Tutorial for python code

on wave packet propagation across materials

User account

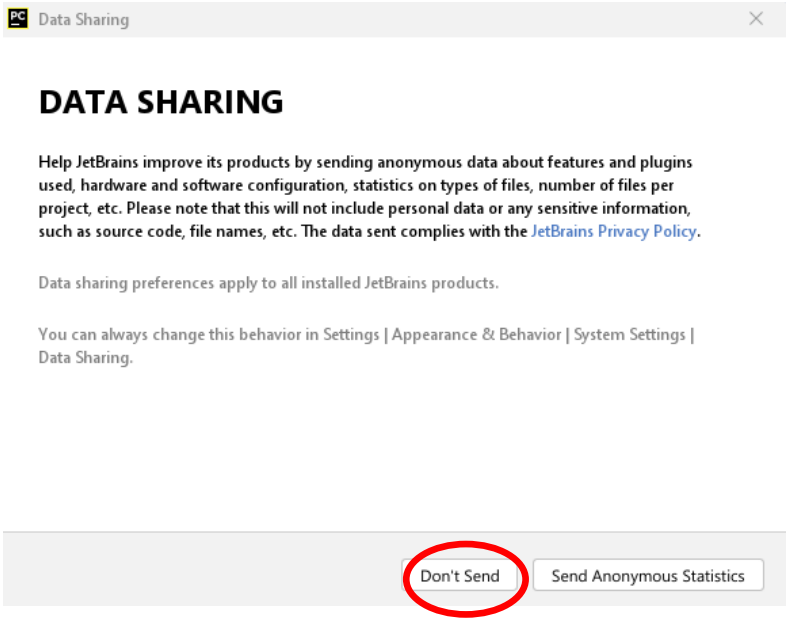
Name: its.usr1

Password: Cost2022:)

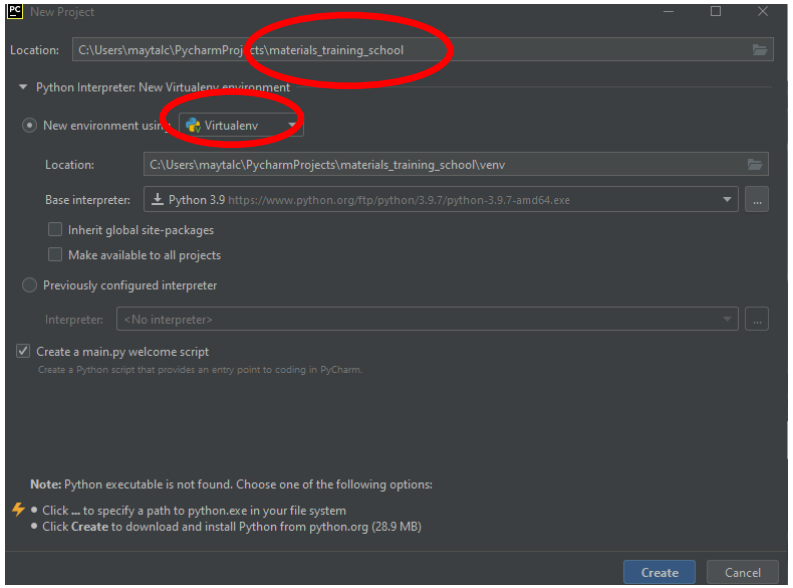
Setting up and installations

- Open pycharm

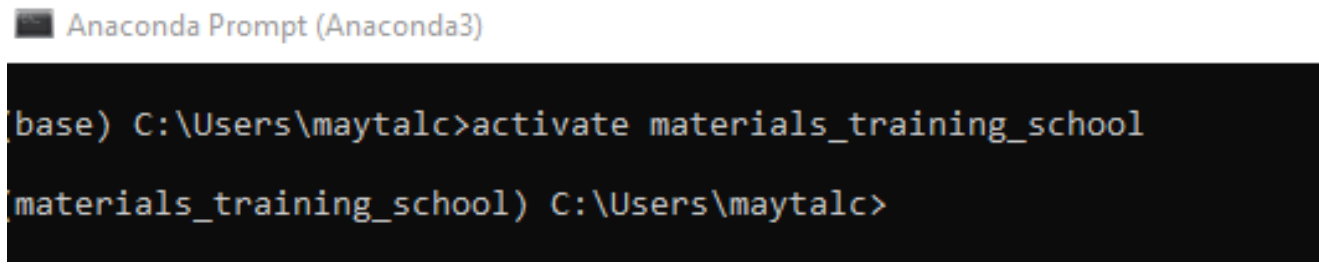
- Click “exit” and afterwards “don’t send”.



- In project, click “new project”, and select a name, and change environment to “conda”.



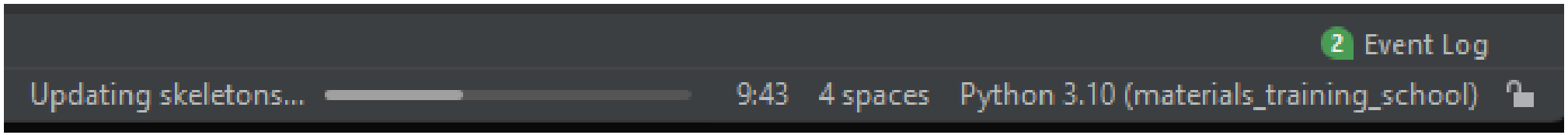
Continued installation



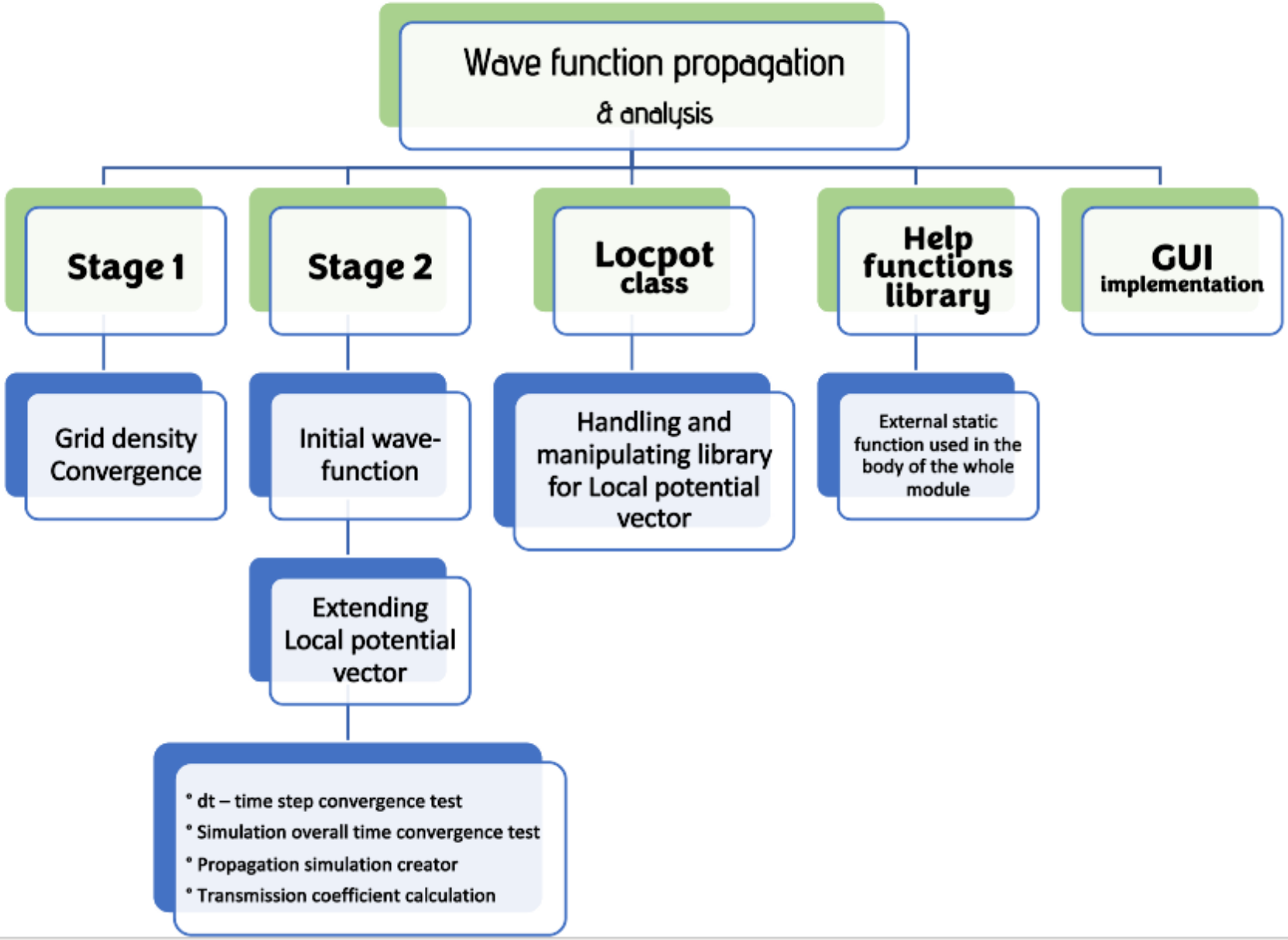
- Open “anaconda prompt”.
- Write “activate <project name>”.
- Write:

```
conda install --channel conda-forge pymatgen
```

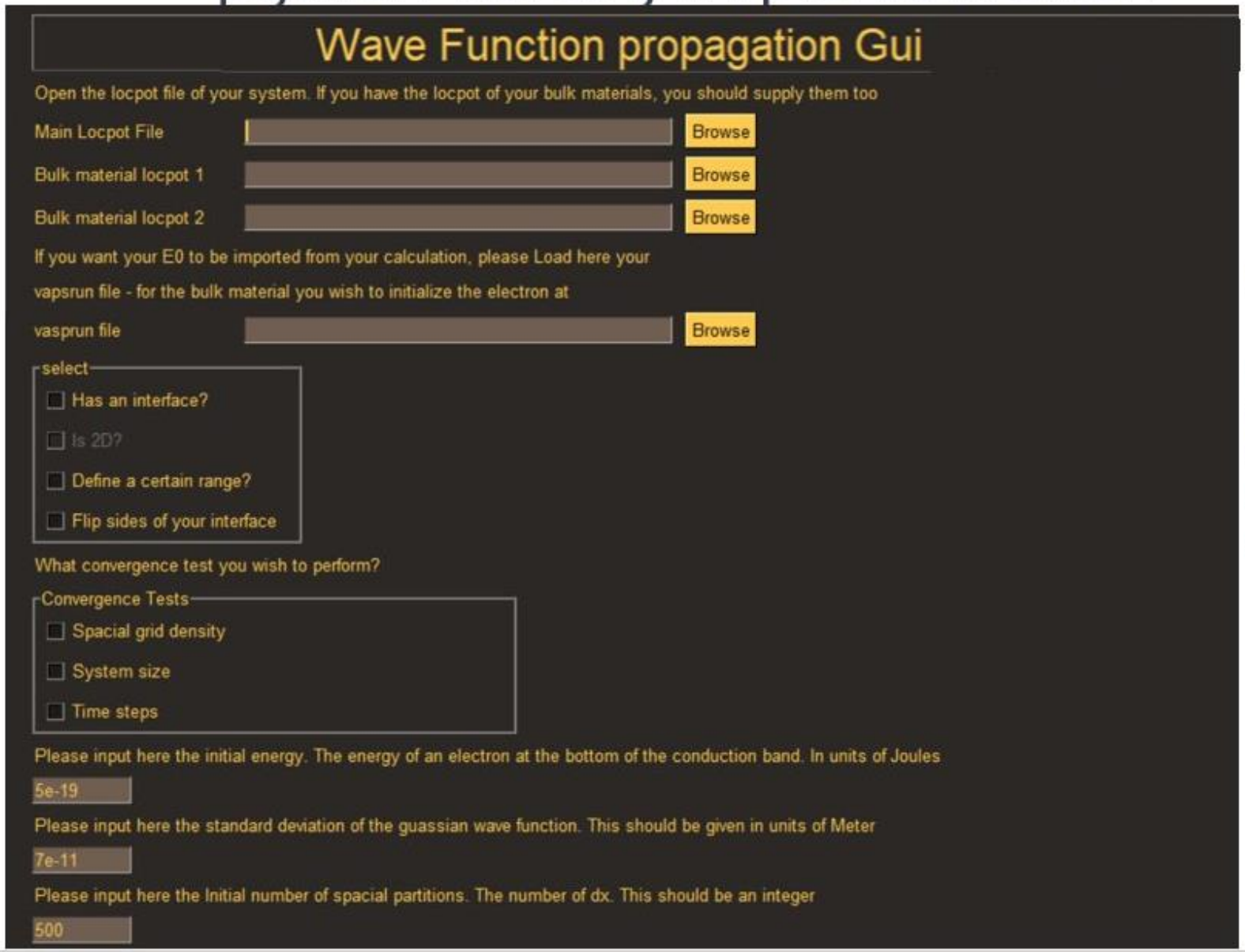
- Write: “y” to proceed when asked.
- Write: “pip install WF-Prop”.
- In Pycharm, there is update that needs to be complete:



Numerical methods & python library implementation



Numerical methods & python library implementation



Python packages:

- Numpy
- Scipy
- Matplotlib
- **Pymatgen**
- **PysimpleGUI**

Using the code GUI

- On the bottom of the pycharm window, click “python consul”.
- To open the GUI write:

```
>>> from WaveFunctionPropagation import Main_execution as m_exe

>>> m_exe.Gui()
```

Downloading the VASP output files

- **LOCPOT** – a file of the material potential from DFT calculations
- **vasprun** – conduction band edge and band gap value

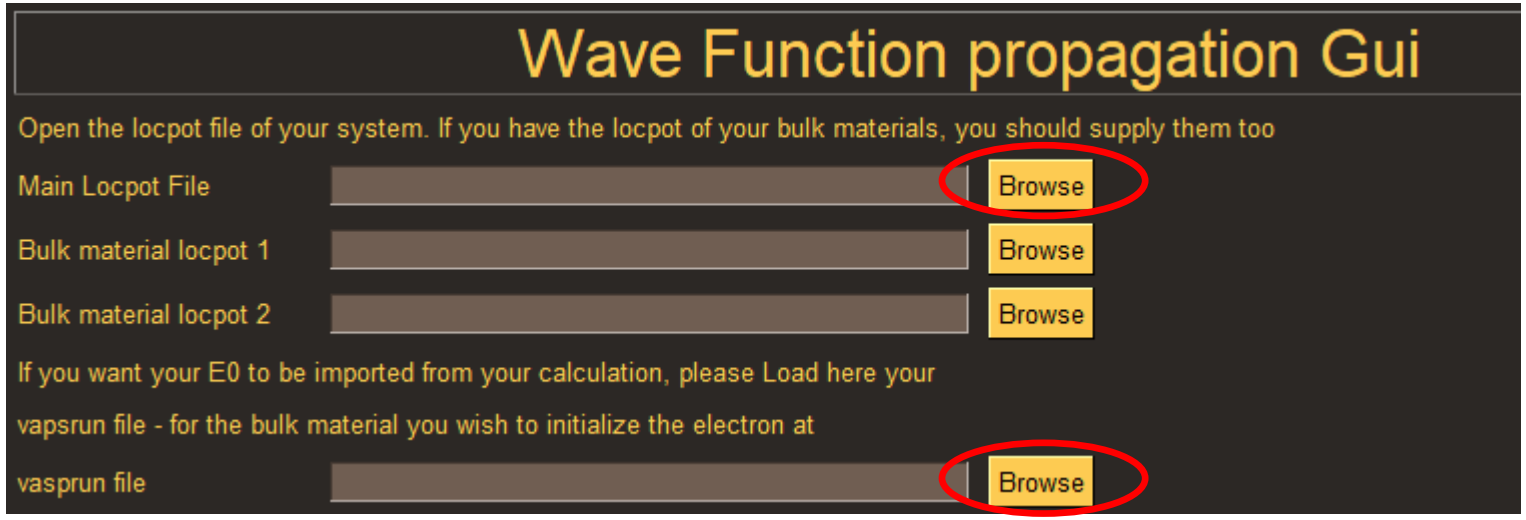
- Location to download: training course web site

