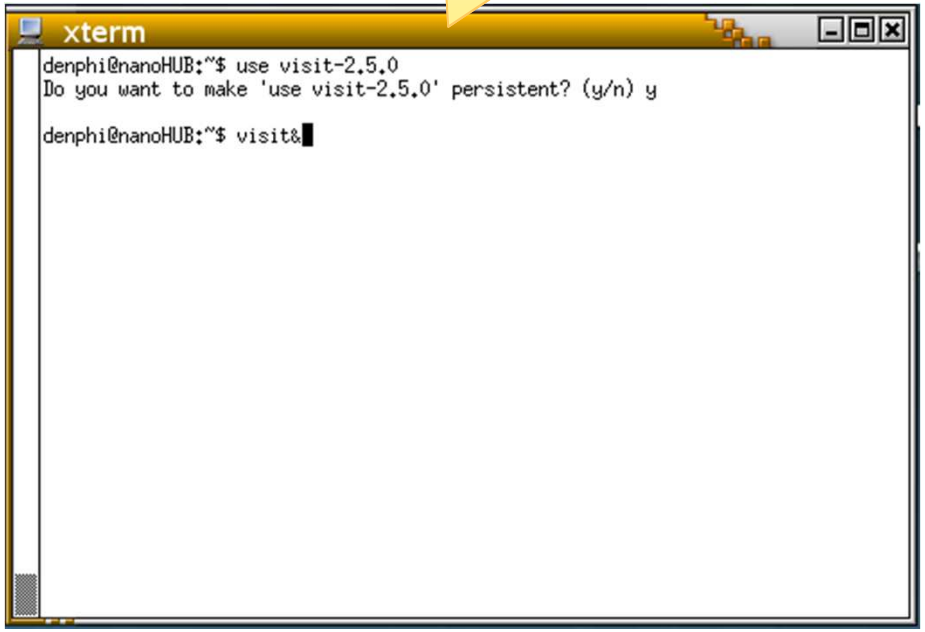
```
Potential[123]:-0.711241071429 - -0.71468656041
Potential[124]:-0.711241071429 - -0.708356163895
Potential[125]:-0.711241071429 - -0.707456438156
Potential[126]:-0.711241071429 - -0.713384328581
Potential[127]:-0.711241071429 - -0.7121059371
Potential[128]:-0.711241071429 - -0.710035799555
Potential[129]:-0.711241071429 - -0.711474255723
Potential[130]:-0.711241071429 - -0.711047785595
Potential[131]:-0.711241071429 - -0.712618402222
Potential[132]:-0.711241071429 - -0.711746789194
Potential[133]:-0.711241071429 - -0.715607662224
Potential[134]:-0.711241071429 - -0.707339627721
Potential[135]:-0.711241071429 - -0.71571539359
Potential[136]:-0.711241071429 - -0.715568649722
Potential[137]:-0.711241071429 - -0.716199576789
```

After Before

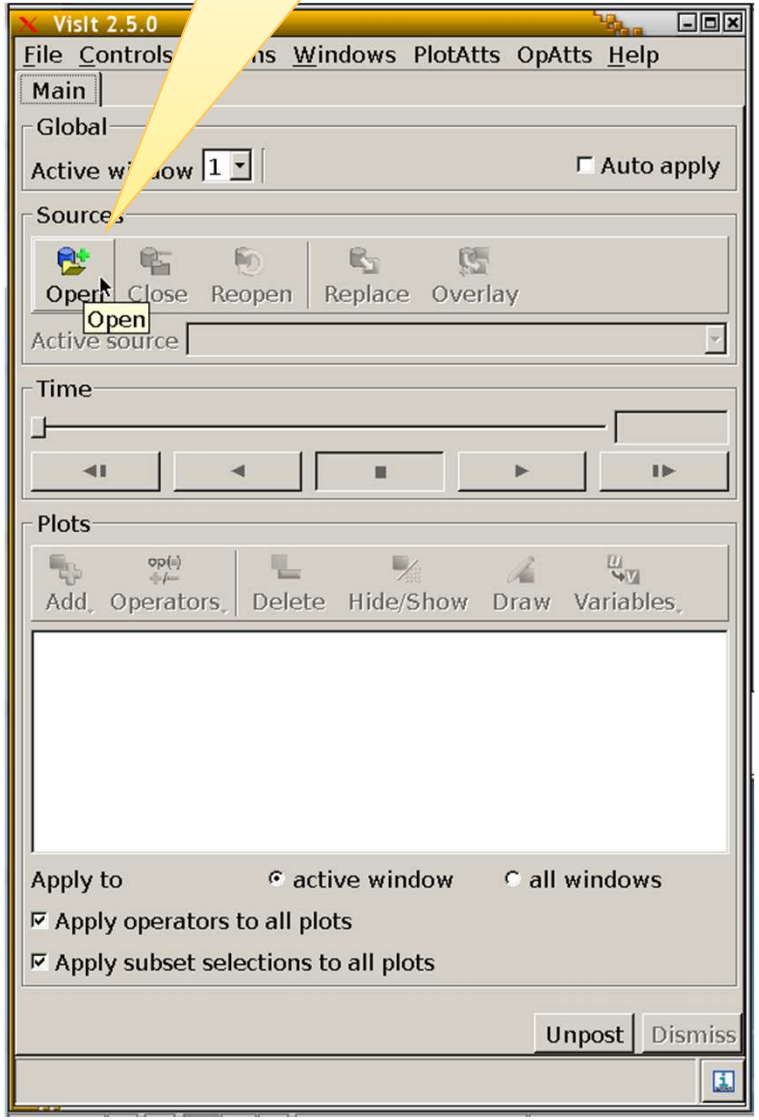



```
def print_potential (pot, ori_pot, new_pot):
"Potential["+str(pot)+"]:"+str(ori_pot)+"-"+str(new_pot)
```

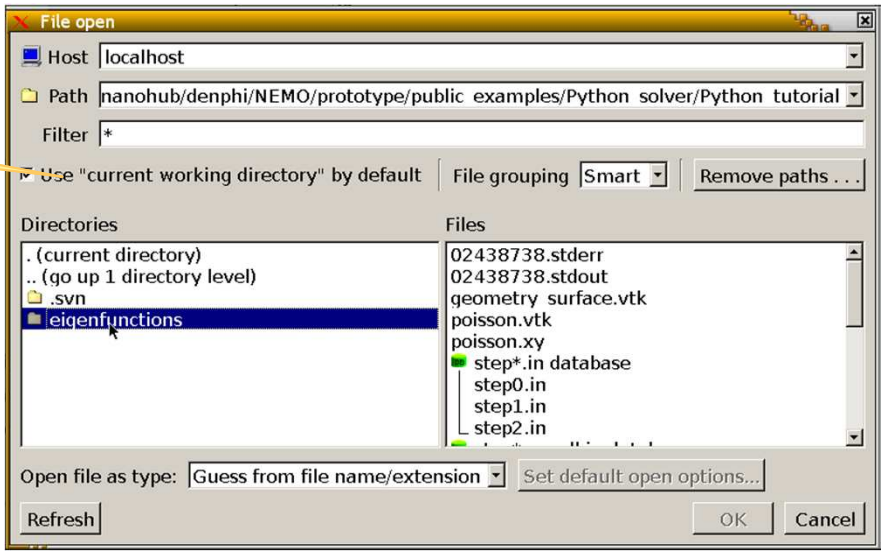
- Load VisIt:
  - use visit-2.5.0 (y)
  - visit &

