

# Tutorial for python code

on wave packet propagation across materials



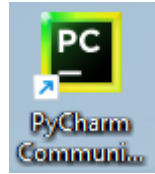
# User account

Name: its.usr1

Password: Cost2022:)

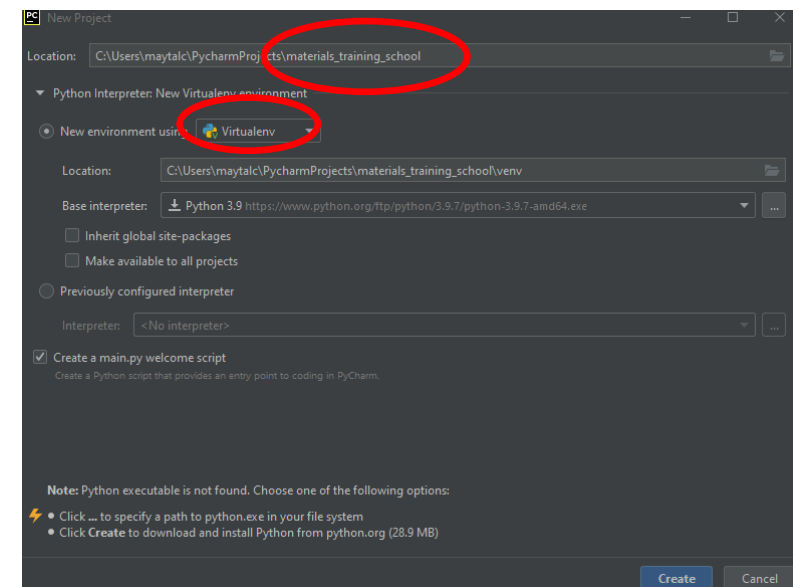
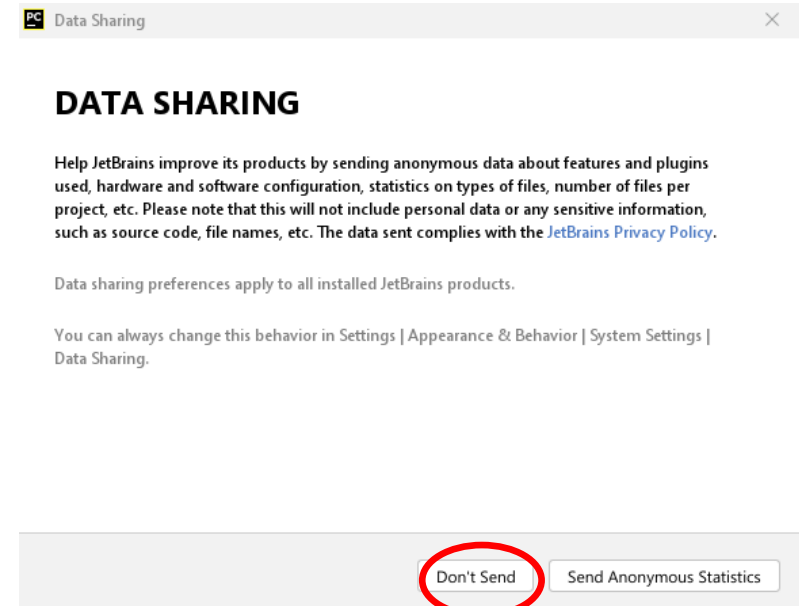
# Setting up and installations

- 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

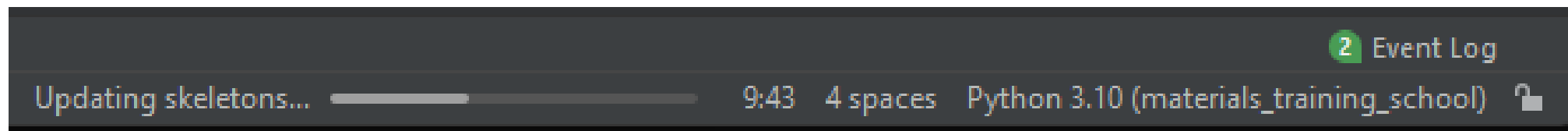
- Open “anaconda prompt”.
- Write “activate <project name>”.
- Write:

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

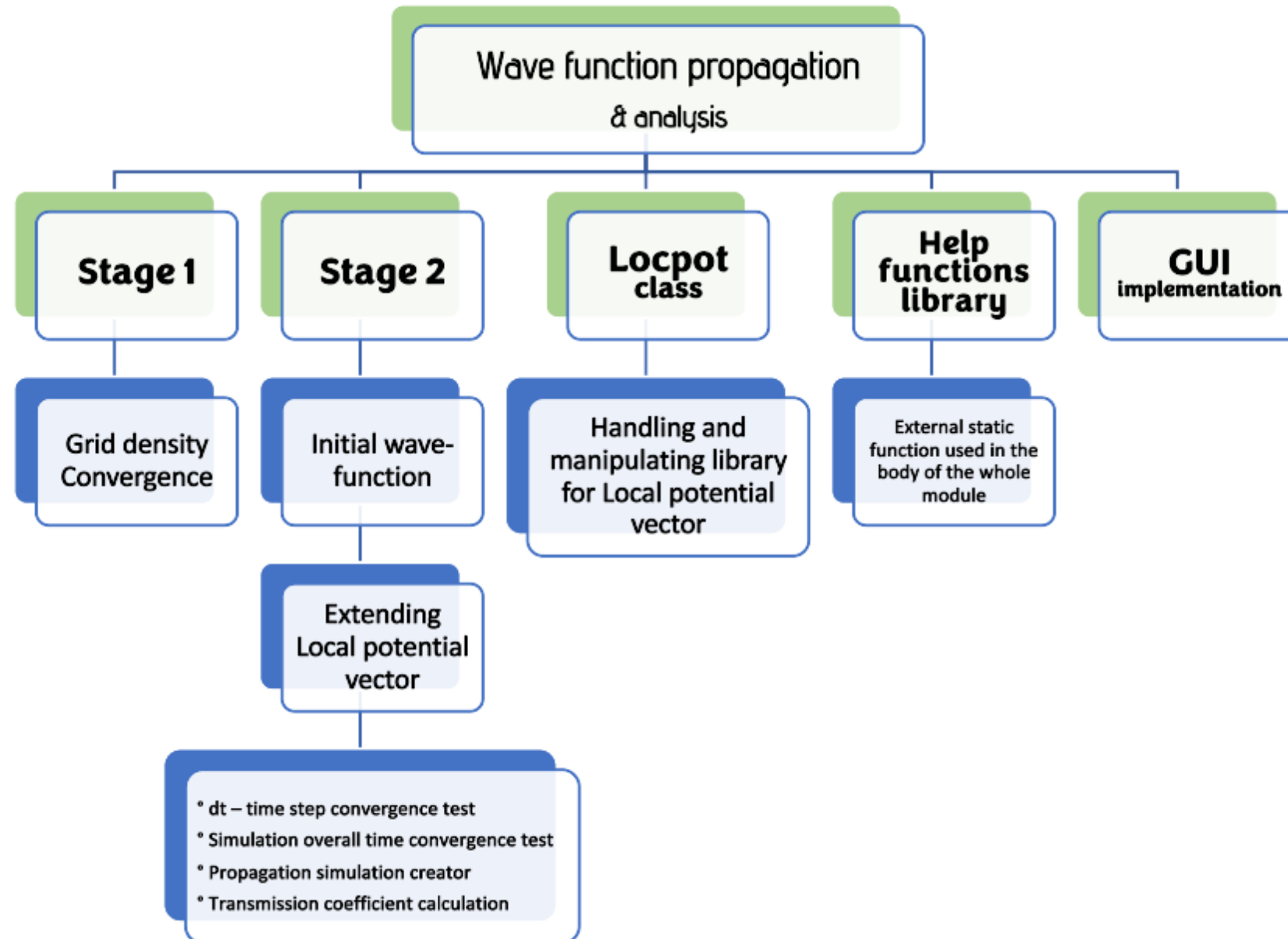
- Write: “y” to proceed when asked.
- Write: “pip install WF-Prop”.
- In Pycharm, there is update that needs to be complete:

Anaconda Prompt (Anaconda3)

```
(base) C:\Users\maytalc>activate materials_training_school  
materials_training_school) C:\Users\maytalc>
```



# Numerical methods & python library implementation



# Numerical methods & python library implementation

## Wave Function propagation Gui

Open the locpot file of your system. If you have the locpot of your bulk materials, you should supply them too

Main Locpot File

Bulk material locpot 1

Bulk material locpot 2

If you want your E0 to be imported from your calculation, please Load here your vasp run file - for the bulk material you wish to initialize the electron at

vasprun file

select

- Has an interface?
- Is 2D?
- Define a certain range?
- Flip sides of your interface

What convergence test you wish to perform?