Type of LOCPOT materials

- GaAs
- AlN
- GaSn

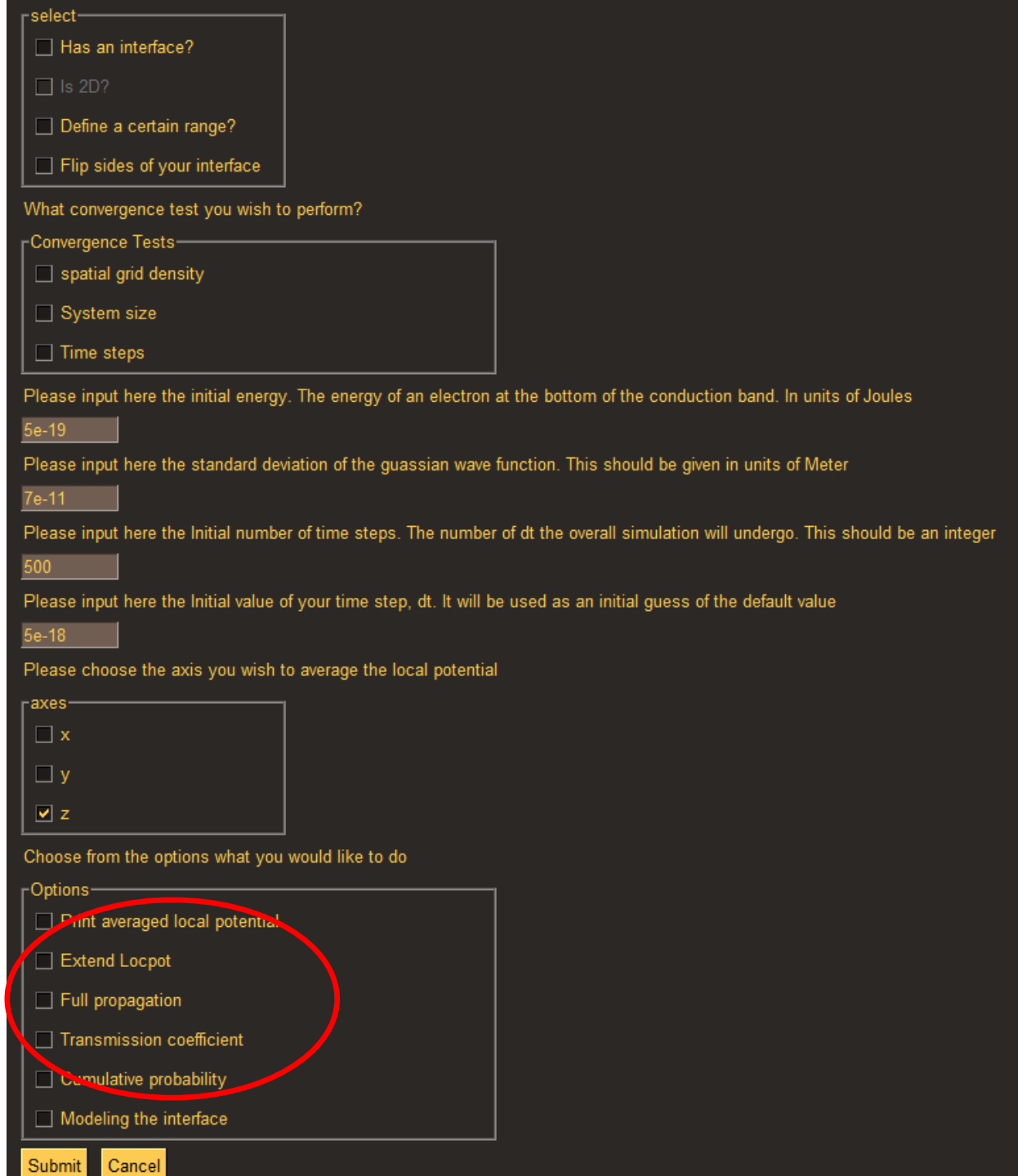
Options for selection on GUI

- Uploading potential energy files:



The rest of the GUI selections

- We can simply tick all output:

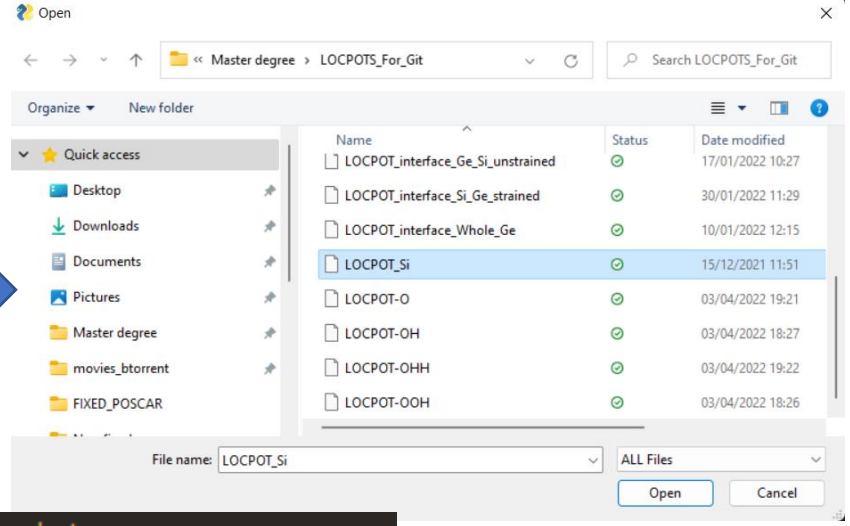


Details on GUI options:

1. Loading Locpot file

If You have bulk-materials locpot files You can load them too, at that level.

Click on 'Browse', Then locate your locpot files



2. Define your system

If you want the code to handle an interface-system, turn on the check box. If you have a vacuum or any kind of slab, turn on the range providing check box.

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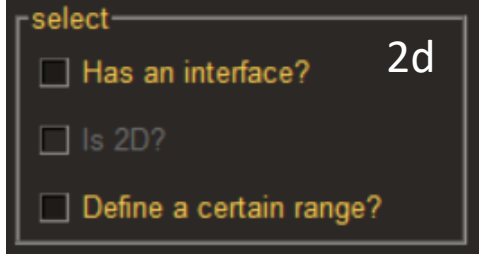
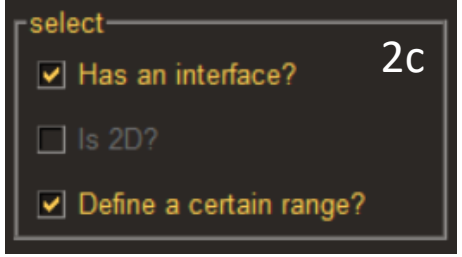
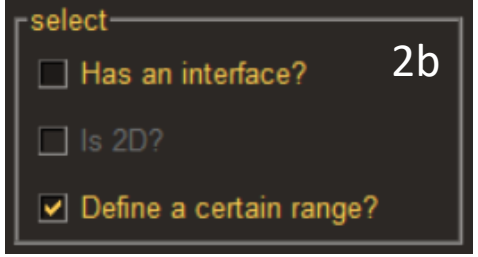
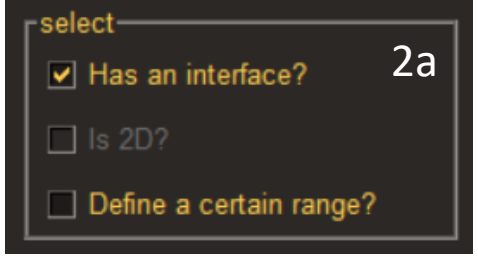
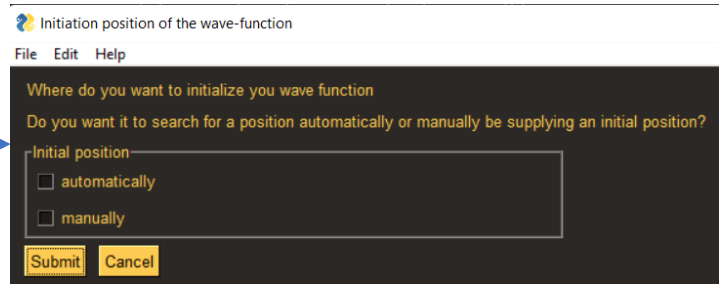






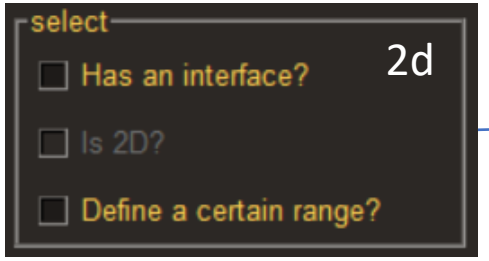


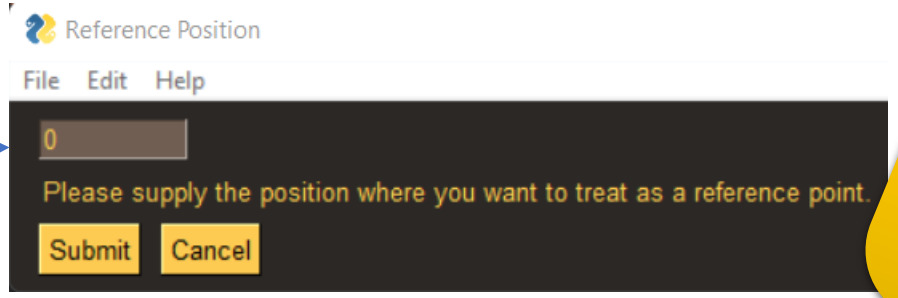
It Doesn't matter what you chose. The next pop-up window will be the first to appear.



Only if you have an interface in your system, you can choose the 'automatically' option.
Otherwise – select manually.

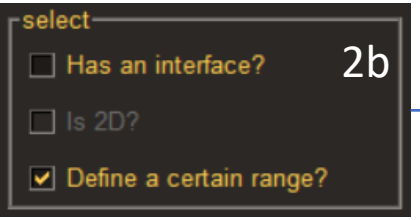
If your selection is as the following, the next pop-up window will appear.

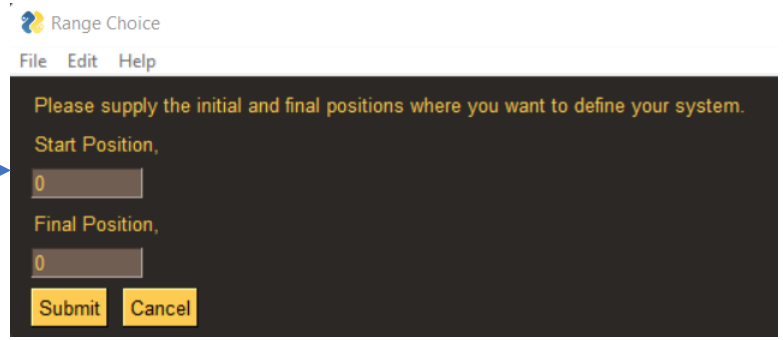




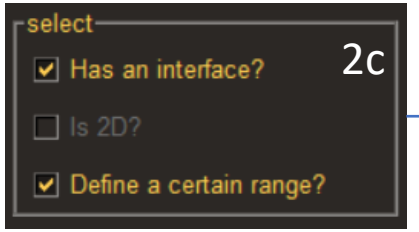
All the positions you asked to provide, must be in the units of **your spacial grid**. Usually it will be in **Meters** (scale of *1e-10*)

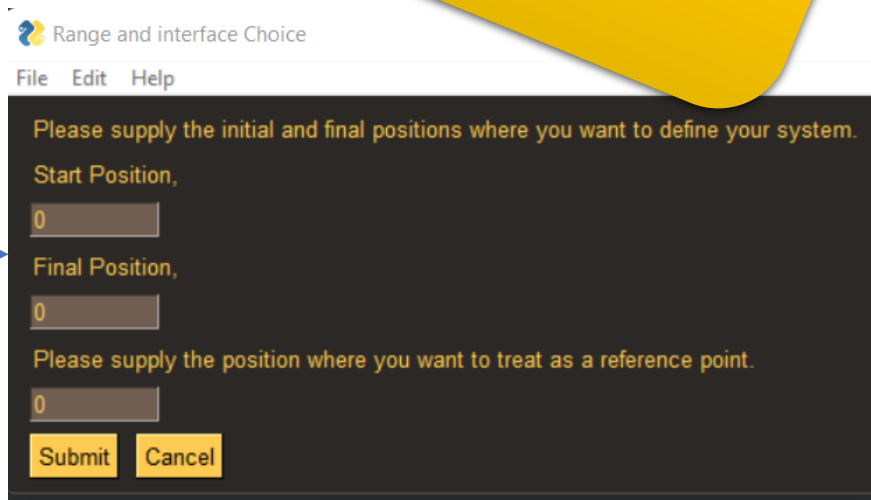
If your selection is as the following, the next pop-up window will appear.





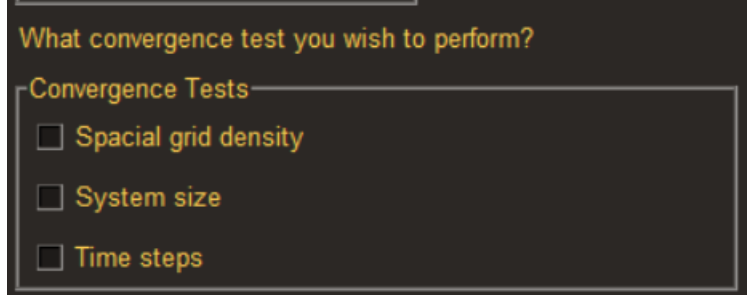
If your selection is as the following, the next pop-up window will appear.





3. Convergence tests

Choose what convergence tests you wish perform.



3a. Grid density

Applies to Stgae_1 sub-module.
Applies to the special grid spacing/partition

Later you will be asked to provide the initial number of measurement points in the space region. This number determines the spacial spacing. If you did not choose to perform the grid density convergence test, it would determine the actual spacial spacing.