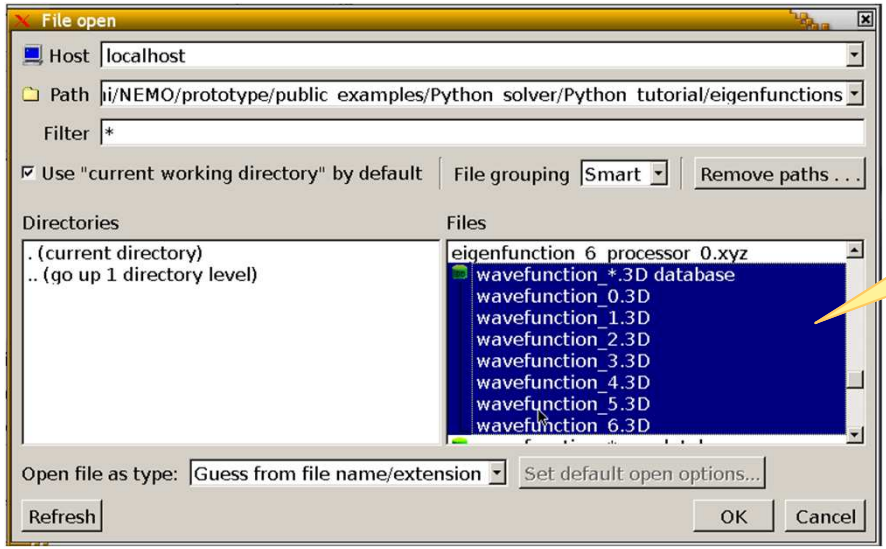


- Open Database



Locate eigenfunctions folder

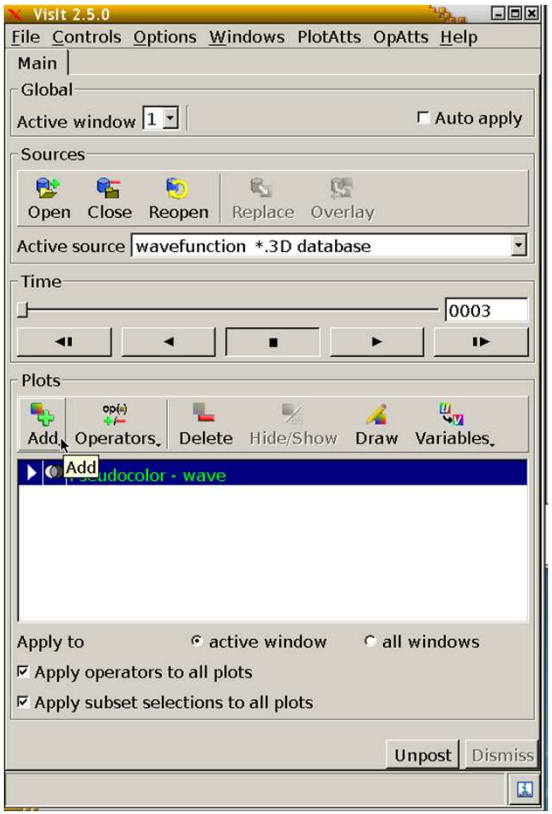


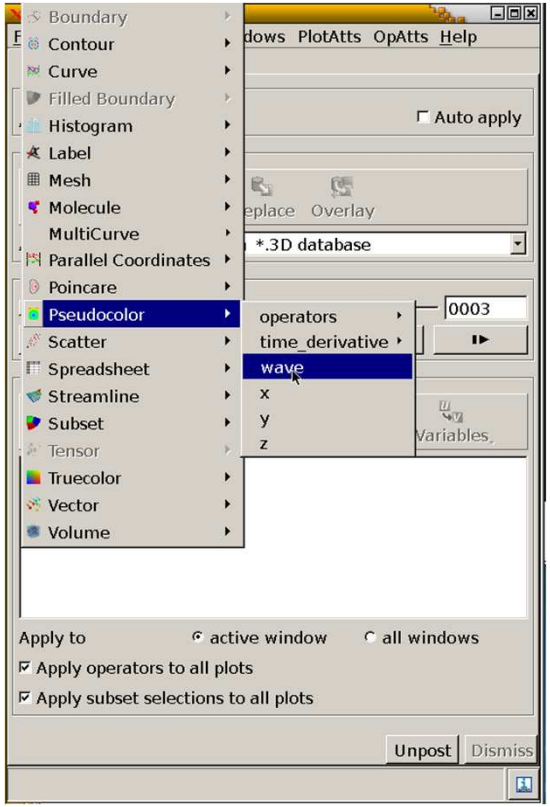


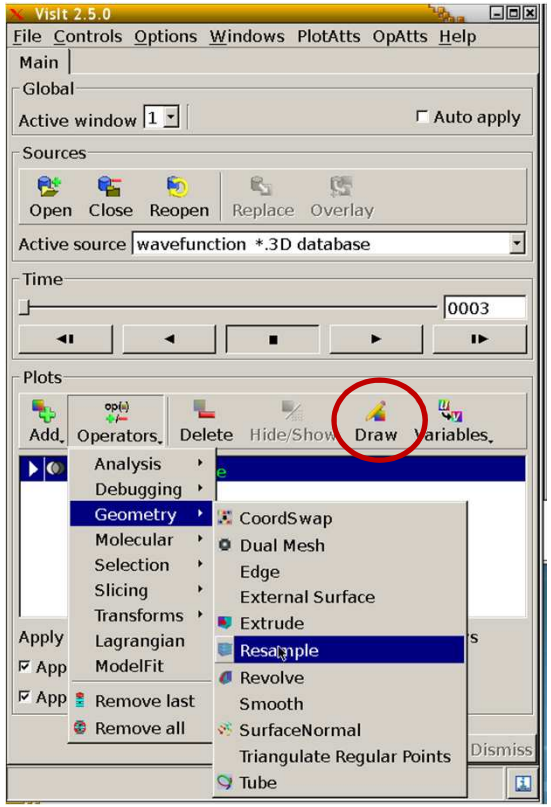
Load wavefunction DB

Visit

1) Add / PseudoColor / Wave