Convergence Tests

- Spacial grid density
- System size
- Time steps

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

Please input here the standard deviation of the gaussian wave function. This should be given in units of Meter

Please input here the Initial number of spacial partitions. The number of dx. This should be an integer

## 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

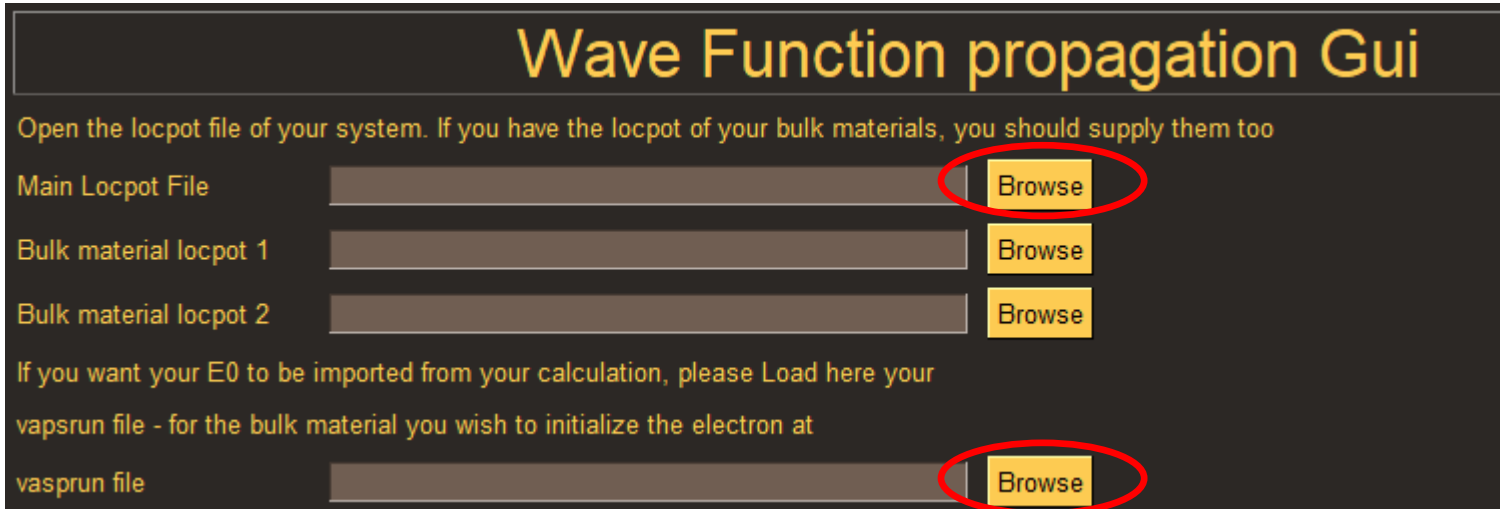


# Type of LOCPOT materials

- GaAs
- AlN
- GaSn

# Options for selection on GUI

- Uploading potential energy files:



**Wave Function propagation Gui**

Open the locpot file of your system. If you have the locpot of your bulk materials, you should supply them too

Main Locpot File

Bulk material locpot 1

Bulk material locpot 2

If you want your E0 to be imported from your calculation, please Load here your vasp run file - for the bulk material you wish to initialize the electron at

vasprun file

The screenshot shows a dark-themed GUI with yellow text. Three 'Browse' buttons are circled in red, highlighting the file selection options for the Main Locpot File, Bulk material locpot 1, and the vasp run file.

# The rest of the GUI selections

- We can simply tick all output:

select

- Has an interface?
- Is 2D?
- Define a certain range?
- Flip sides of your interface

What convergence test you wish to perform?

Convergence Tests

- spatial grid density
- System size
- Time steps

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 standard deviation of the gaussian wave function. This should be given in units of Meter

7e-11

Please input here the Initial number of time steps. The number of dt the overall simulation will undergo. This should be an integer

500

Please input here the Initial value of your time step, dt. It will be used as an initial guess of the default value

5e-18

Please choose the axis you wish to average the local potential

axes

- x
- y
- z

Choose from the options what you would like to do

Options

- Print averaged local potential
- Extend Locpot
- Full propagation
- Transmission coefficient
- Cumulative probability
- Modeling the interface

Submit Cancel

# Details on GUI options:

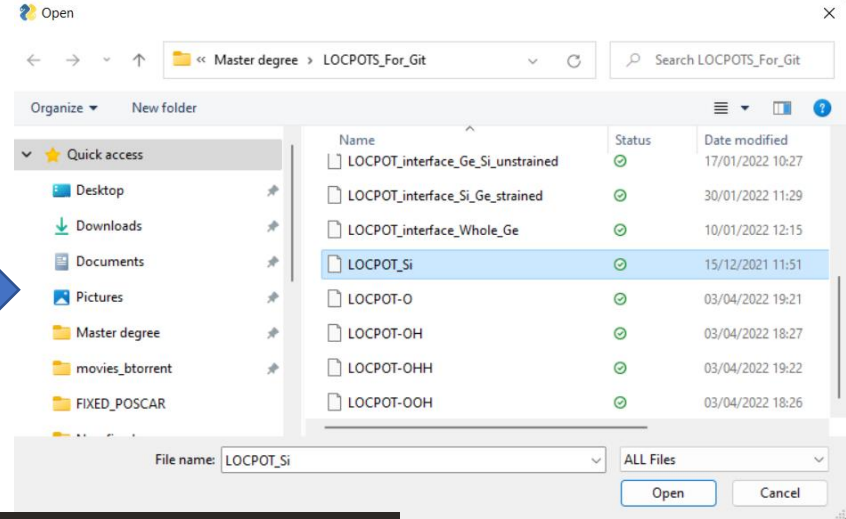
Click on 'Browse',  
Then locate your  
locpot files