3b. System size

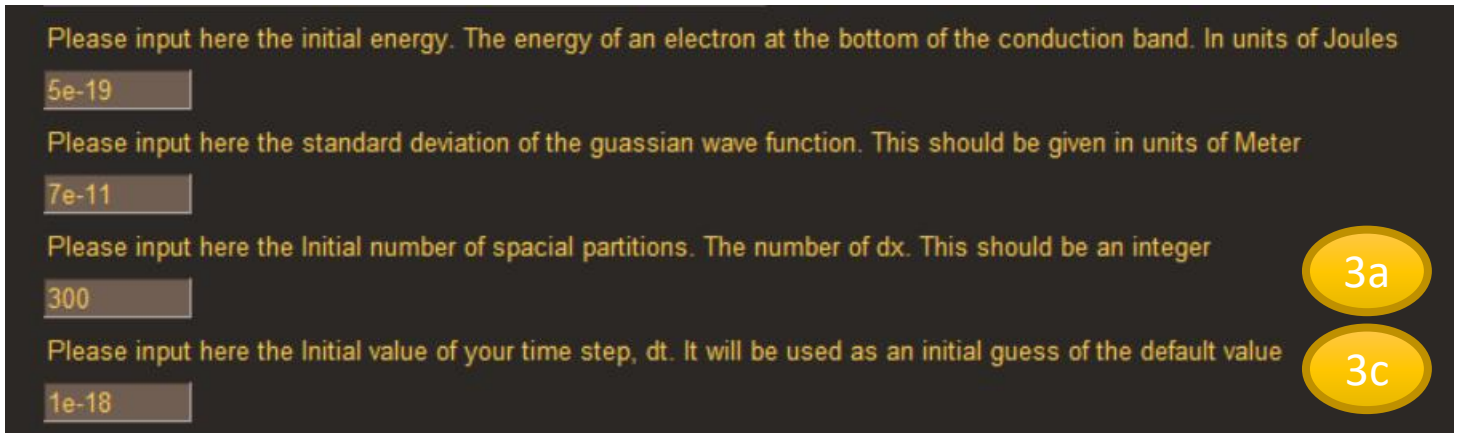
Applies to Stgae_2 sub-module
Basically – determines to system's length.

Determines the system length by iterating over increasing lengths of the system and increasing simulation times. It is calculated from the parameters that fits the point where the transmission coefficient reaches plateau with respect to simulation time

3c. Time step - dt

Determines the time-step value for the propagation

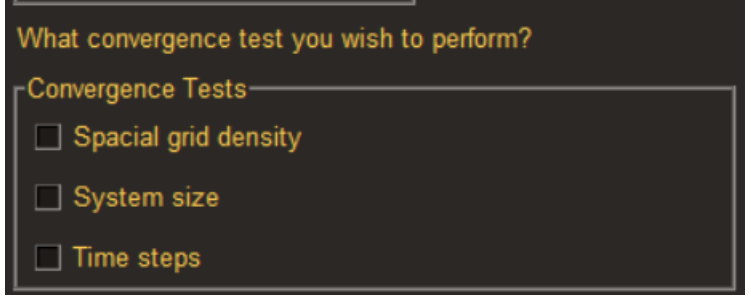
Later, you will be asked to provide an initial guess for the time-step convergence test, if it was checked true.
If you rather not to perform the time-step convergence test, this value will be the time-step value that will be used through the propagation.



At this point, you should provide some crucial information about your desired initial wave-function.
Those would be the **gaussian width** (the sigma of the Gauss-function) and the **initial total energy** of an electron at the bottom of the conduction band.

3. Convergence tests

Choose what convergence tests you wish perform.



3a. Grid density

Applies to Stgae_1 sub-module

3b. System size

Applies to Stgae_2 sub-module
Basically – determines to system's length.

3c. Time step - dt

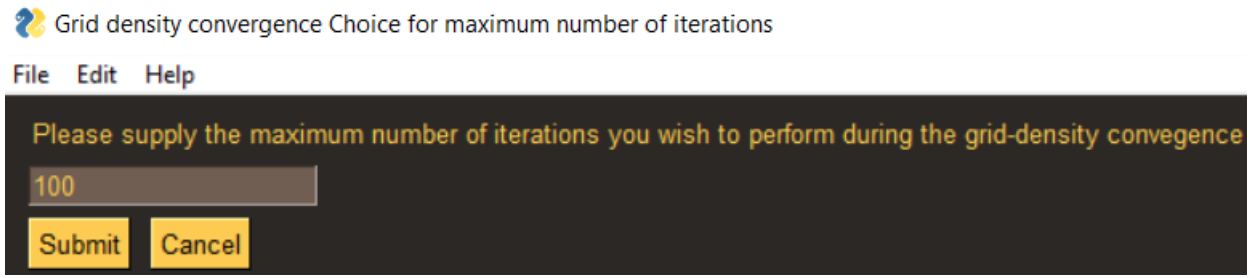
Determines the time-step value for the propagation proccess

The other convergence tests selection will take place with respect to the operations you would like to perform. It will be explained in later slides.

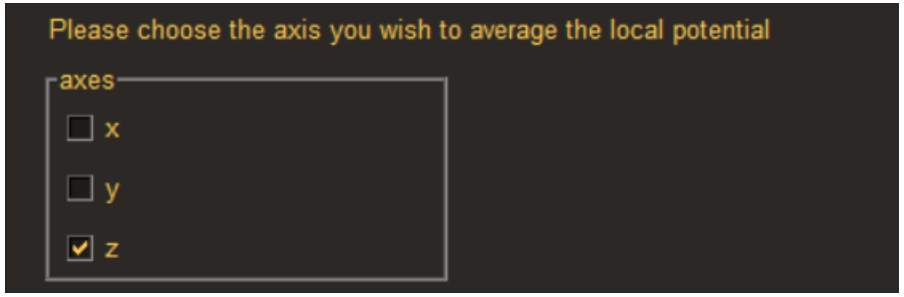
3a. Grid density

Applies to Stgae_1 sub-module

If you chose to perform the grid-density convergence test, then you will be asked to provide the maximum number of iterations that the algorithm will be going through.



4. Axis grid

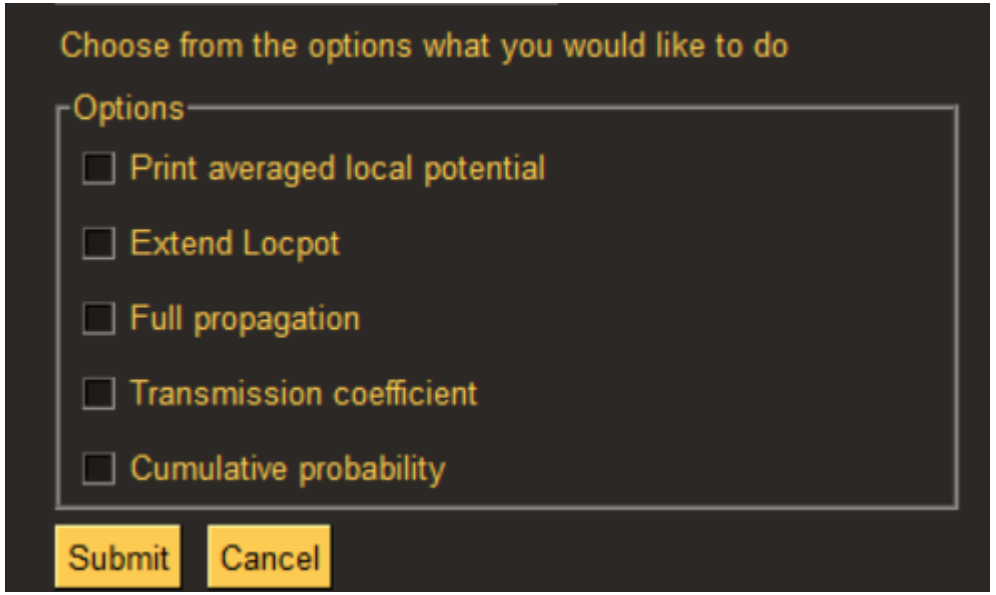


This module version is not yet to support 2D calculations. Only 1D's calculations.

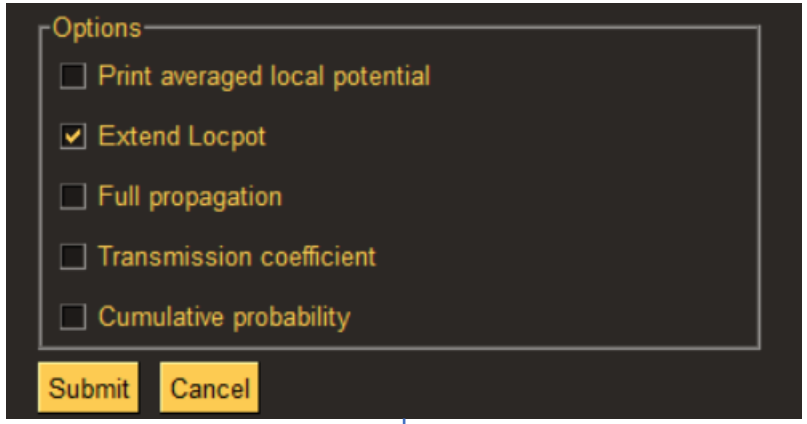
The following step is to choose the parallel direction where the wave function will be propagated along. This also will be the direction where all the local potential will be averaged to for yielding 1D local potential. The default axis grid is Z.

5. Optional operations choice

The last part of the form. Enables to choose what you wish the module to perform. If you do not choose any of these, nothing is going to happen (if you chose to perform the a convergence test, it will run the test and then will finish without doing anything else).

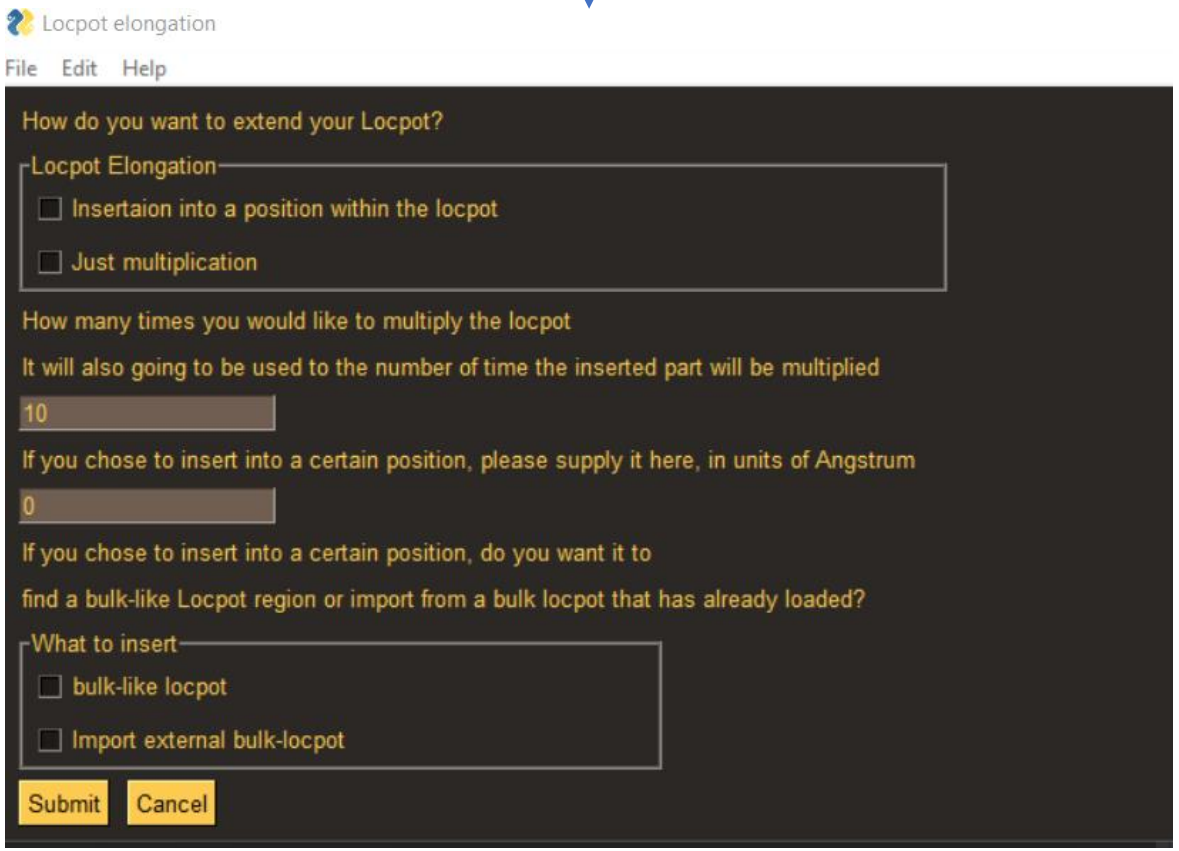


5. Optional operations choice



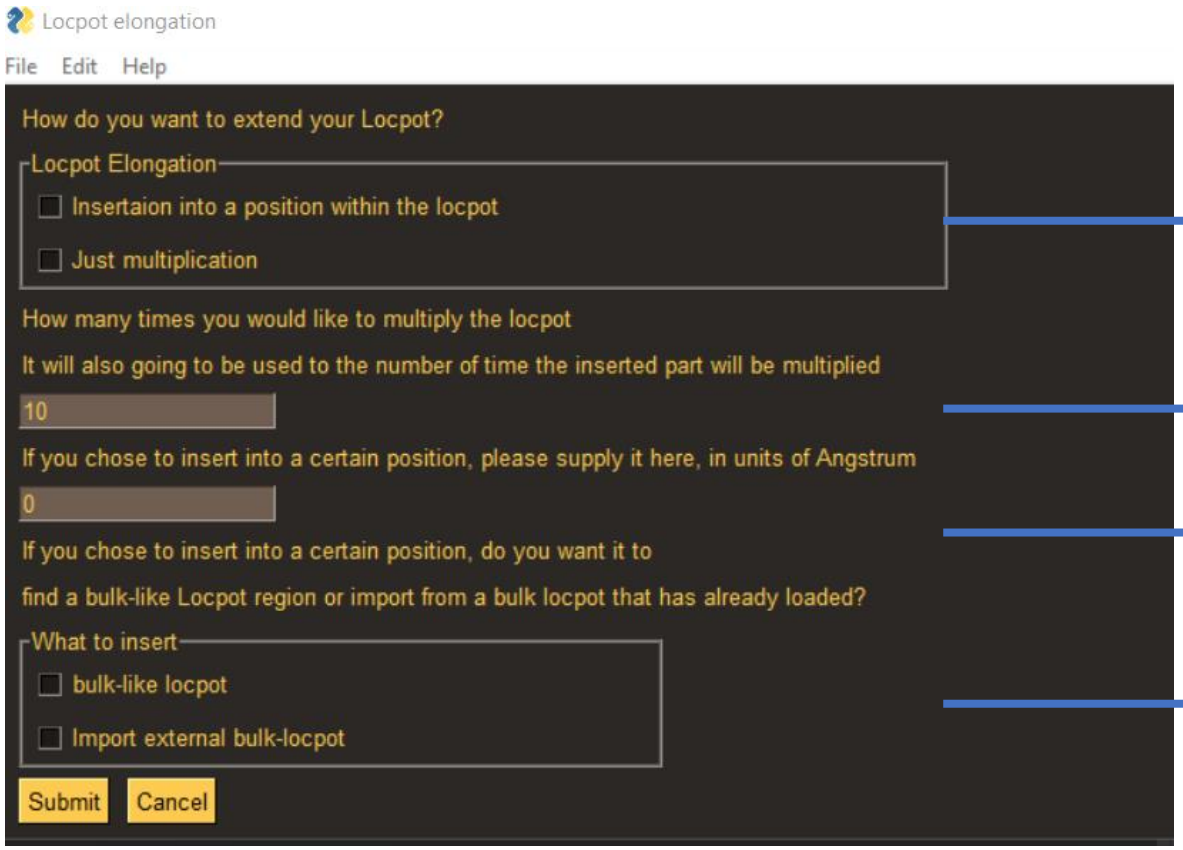
The Only operation that might affect the course of the convergence test is extending of the local potential.