2) Operators / Geometry / Resample
3) Draw

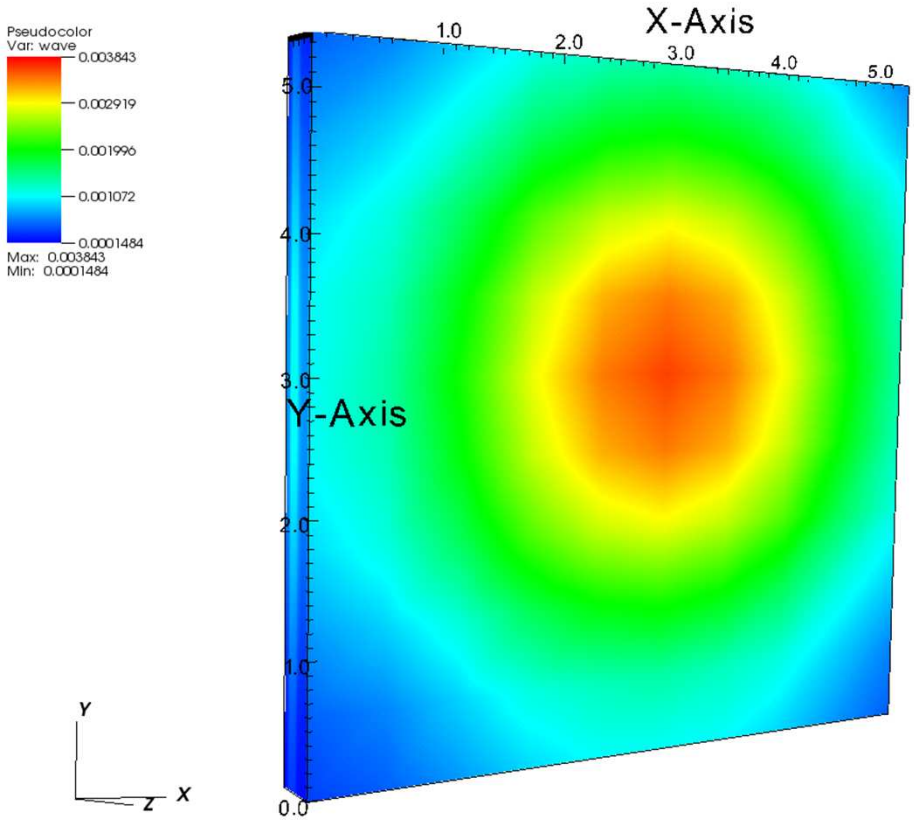




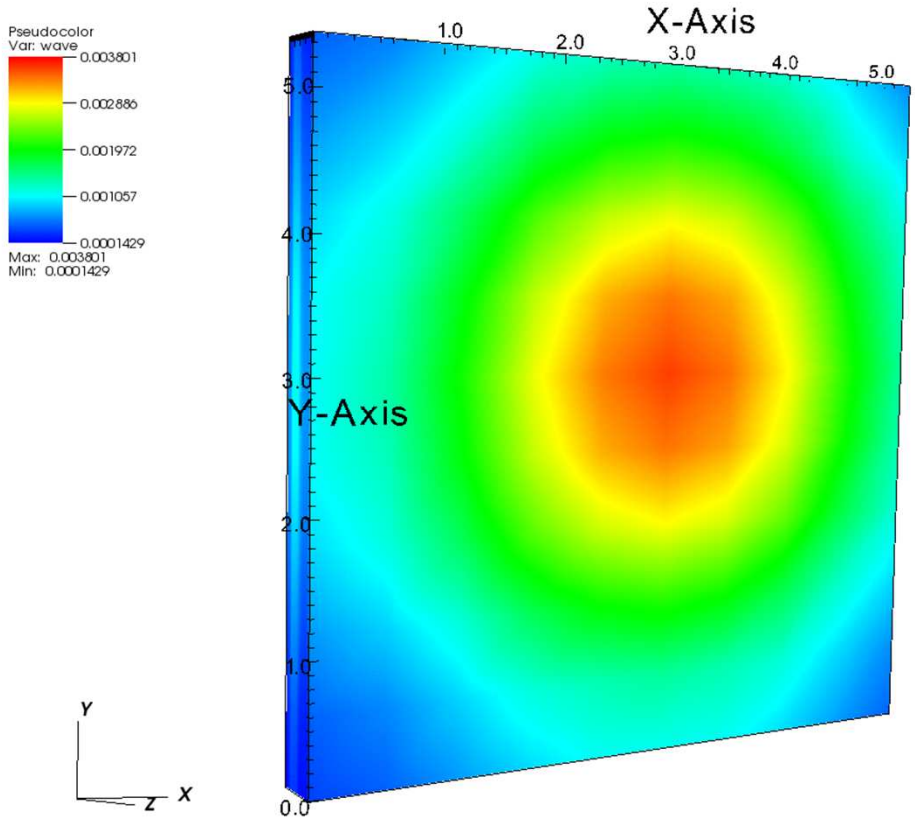


step0 vs step1

eigenfunctions/wavefunction_0.xyz

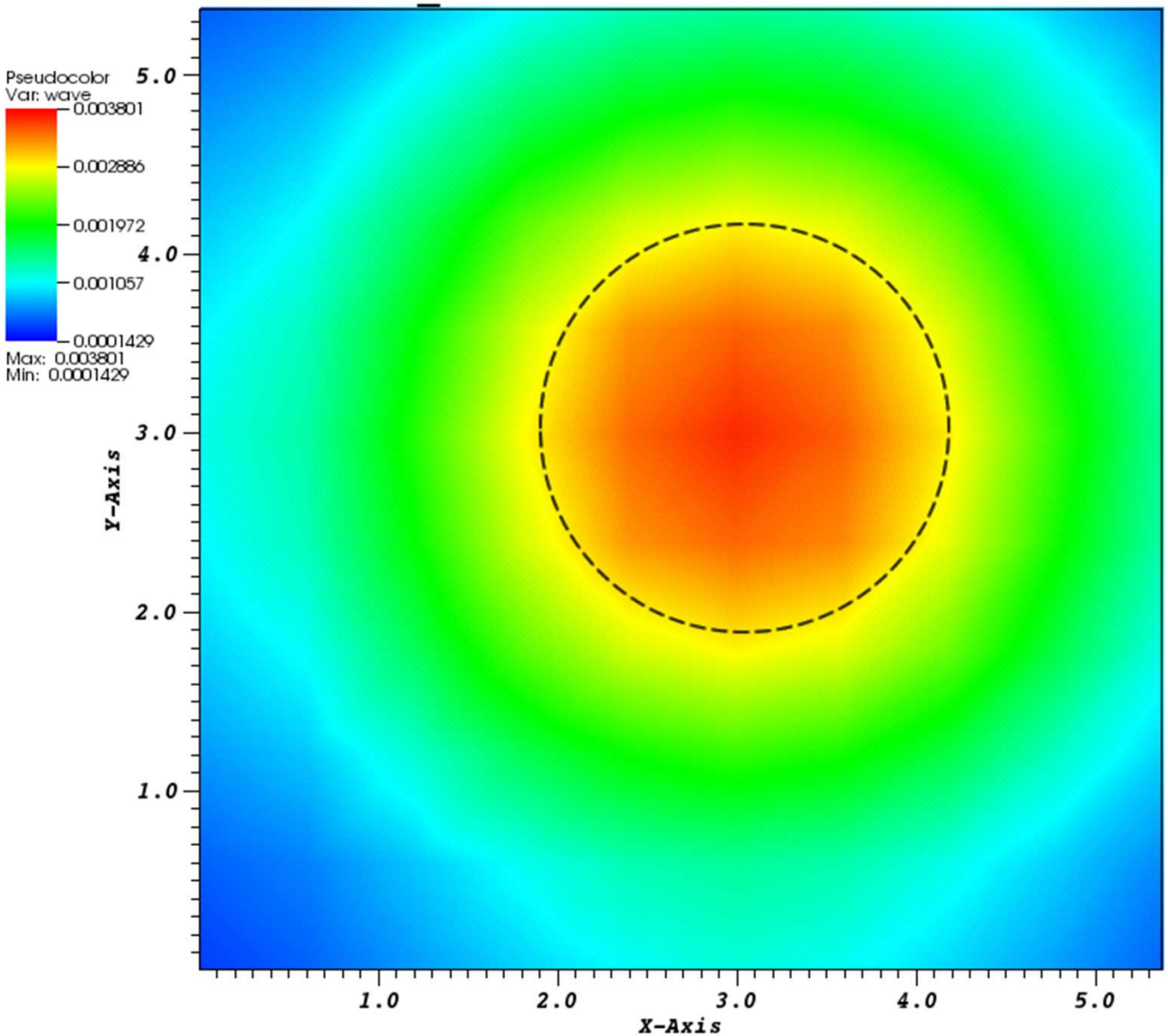


step0.py



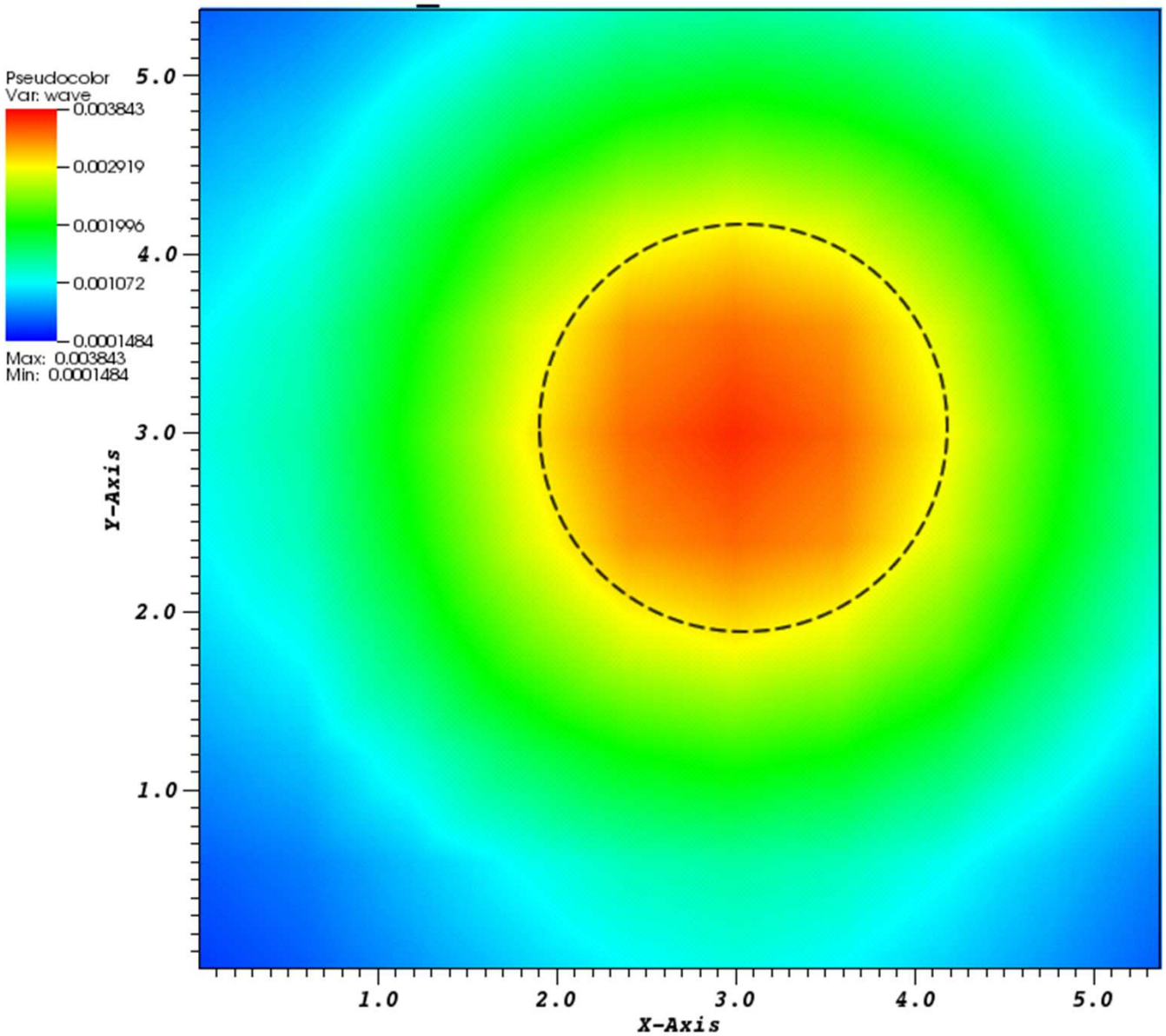
step1.py

step0 vs step1



PURDUE UNIVERSITY

step0 vs step1



PURDUE UNIVERSITY

Exercise

- Edit random_perturbation function. File (step1.py)

- Examples:
  - return (random.random()-0.5)
  - return random.random()
  - return (random.random()-0.5)*2

step1.py (~/NEMO/prototype/public_examples/Python_solver/Pyt...

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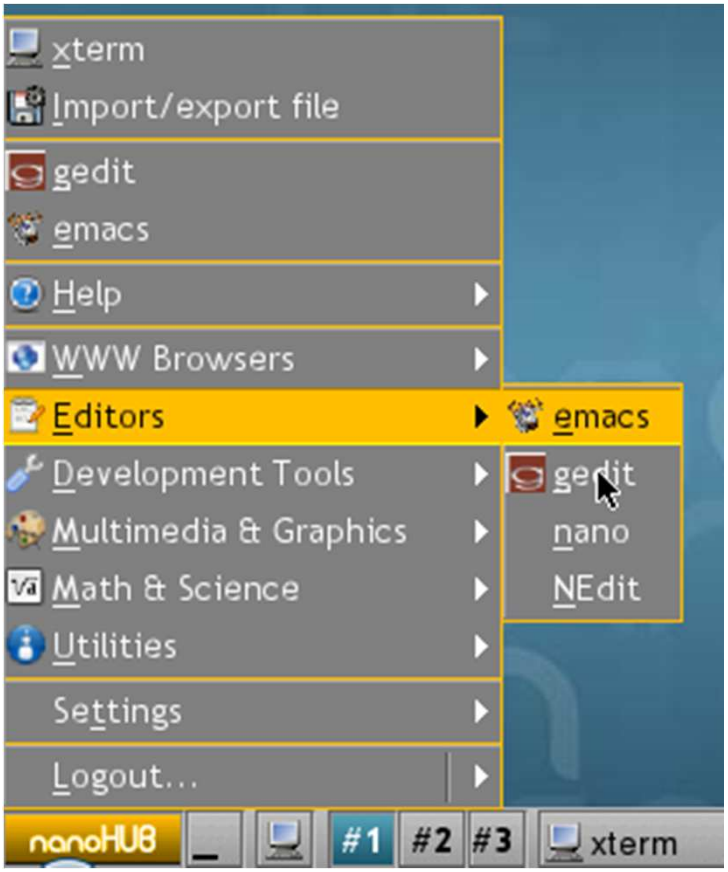
New Open Save Print Undo Redo Cut Copy Paste Find Replace

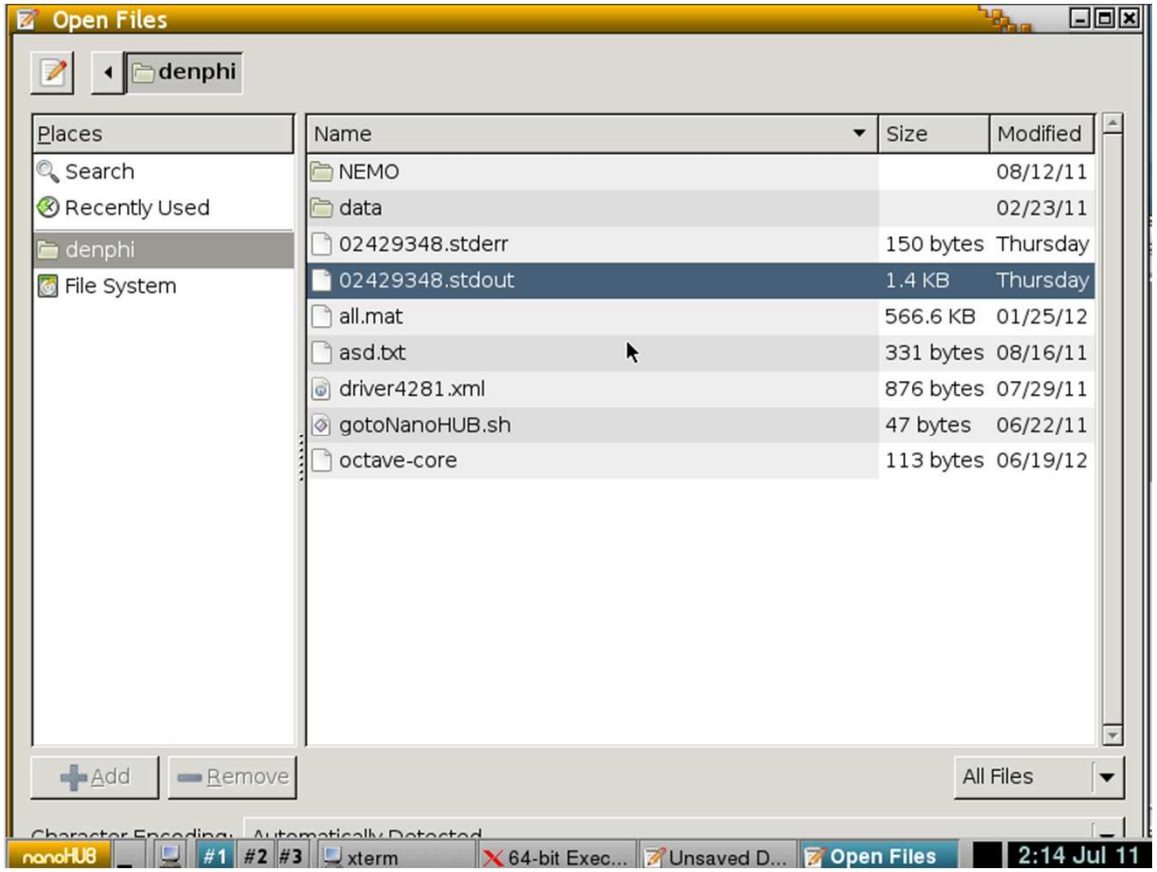
step1.py

```python
import math
import random
def do_init(self):
  self.potentials = {}
  if self.check_option( "poisson" ):
    poisson_str = self.get_option( "poisson" )
    self.poisson = self.find_simulation( poisson_str )
  else:
    self.poisson = None

def random_perturbation ():
  return (random.random()-0.5)/10

#pot = Atom Id
#ori_pot = Original Potential
#new_pot = Perturbated Potential
def print_potential (pot, ori_pot, new_pot):
  txt = ""
  txt += "Potential[" + str(pot) + "]:" + str(ori_pot)
  txt += " - " + str(new_pot)
  print txt

def get_list_uint_data_list_double ( self, params, variables ):
  result = []
  if self.poisson is not None:
    self.poisson.get_multidata(params, variables, result,
"list<uint>:list<double>")
    for i, v in enumerate(variables[0]):
      original_potential = result[0][i]
      if v in self.potentials:
        result[0][i] = self.potentials[v]
      else :
        result[0][i] += random_perturbation()
        self.potentials[v] = result[0][i]
      print_potential(v, original_potential, result[0][i])
  return result
```