5a. Locpot elongation



Choosing this option will lead to the following pop-up window to appear.

5a. Locpot elongation



You can choose just the take the original local potential vector and multiply it – putting together side by side the local potential vectors as many times you wish.
Or you can take a certain range of local potential and insert it into a position within the original locpot vector.

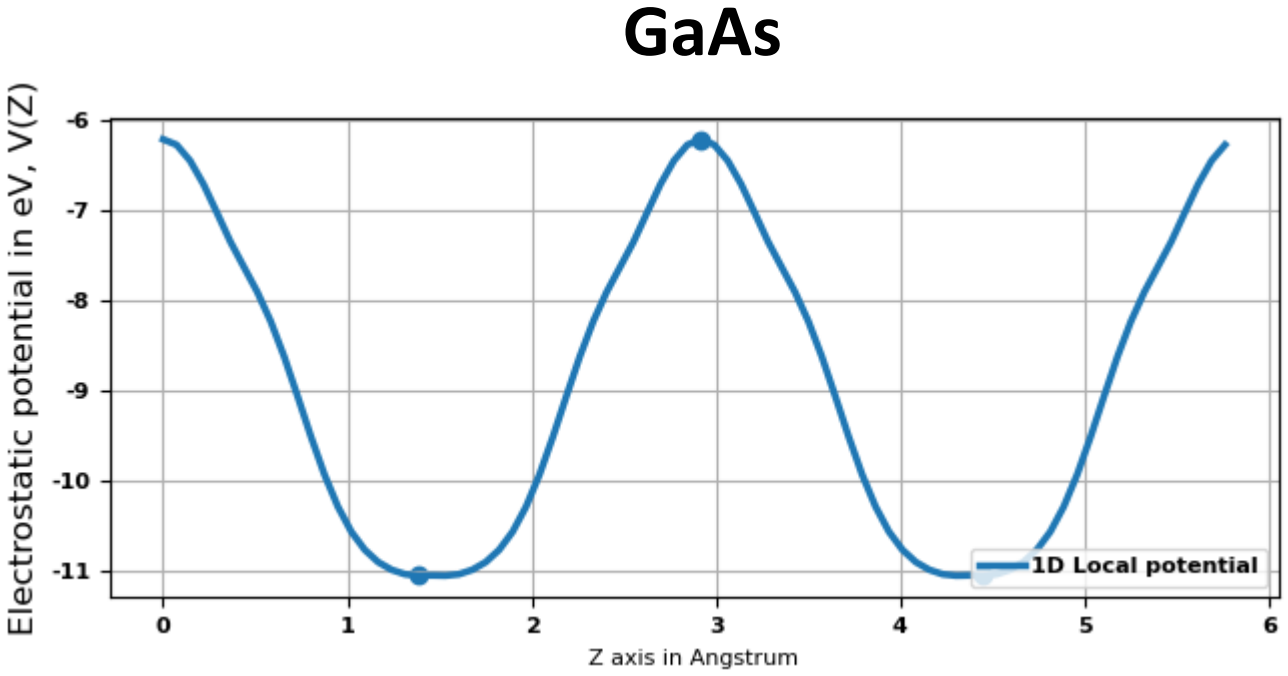
It asks the user to provide the number of the multiplications the local potential vector is going be multiplied at. It is utilized both for the cases when the user asked the elongation of the locpot to be ‘just a multiplication’ or ‘insertion into a position’ (the inserted part will be multiplied).

If the option of ‘insertion into a position’ was chosen, the user is required to provide the position where he wish insert the vector.

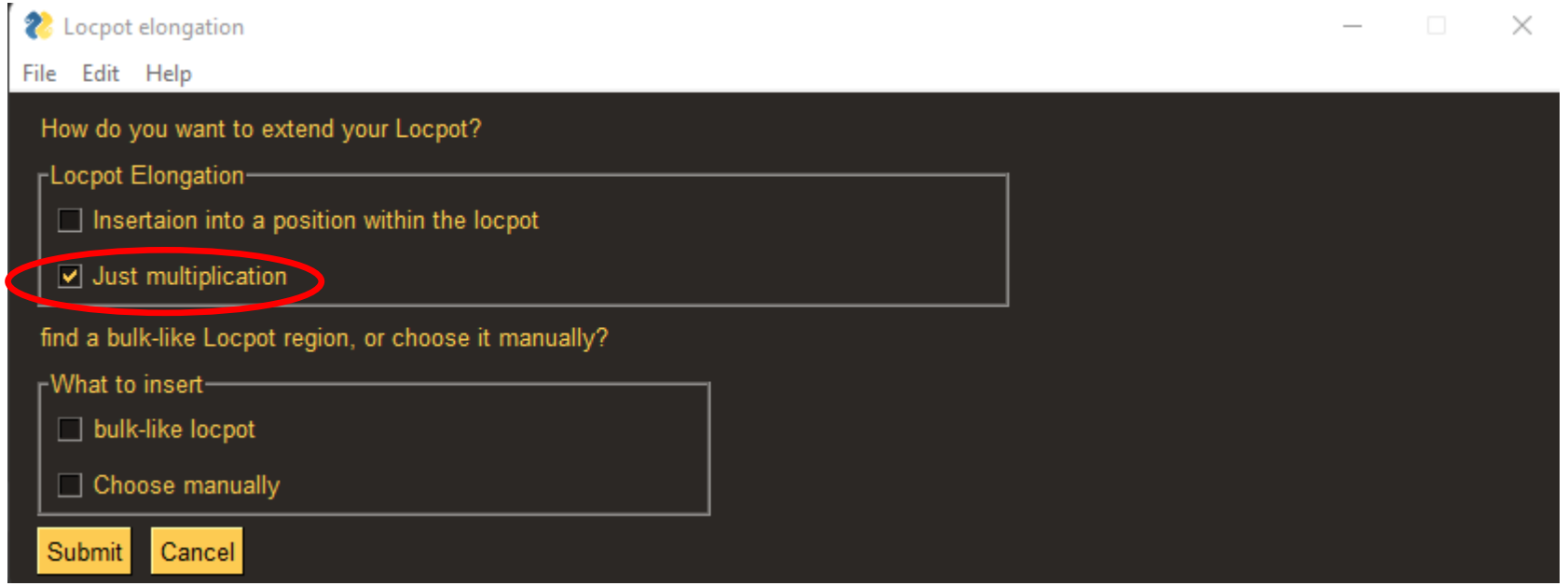
If the option of ‘insertion into a position’ was chosen,
It asks the user to tell what exactly to insert. It can insert a bulk locpot vector or search for a bulk-like local potential (which is taken from the far mid-range local potential of each material).

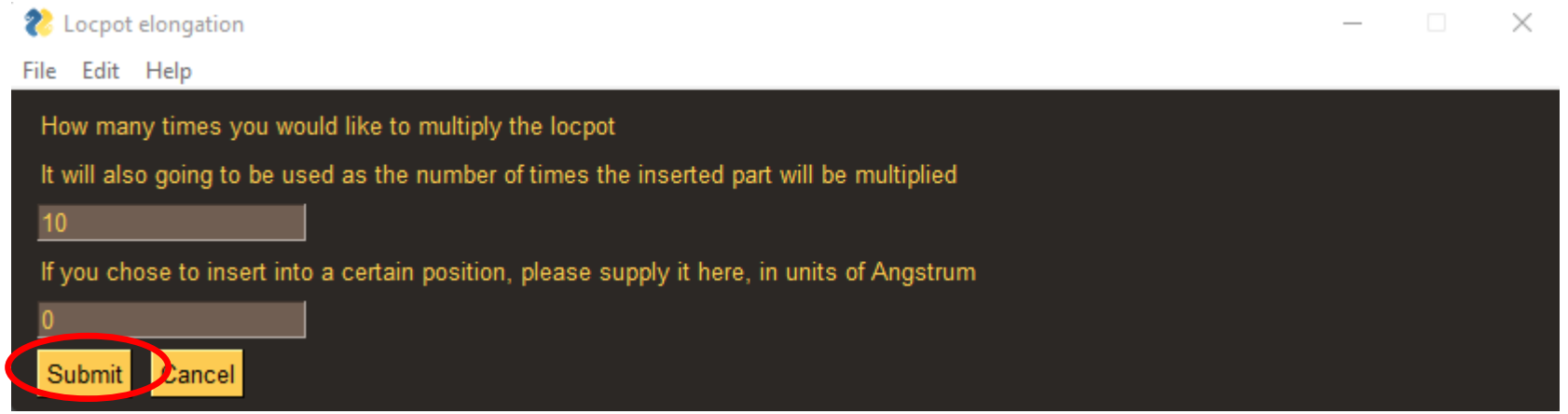
Printing potential

- After uploading files, select “print average potential” at the end.



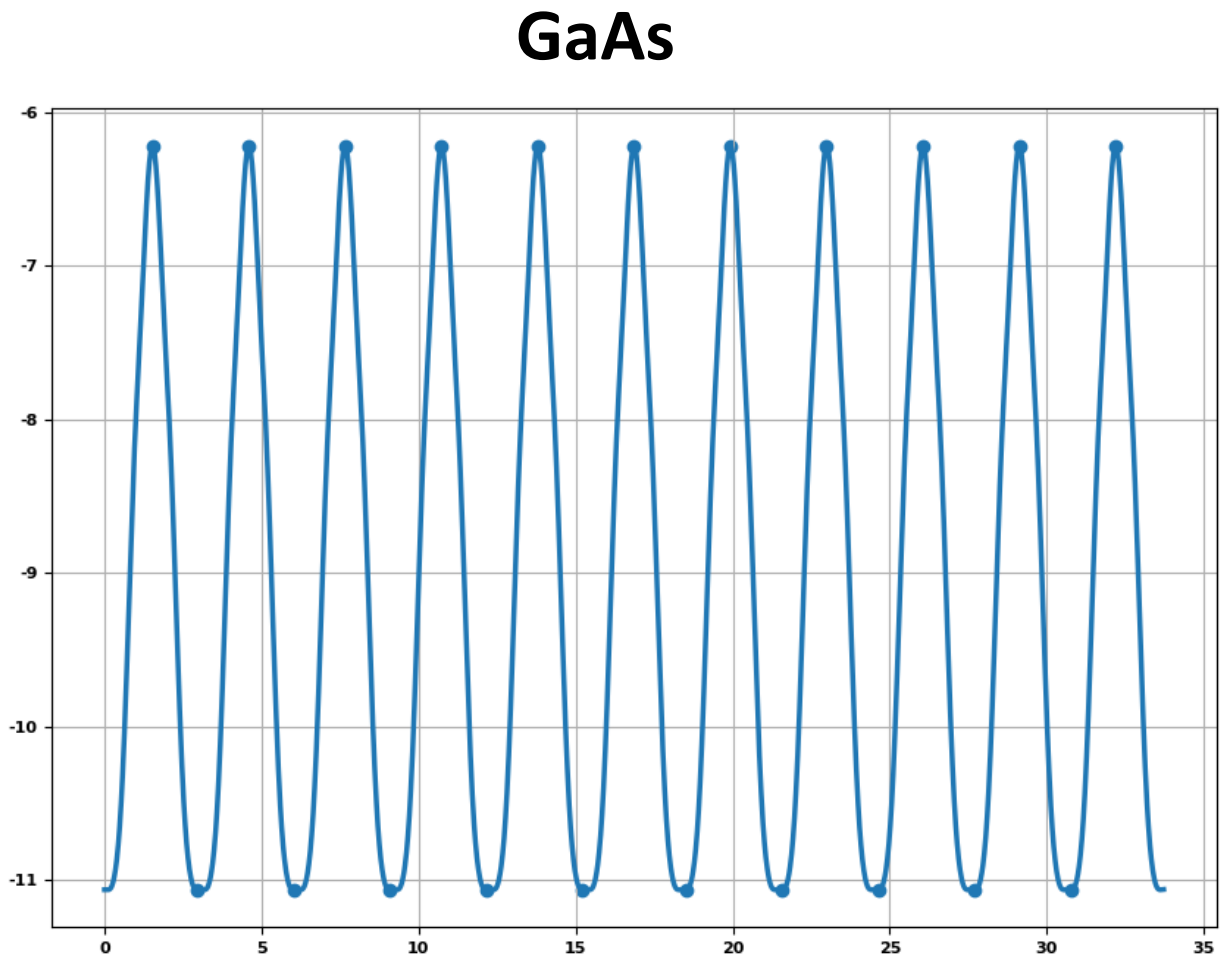
Next GUI pop-ups: multiplying potential



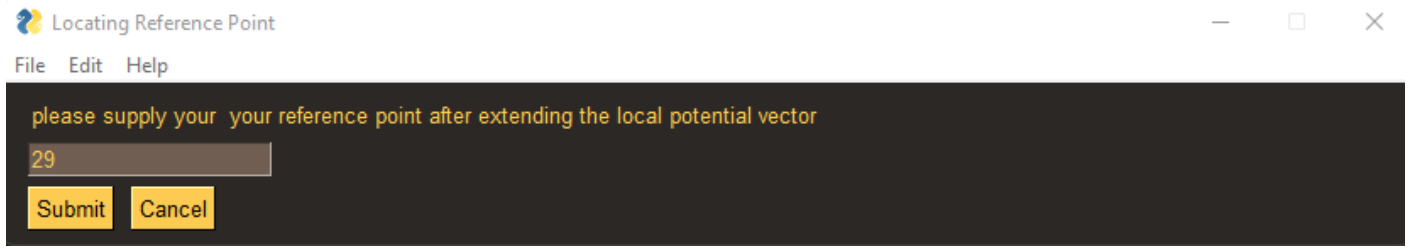


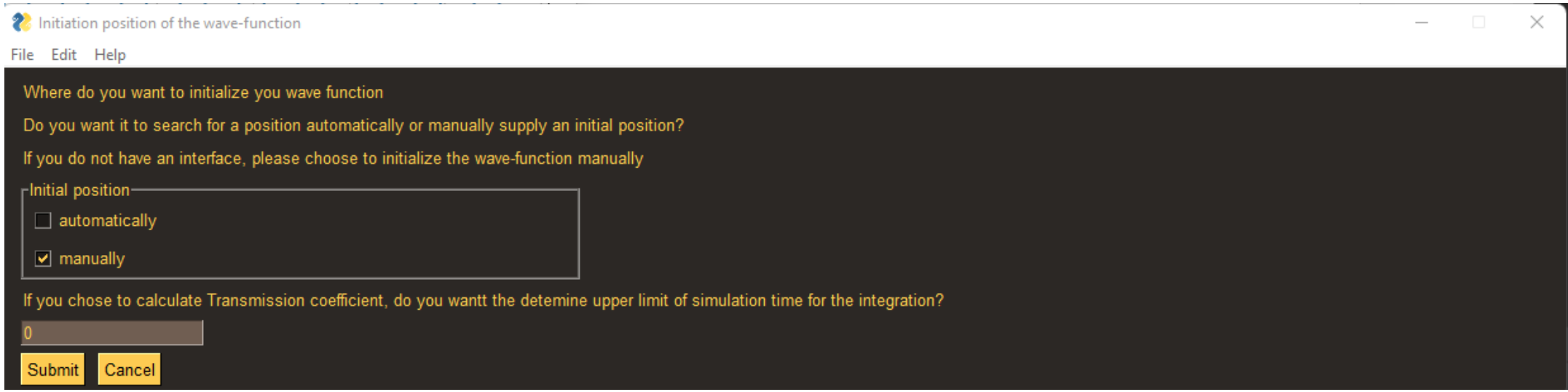
Extending the potential

- After selecting “just multiply” the potential, write: multiply 10 times



Selections for flux position and initial wavefunction:



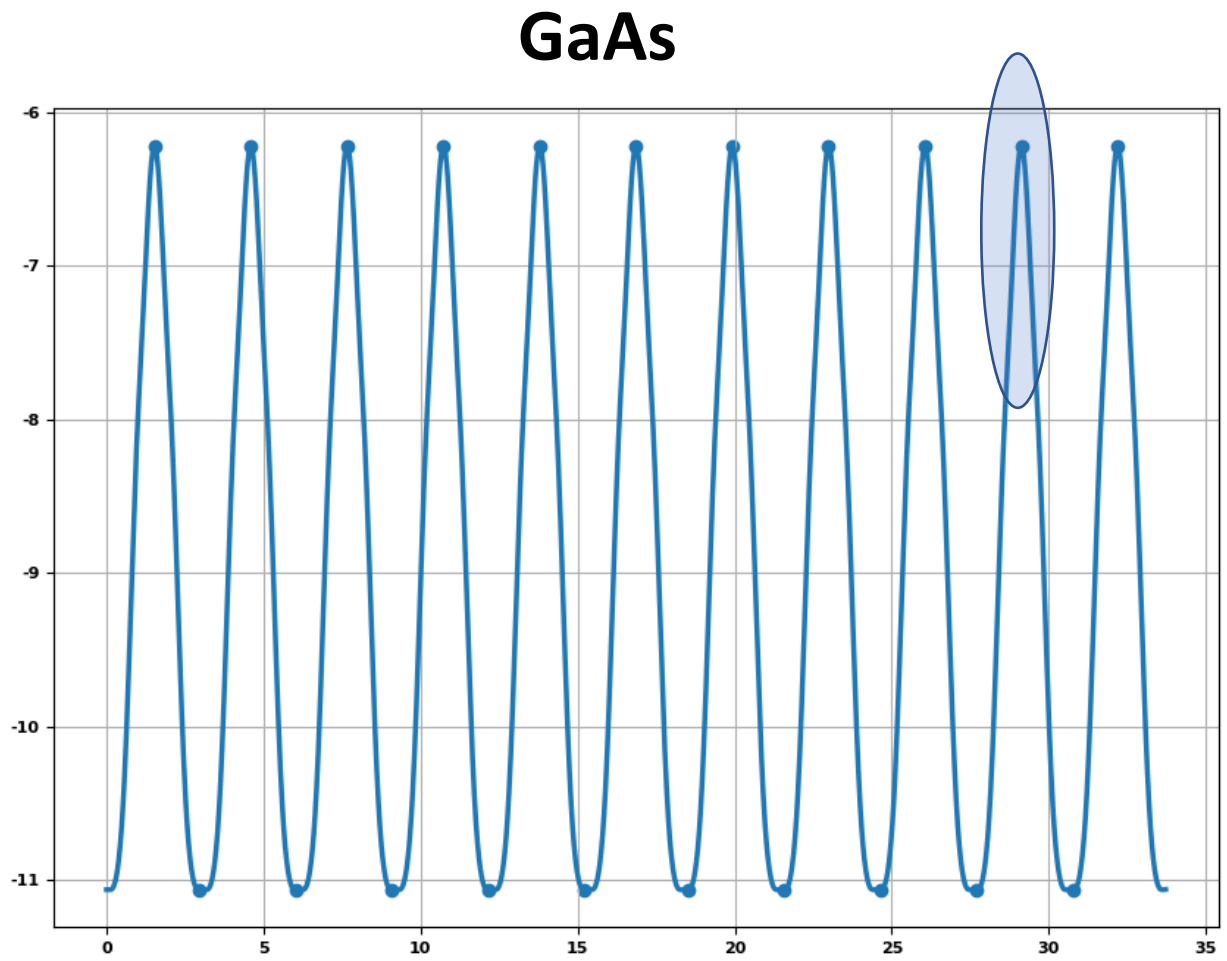


When asked where to **store the movie file**, you may select one of the LOCPOT files.

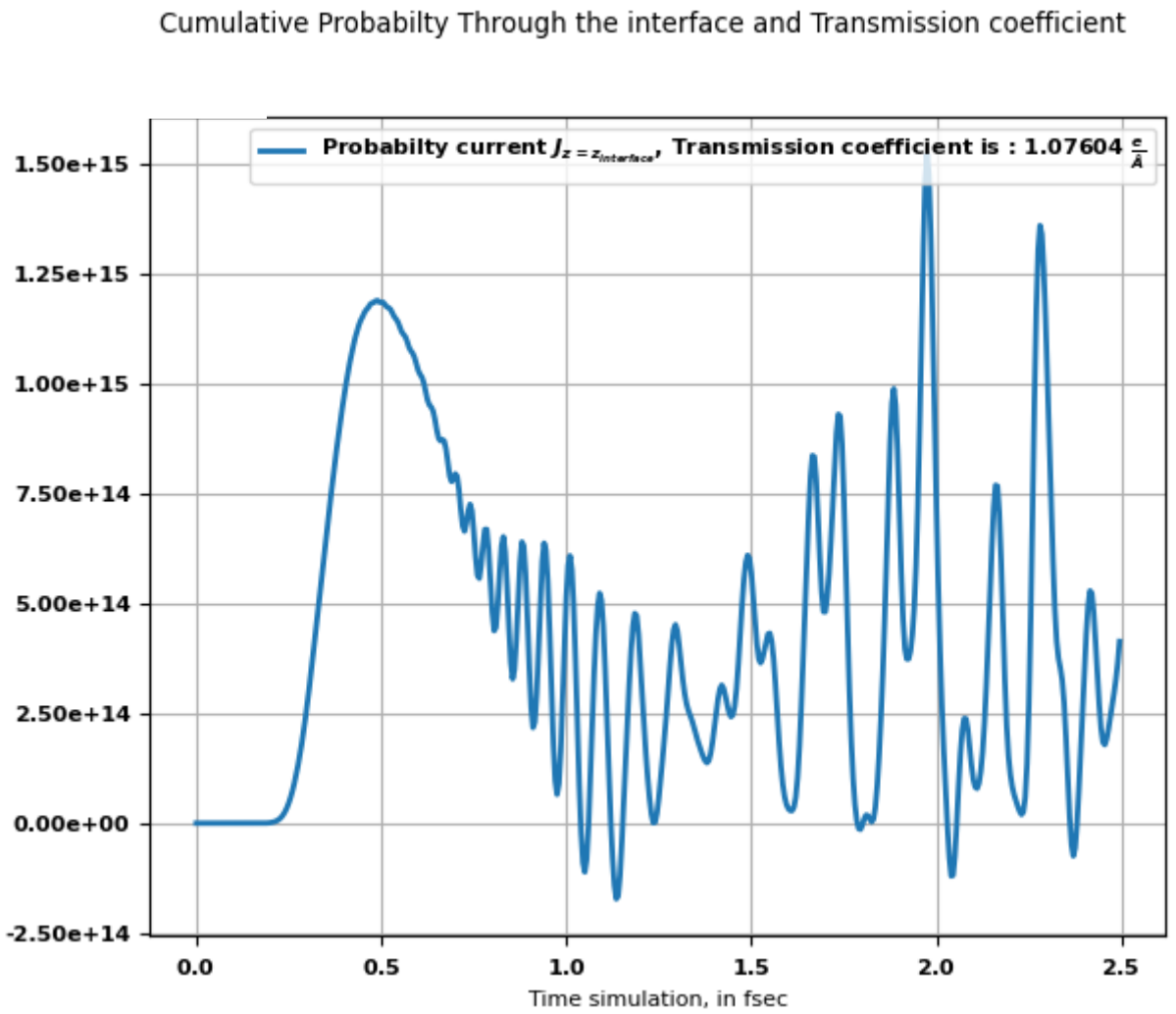
Charge time evolution

* Choose a reference location to calculate flux: write “29”.

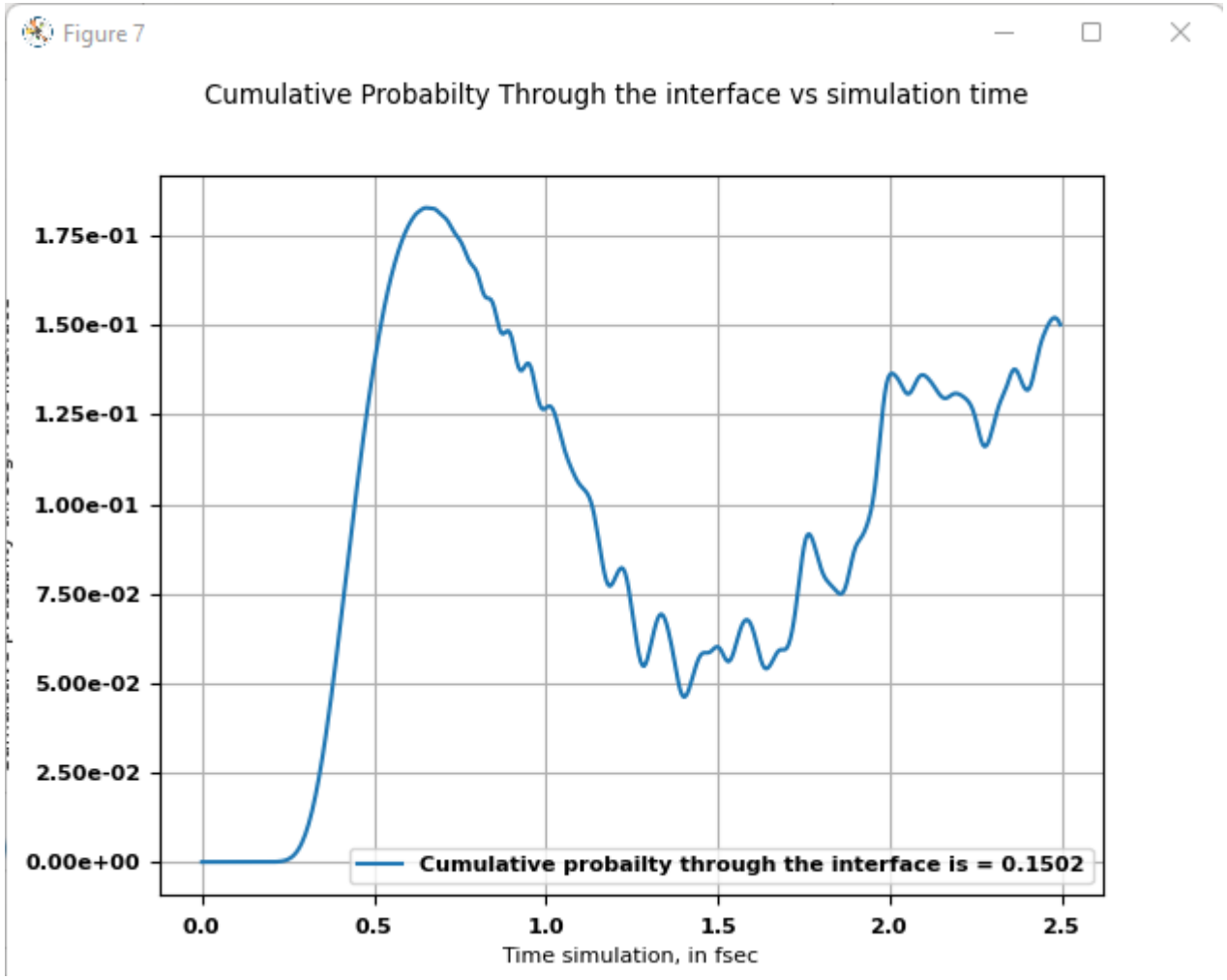
- Manually select initial position: write “15” at the center of the grid.



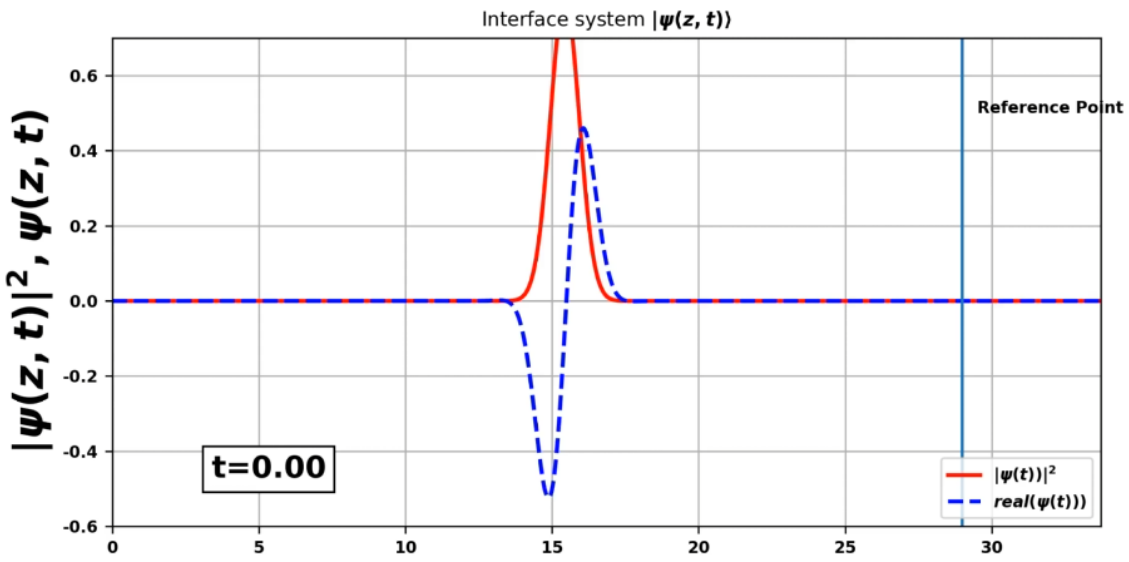
Time-dependent flux

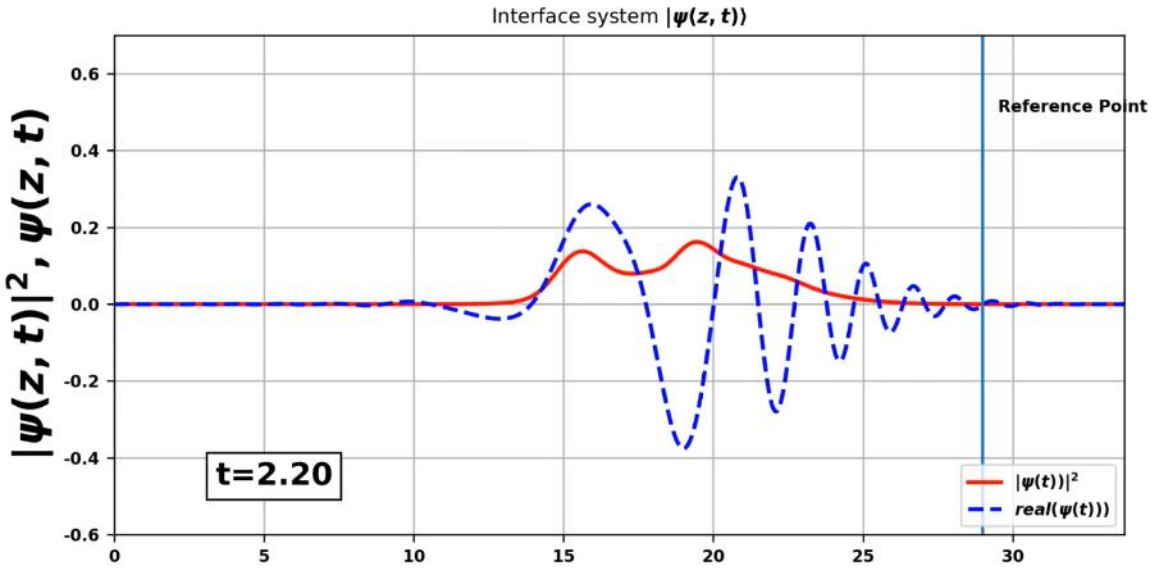


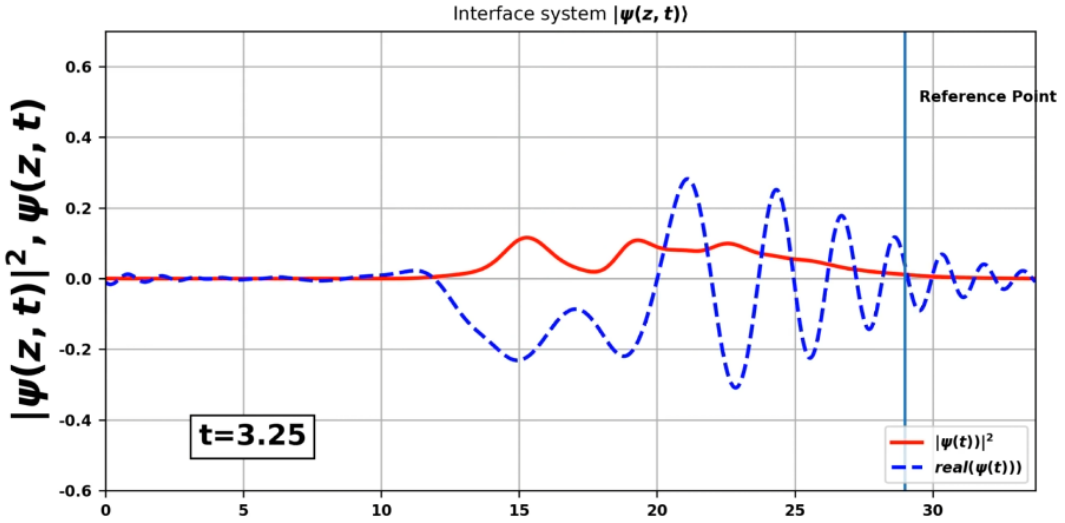
Cumulative time-dependent Flux



Watching the movie (checking the file MP4)

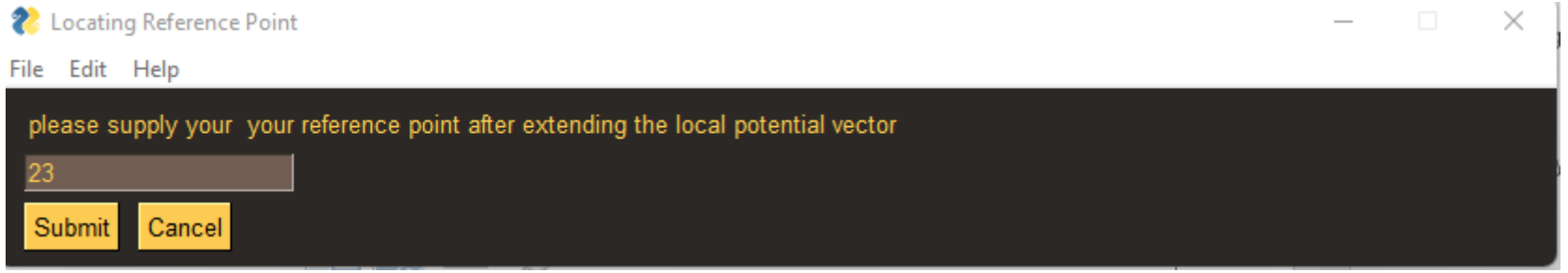




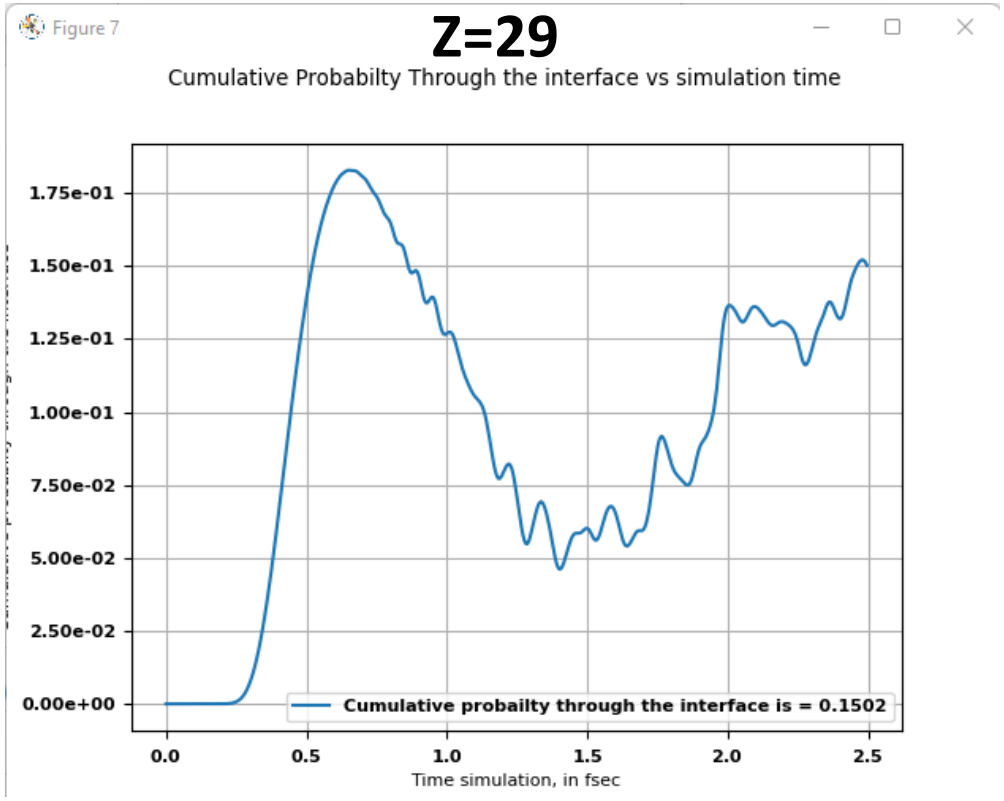


Comparing between different flux positions

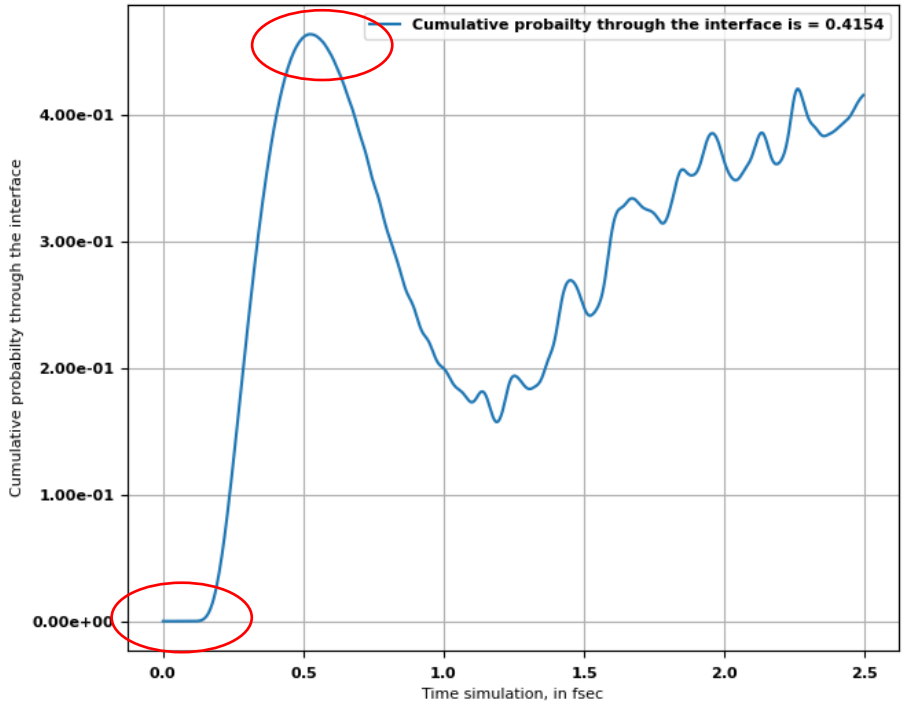
- Choose a reference location to calculate flux: write “23” instead of “29”. The start of the flux increase and maxima start earlier.



Z=29



Z=23

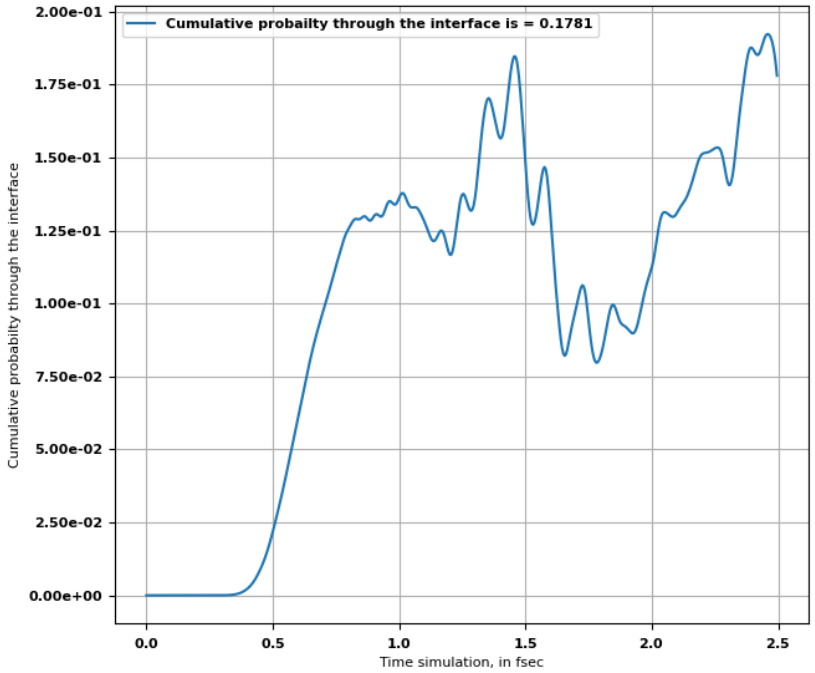


Comparing between different initial positions

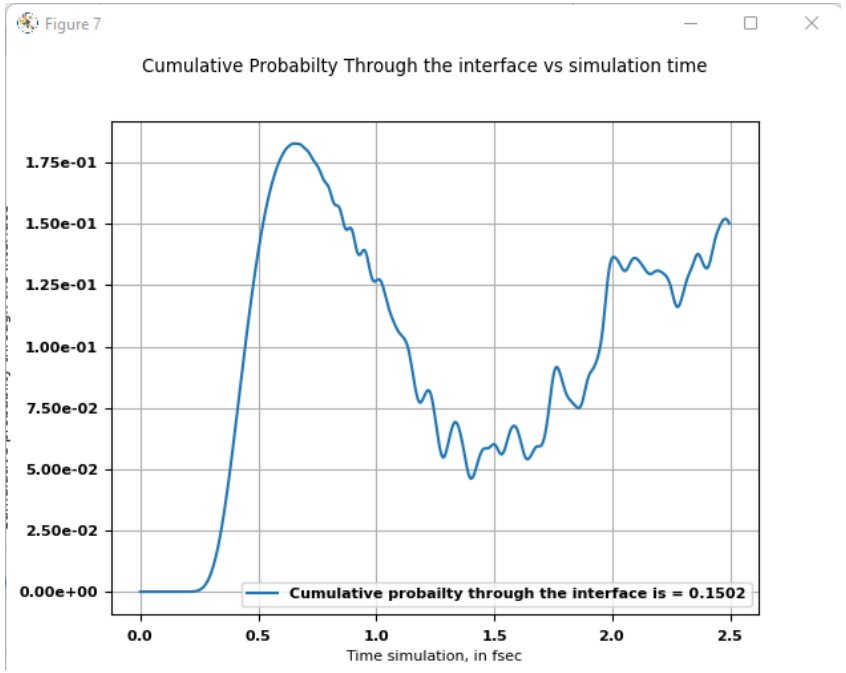
- Manually select initial position: write “9” instead of “15”.

Late and less sharp rise.

Z_0=9



Z_0=15



Comparing different initial energies

Please input here the initial energy. The energy of an electron at the bottom of the conduction band. In units of Joules

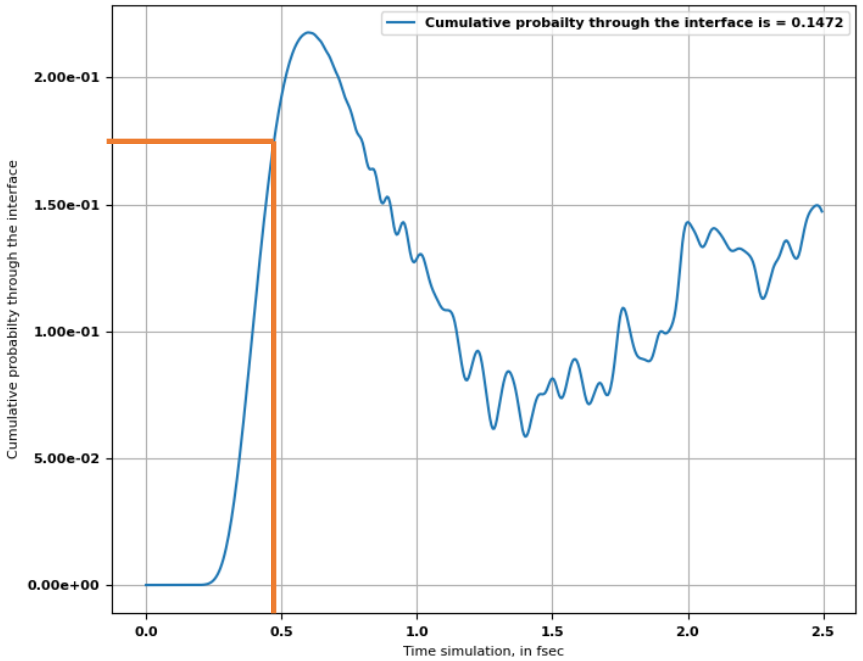
5e-19

Please input here the initial energy. The energy of an electron at the bottom of the conduction band. In units of Joules

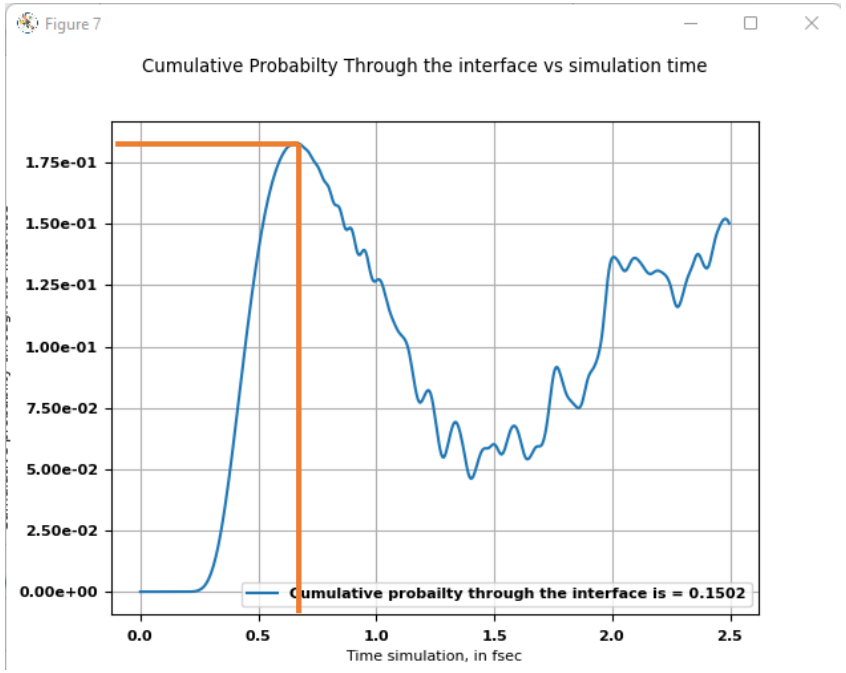
10e-19

- More and faster transmission.