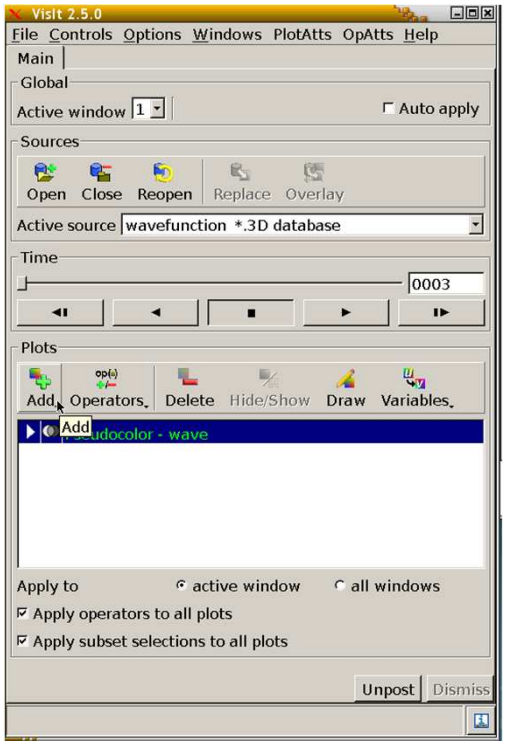
Python | Tab Width: 8 | Ln 22, Col 3 | INS

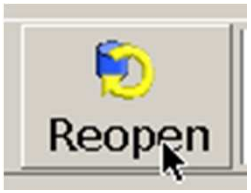
step1_small.py





```
submit -v coates \
    -i /apps/share64/nemo/examples/current/materials/all.mat \
    -i ./step1_small.in \
    -i ./step1.py \
    nemo-r7962 step1_small.in
```