Initial energy 10e-19J



Initial energy 5e-19J

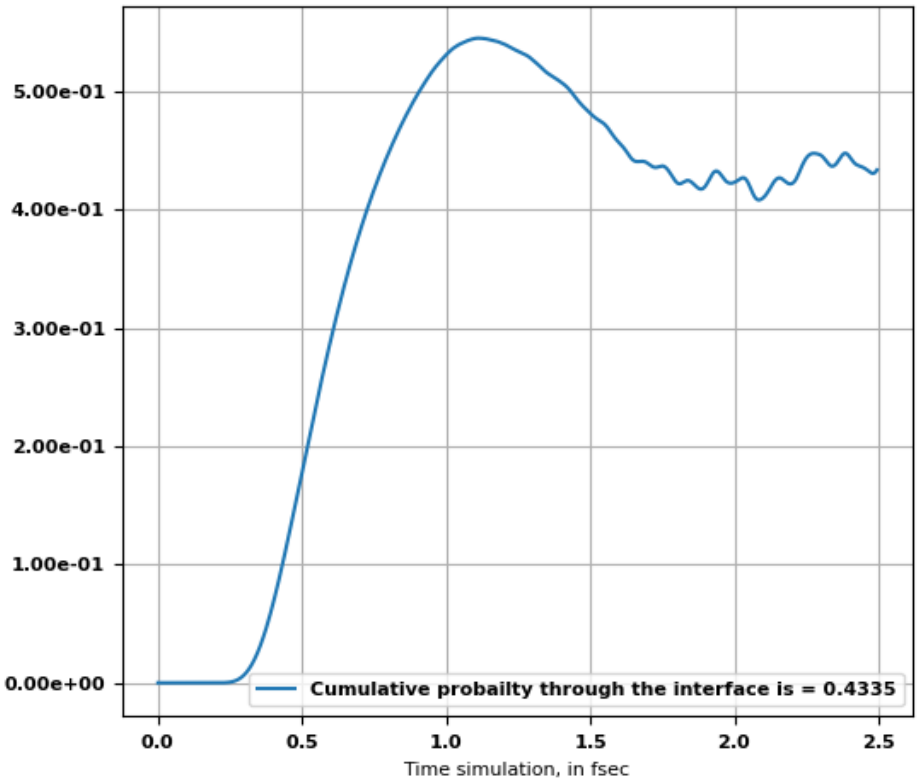


Comparing between different sizes of potential multiplications

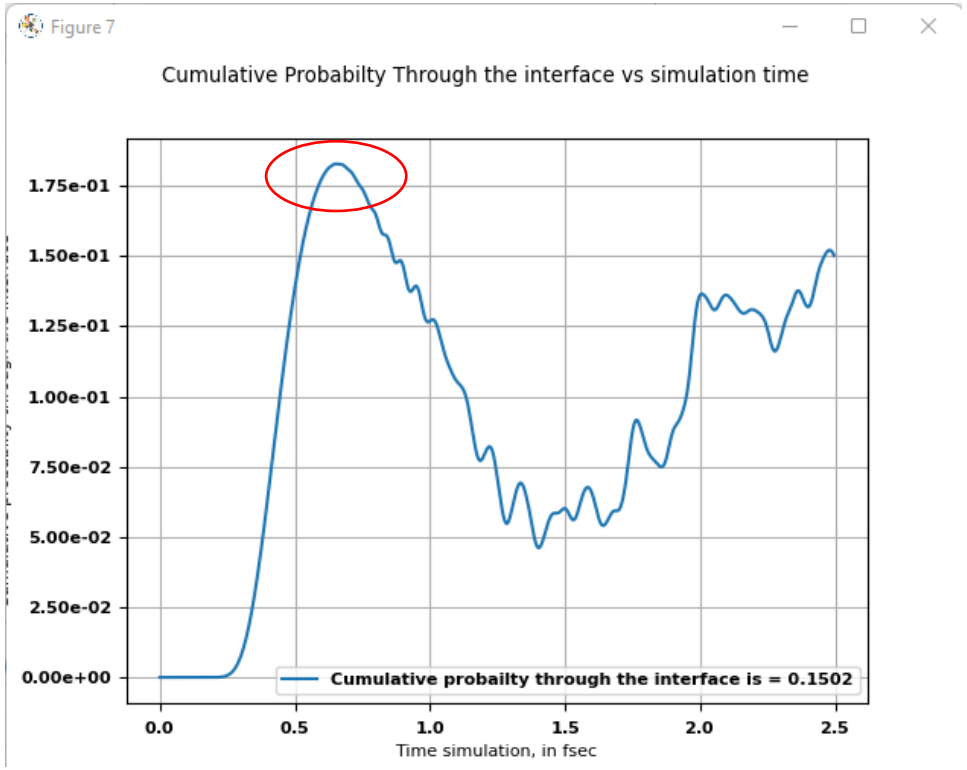
- Multiply the potential 20 times (instead of 10).

Not converged yet, noise scattering from grid edges.

Multiplied 20



Multiplied 10



Comparing between materials

experiment	http://www.ioffe.ru/SVA/NSM/Semicond/GaAs/electric.html
GaAS	≤8500 $cm^2 V^{-1}s^-$
GaSb	3000 $cm^2 V^{-1} s^{-1}$

- GaSn has larger widths and heights in the potential.
- Note: multiply GaSn x5 times instead of x10 (since the GaAs starts at maxima the initial maxima are deleted before multiplication from minima).

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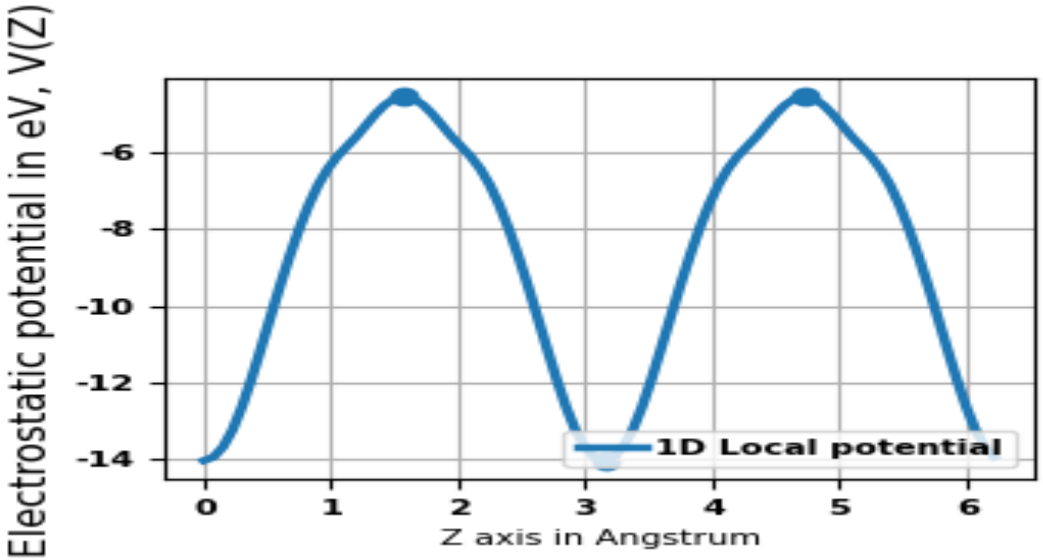
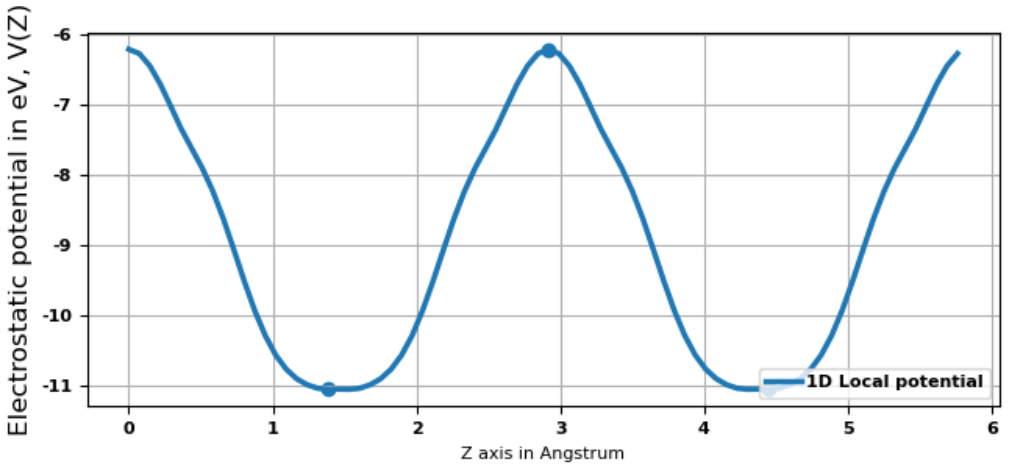
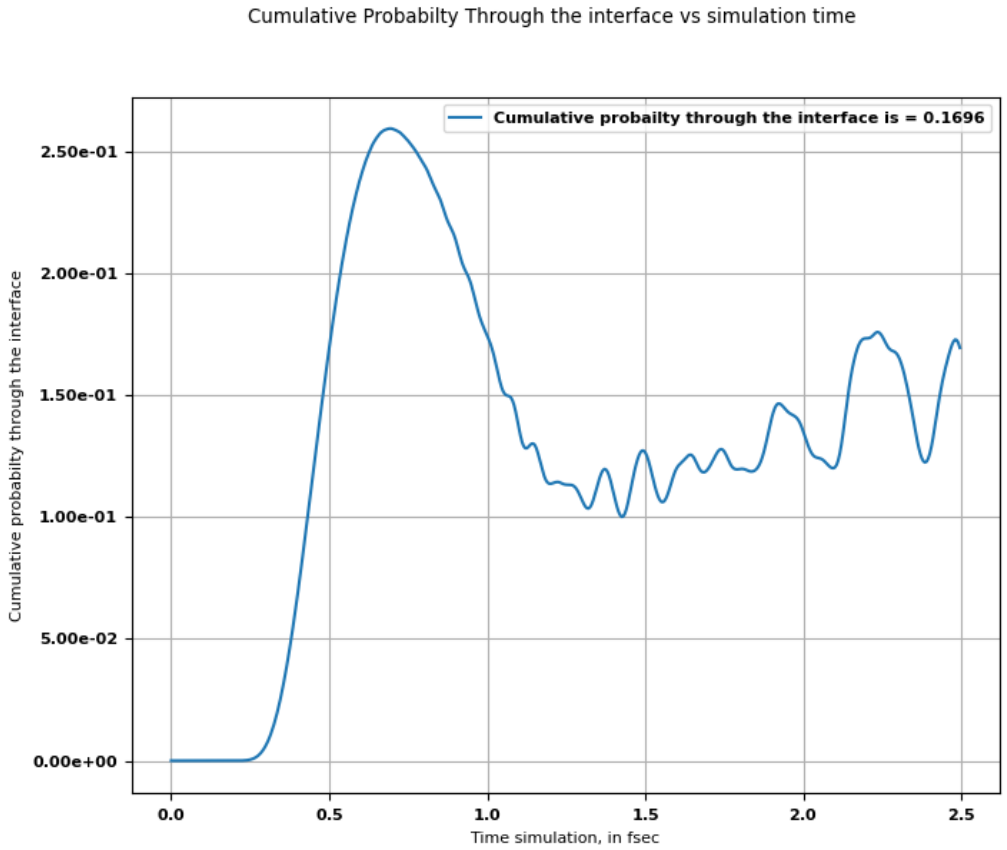
GaSb



GaAs



GaSb


Cumulative Probabilty Through the interface vs simulation time
Cumulative probailty through the interface is = 0.1696
Cumulative probability through the interface
2.50e-01
2.00e-01
1.50e-01
1.00e-01
5.00e-02
0.00e+00
0.0
0.5
1.0
1.5
2.0
2.5
Time simulation, in fsec

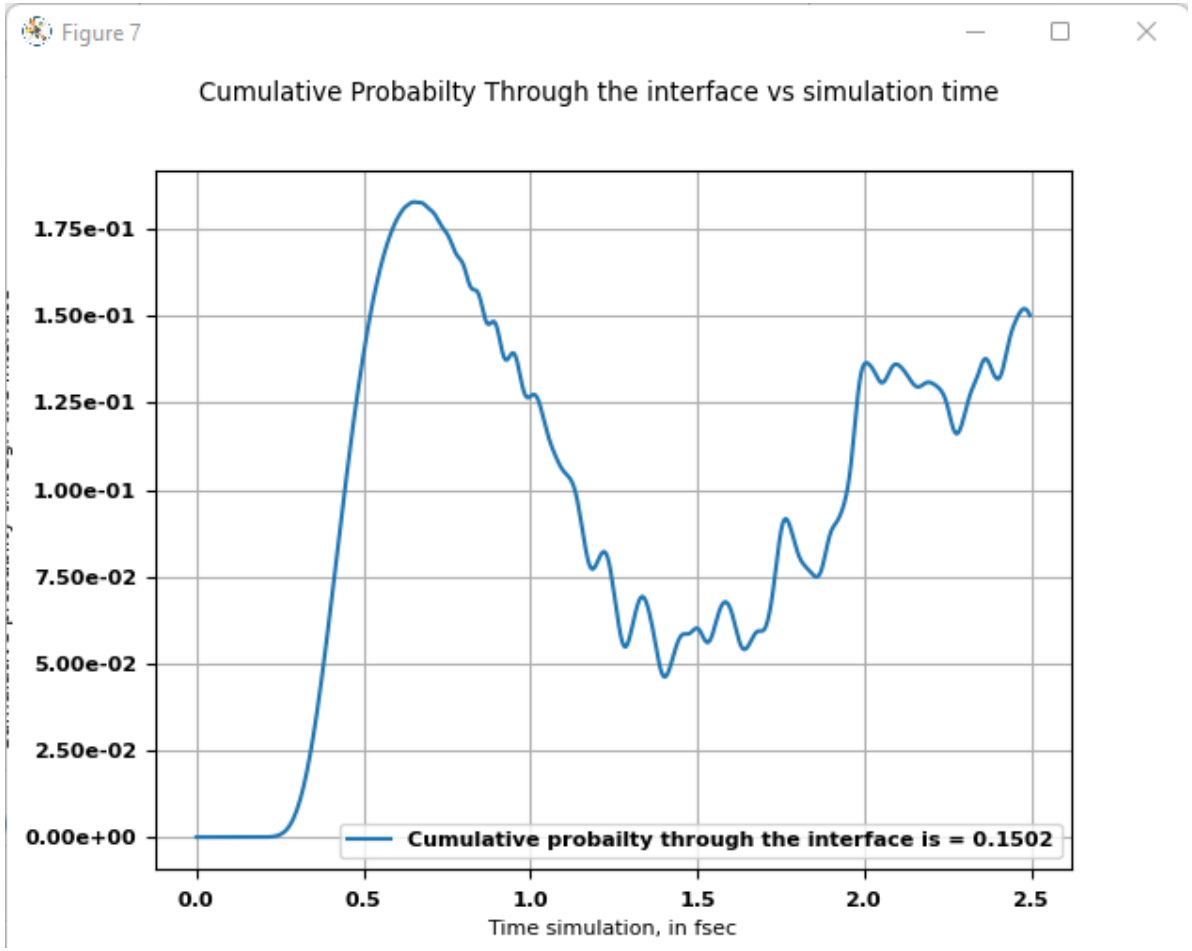
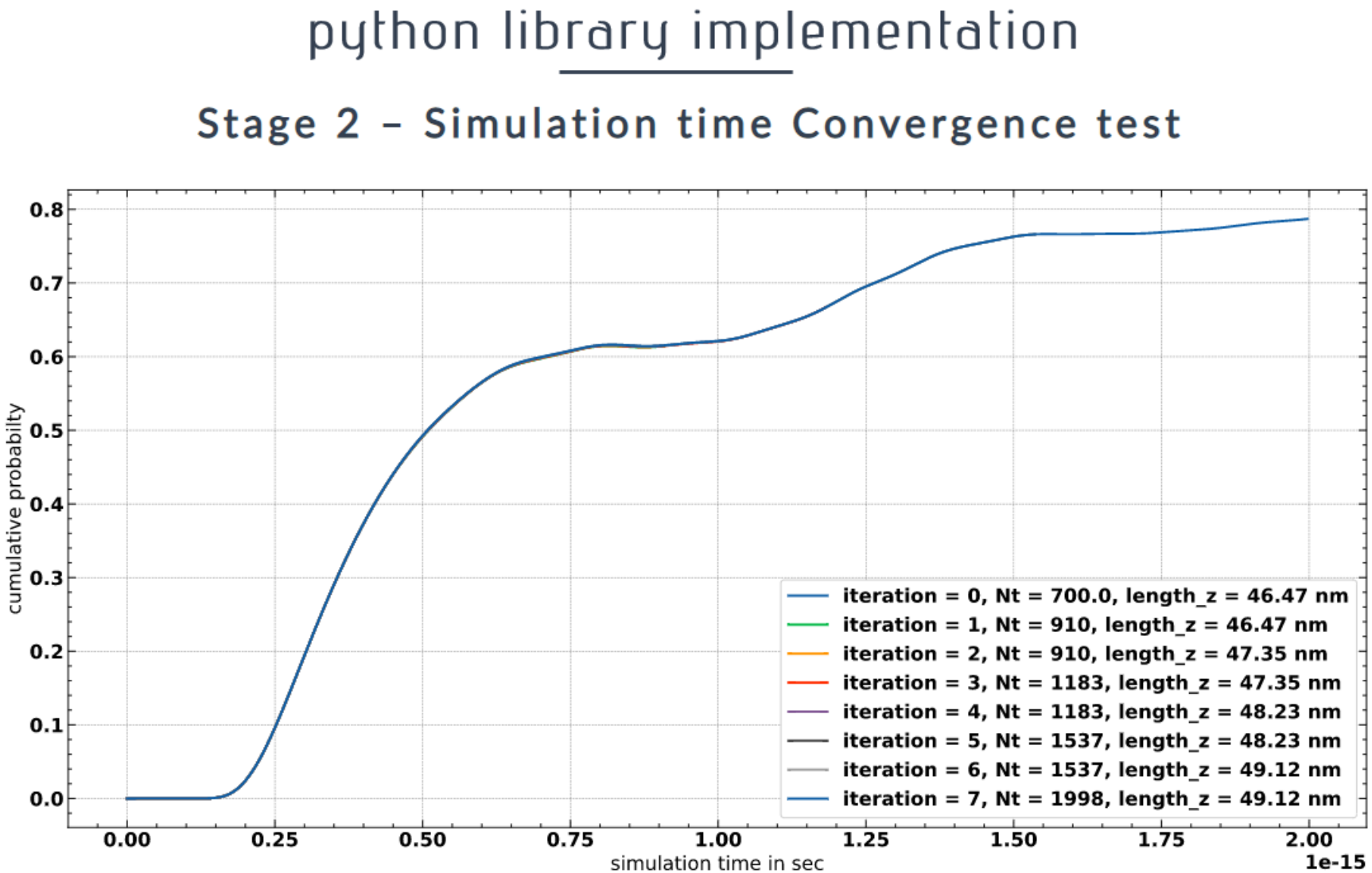


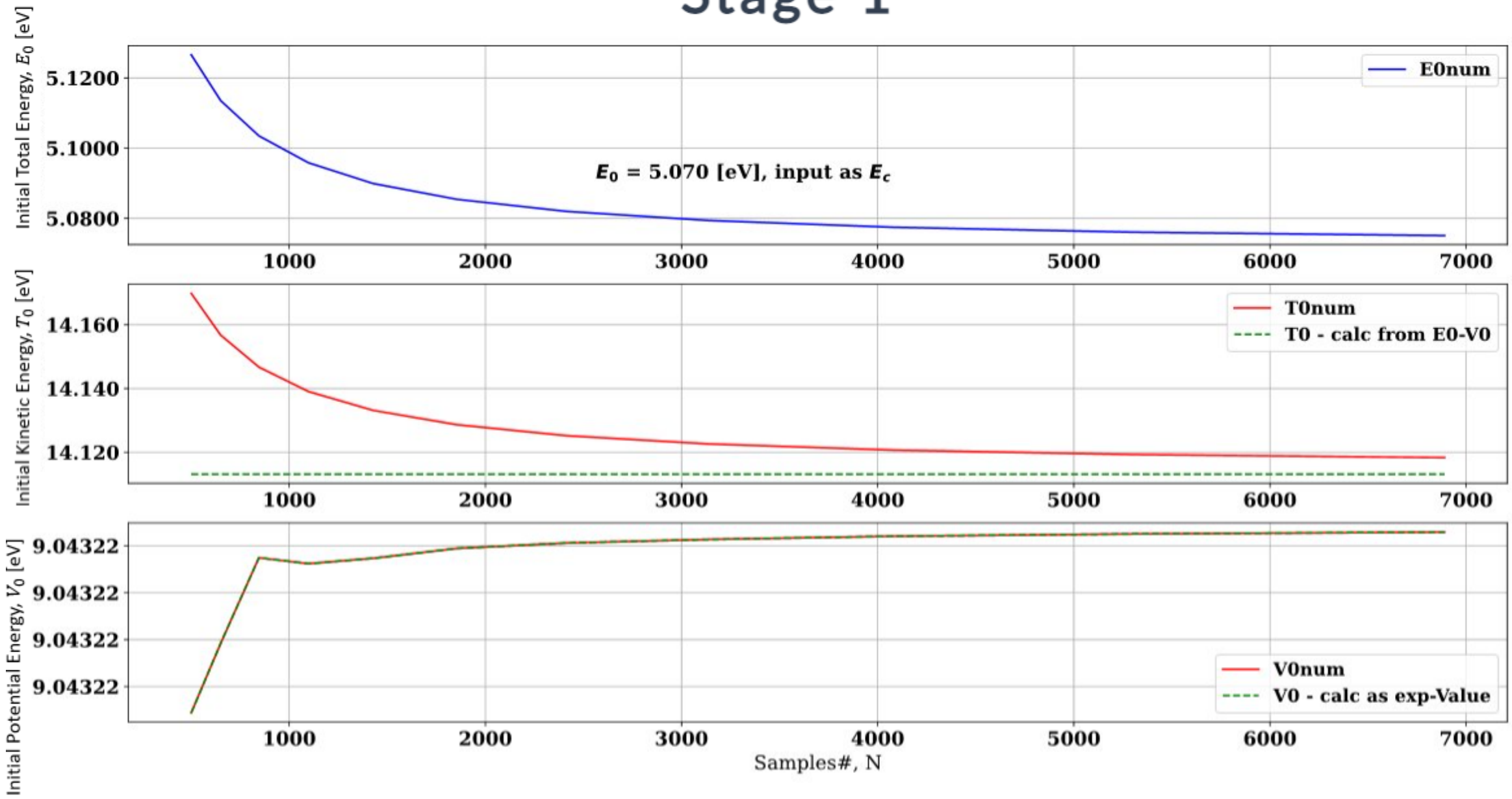
Figure 7
Cumulative Probabilty Through the interface vs simulation time
1.75e-01
1.50e-01
1.25e-01
1.00e-01
7.50e-02
5.00e-02
2.50e-02
0.00e+00
Cumulative probailty through the interface is = 0.1502
0.0
0.5
1.0
1.5
2.0
2.5
Time simulation, in fsec

Examples for convergence tests



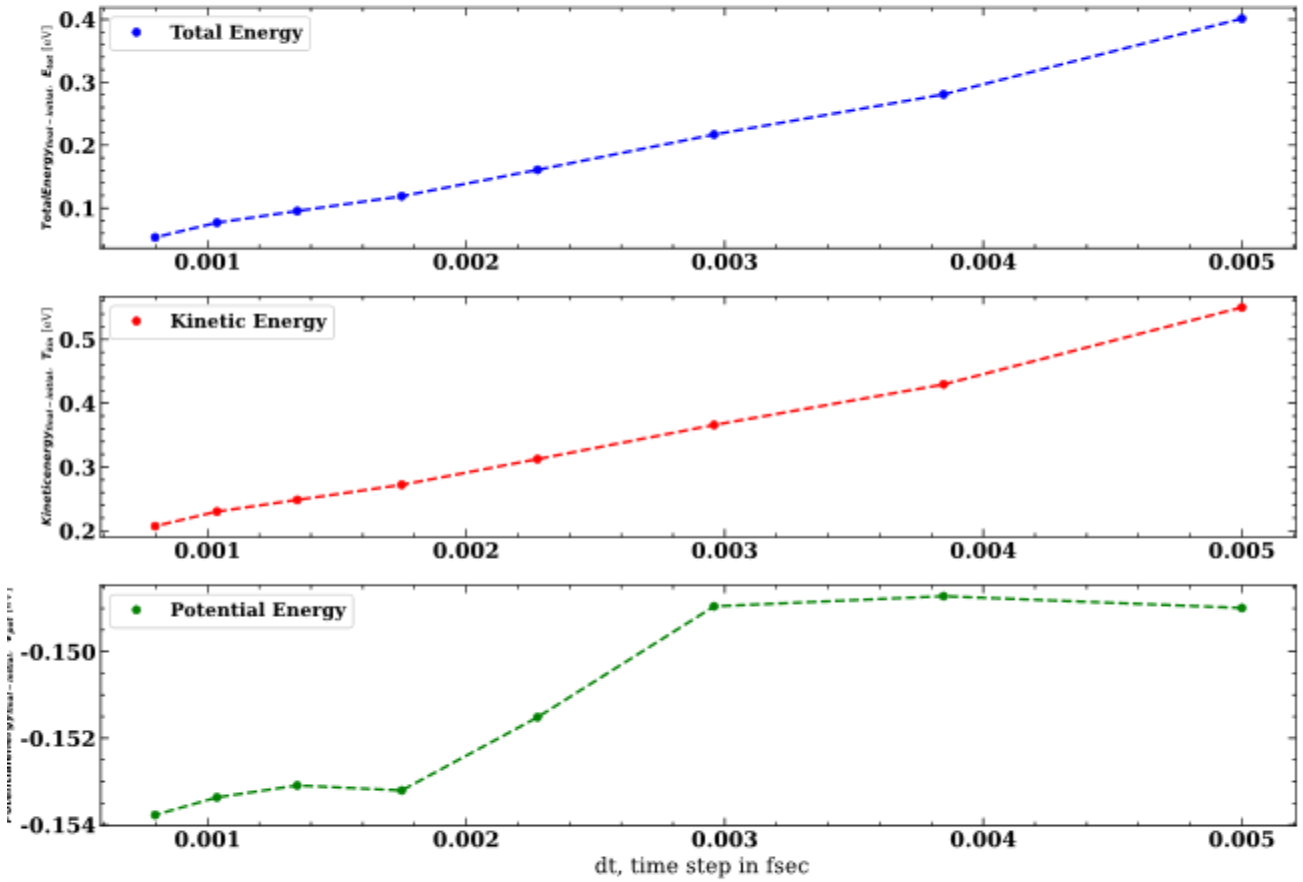
python library implementation

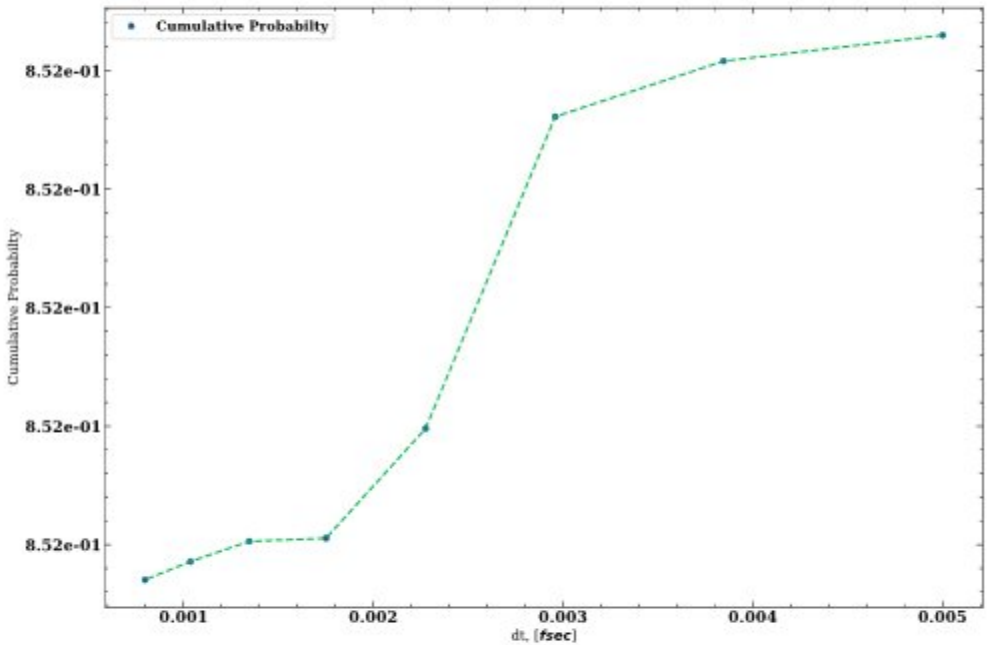
Stage 1



python library implementation

Stage 2 – time step convergence tests





$E_{tot}(Last\ propagation\ step) - E_{tot}(First\ propagation\ step) \leq 1\text{meV}$

$\Phi(Last\ propagation\ step) - \Phi(First\ propagation\ step) \leq 0.001$