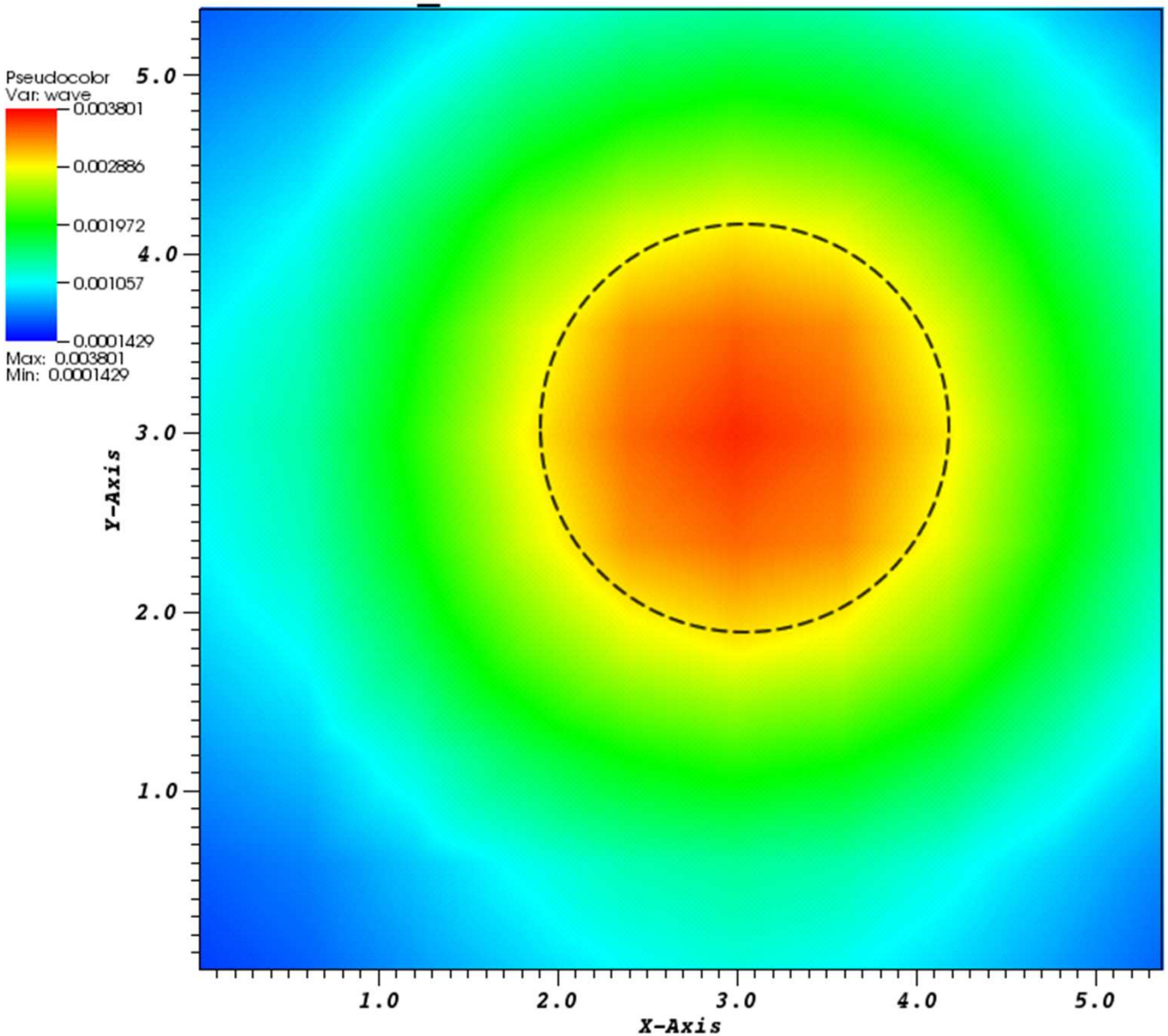




Reload database

Visualize next Wavefunction

step0 vs step1



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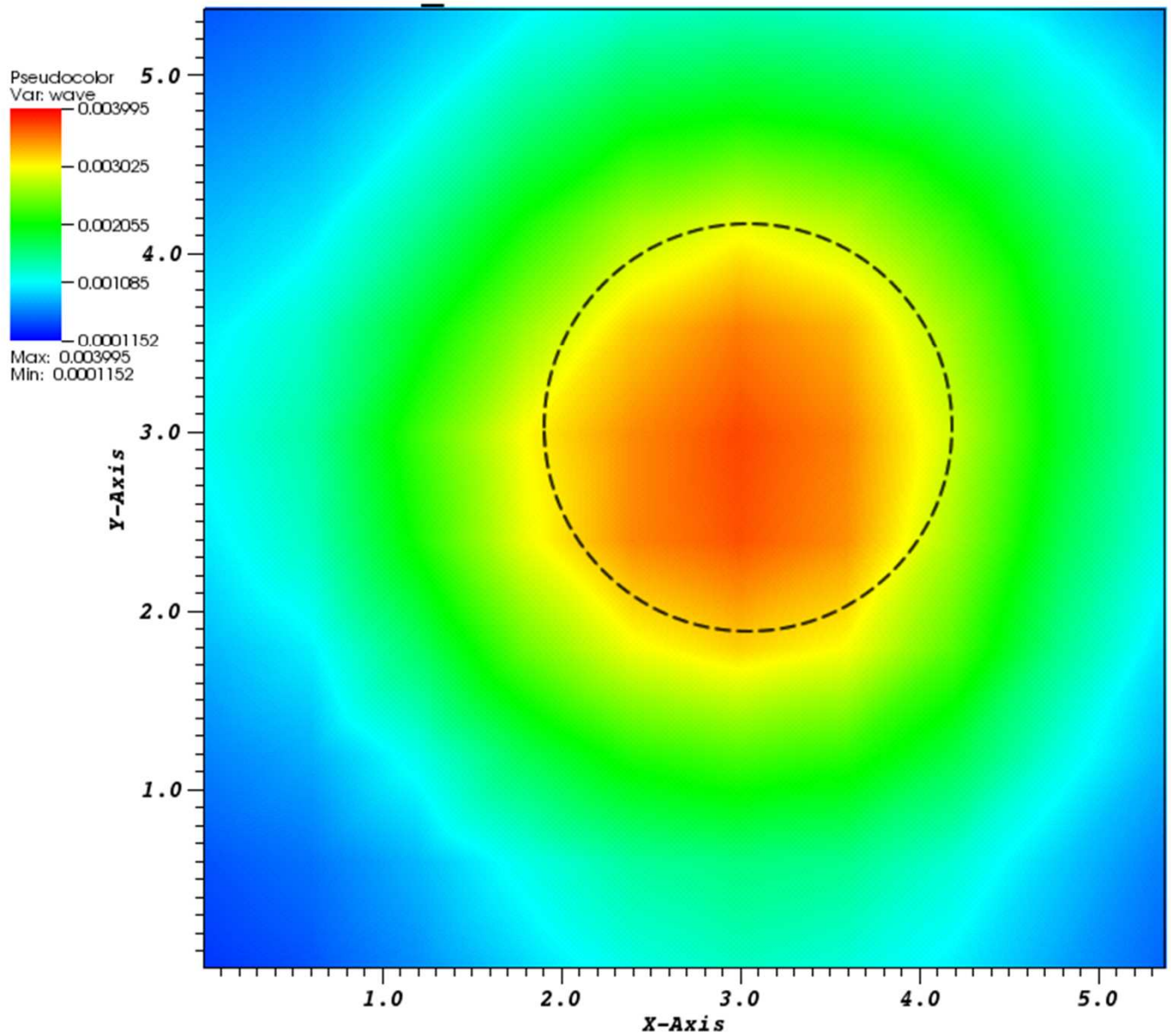
step0 vs step1



PURDUE UNIVERSITY

~100 Nemo5 features

PythonSolverInterface() //N5_Solver
- str get_name()
- str get_type()
- list get_options()
- bool check_option(str)
- str get_option (str)

- N5_VecDouble/N5_VecComplex()
  - » int get_size()
  - » int get_local_size()
  - » void get_values(list, list)
  - » void set_values(list, list)
  - d_values(list, list)
  - (double/complex)
  - ale(double)
  - _product(N5_Vec*, N5
  - ble_Sequential

- **N5_MatDouble/Complex_Parallel()**
  - » void set_num_nonzeros (int, int, int)
  - » void allocate_memory()
  - » bool is_ready()
  - » void add(int, int, double/complex)
  - » v
  - » c
  - » i
  - » i
  - » v

- N5_Output()
  - » void add_dataset(str name, list values
  - » void remove_dataset(str)
  - » void write_to_file(str)

- N5_Utils (static)
  - » **void db_set_parameter(str, str, s**
  - » **string db_get_parameter(str,str)**

- N5_P(object) // pointer
  - » setValue(object)
  - » .value // object

- N5_MPI (static)
  - » void N5_MPI_Comm_rank(N5_P, int)
  - » void N5_MPI_Comm_size(N5_P, int)
  - » **void N5_MPI_Bcast(object, int**
  - » void N5_MPI_Barrier()
  - » void N5_MPI_COMM_WORLD()

- **N5_Atom()**
  - » str get_atom_type ()
  - » str get_atom_tight_binding()
  - » **.position // list[3]**
  - » .ideal_position // list[3]
  - » .id // int
  - » .proc_id //int
  - » .region // int
  - » .active // bool

N5_Output create_output( )
void init_material_properties()
void reinit_material_properties()

- N5_Material()
  - » str get_name()
  - » list get_options()
  - » bool check_option(str)
  - » str get_option(str)
  - » void set_option(str, str)

- N5_Domain()
  - » list get_domain_options ()
  - » str get_name()
  - » bool if_atomistic()
  - » bool if_intialized()

- N5_AtomisticDomain (N5_Domain)
  - » int num_atoms()
  - » list get_atoms_info()
  - » list get_atoms_info_CPU(int)
  - » int get_size_CPU()

Thanks!

step2.py(add potential due an impurity)

~/public_samples/Python_solver/Python_tutorial/step2.py

Initialization (do_init)

```
def do_init(self):
  self.potentials = {}
  self.done = False
  self.charged_id_atom = 1
  self.charge_atom = -1.60217646e-19  #boron charge
  self.charged_pos_atom = [0,0,0]
  if self.check_option( "poisson" ):
    poisson_str = self.get_option( "poisson" )
    self.poisson = self.find_simulation( poisson_str )
  else:
    self.poisson = None
```

step2.py

Solution (do_solve)

$$V_{\mathbf{E}} = \frac{1}{4\pi\varepsilon_0}\frac{Q}{r}$$

Electric potential due to a point charge

Searching "impurity"

Calculating potential

```
def do_solve (self):
  if self.done is False :
    K = 8.988e9 # Nm2/C2
    domain = self.get_domain()
    atomistic_domain = N5_AtomisticDomain(domain)
    atoms = atomistic_domain.get_atoms_info();
    for atom in atoms:
      if atom.id == self.charged_id_atom:
        self.charged_pos_atom[0] = atom.position[0]
        self.charged_pos_atom[1] = atom.position[1]
        self.charged_pos_atom[2] = atom.position[2]
        self.potentials[atom.id] = 0
        break;
    #endfor
    for atom in atoms:
      if not atom.id == self.charged_id_atom:
        X = atom.position[0]-self.charged_pos_atom[0]
        Y = atom.position[1]-self.charged_pos_atom[1]
        Z = atom.position[2]-self.charged_pos_atom[2]
        dist = math.sqrt(X*X + Y*Y + Z*Z) * 1e-9 # nm to m
        Pi = ( K * (self.charge_atom) ) / (dist)
        self.potentials[atom.id] = Pi
  self.done = True
```

Communication
(get_data)

```
def get_list_uint_data_list_double ( self, params, variables ):
  result = []
  if self.poisson is not None:
    self.poisson.get_multidata(params, variables, result, "list<uint>:list<double>")
    for i, v in enumerate(variables[0]):
        result[0][i] += self.potentials[v]
  return result
```

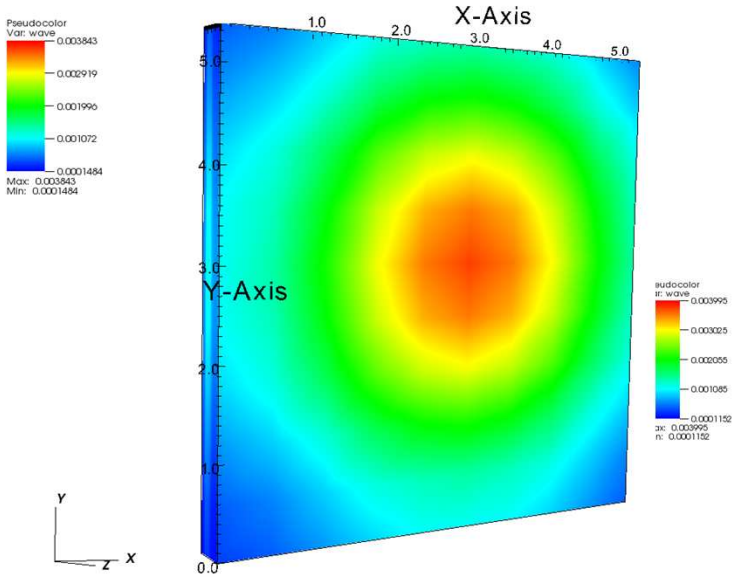
Run step2.py

```
submit -v coates \
    -i /apps/share64/nemo/examples/current/materials/all.mat \
    -i ./step2_small.in \
    -i ./step2.py \
    nemo-r7962 step2_small.in
```

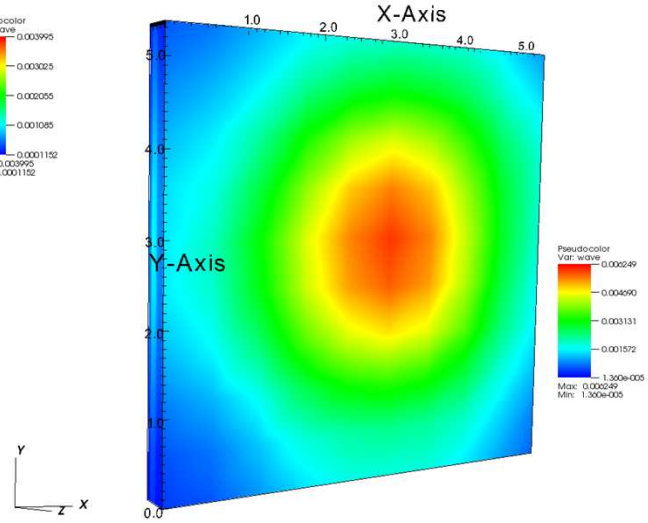
Run step2.py

submit -v coates -i ./all.mat -i ./step2.in -i ./step2.py nemo-rXXXX step2.in

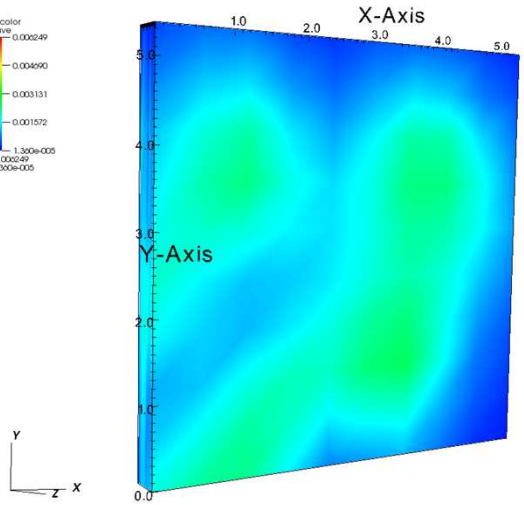
eigenfunctions/wavefunction_0.xyz



step0.py

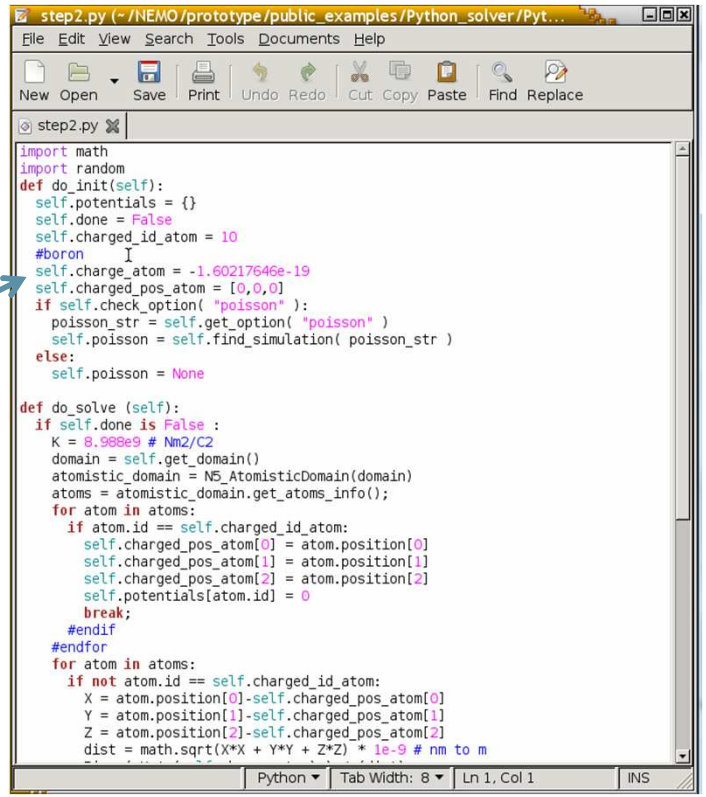


step1.py



step2.py

- File (step2.py)
  - Edit charge_atom value.
  - Edit charge_id_atom value.




```
submit -v coates \
    -i /apps/share64/nemo/examples/current/materials/all.mat \
    -i ./step2_small.in \
    -i ./step2.py \
    nemo-r7962 step2_small.in
```