**1. Loading Locpot file**  
If You have bulk-materials locpot files  
You can load them too, at that level.

Main Locpot File

Bulk material locpot 1

Bulk material locpot 2



**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.

select

Has an interface?

Is 2D?

Define a certain range?

select

Has an interface?

Is 2D?

Define a certain range?

select

Has an interface?

Is 2D?

Define a certain range?

select

Has an interface?

Is 2D?

Define a certain range?

select

Has an interface?

Is 2D?

Define a certain range?

## 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.

select

Has an interface? 2d

Is 2D?

Define a certain range?

select

Has an interface? 2c

Is 2D?

Define a certain range?

select

Has an interface? 2b

Is 2D?

Define a certain range?

select

Has an interface? 2a

Is 2D?

Define a certain range?

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

Initiation position of the wave-function

File Edit Help

Where do you want to initialize you wave function  
Do you want it to search for a position automatically or manually be supplying an initial position?

Initial position

automatically

manually

Submit Cancel

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.

select

Has an interface? 2d

Is 2D?

Define a certain range?

Reference Position

File Edit Help

0

Please supply the position where you want to treat as a reference point.

Submit Cancel

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.

select

Has an interface? 2b

Is 2D?

Define a certain range?

Range Choice

File Edit Help

Please supply the initial and final positions where you want to define your system.

Start Position,  
0

Final Position,  
0

Submit Cancel

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

select

Has an interface? 2c

Is 2D?

Define a certain range?

Range and interface Choice

File Edit Help

Please supply the initial and final positions where you want to define your system.

Start Position,  
0

Final Position,  
0

Please supply the position where you want to treat as a reference point.

0

Submit Cancel

### 3. Convergence tests

Choose what convergence tests you wish perform.

What convergence test you wish to perform?

Convergence Tests

- Spatial grid density
- System size
- Time steps

#### 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.

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 standard deviation of the gaussian wave function. This should be given in units of Meter

7e-11

Please input here the Initial number of spacial partitions. The number of dx. This should be an integer

300

Please input here the Initial value of your time step, dt. It will be used as an initial guess of the default value

1e-18

3a

3c

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.

What convergence test you wish to perform?

#### Convergence Tests

- Spatial grid density
- System size
- Time steps

#### 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 process

#### 3a. Grid density

Applies to Stgae\_1 sub-module

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.

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.

Grid density convergence Choice for maximum number of iterations

File Edit Help

Please supply the maximum number of iterations you wish to perform during the grid-density convergence

100

Submit

Cancel

## 4. Axis grid

Please choose the axis you wish to average the local potential

axes

- x
- y
- z

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.

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

## 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).

Choose from the options what you would like to do

Options

- Print averaged local potential
- Extend Locpot
- Full propagation
- Transmission coefficient
- Cumulative probability

Submit Cancel



## 5. Optional operations choice

Options

- Print averaged local potential
- Extend Locpot
- Full propagation
- Transmission coefficient
- Cumulative probability

Submit Cancel

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

## 5a. Locpot elongation

Locpot elongation

File Edit Help

How do you want to extend your Locpot?

Locpot Elongation

- Insertaion into a position within the locpot
- Just multiplication

How many times you would like to multiply the locpot

It will also going to be used to the number of time the inserted part will be multiplied

10

If you chose to insert into a certain position, please supply it here, in units of Angstrum

0

If you chose to insert into a certain position, do you want it to find a bulk-like Locpot region or import from a bulk locpot that has already loaded?

What to insert

- bulk-like locpot
- Import external bulk-locpot

Submit Cancel

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

## 5a. Locpot elongation

You can choose just to 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 to 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 wishes to 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).

Locpot elongation

File Edit Help

How do you want to extend your Locpot?

Locpot Elongation

Insertion into a position within the locpot

Just multiplication

How many times you would like to multiply the locpot

It will also go to be used to the number of times the inserted part will be multiplied

10

If you chose to insert into a certain position, please supply it here, in units of Angstrom

0

If you chose to insert into a certain position, do you want it to

find a bulk-like Locpot region or import from a bulk locpot that has already loaded?

What to insert

bulk-like locpot

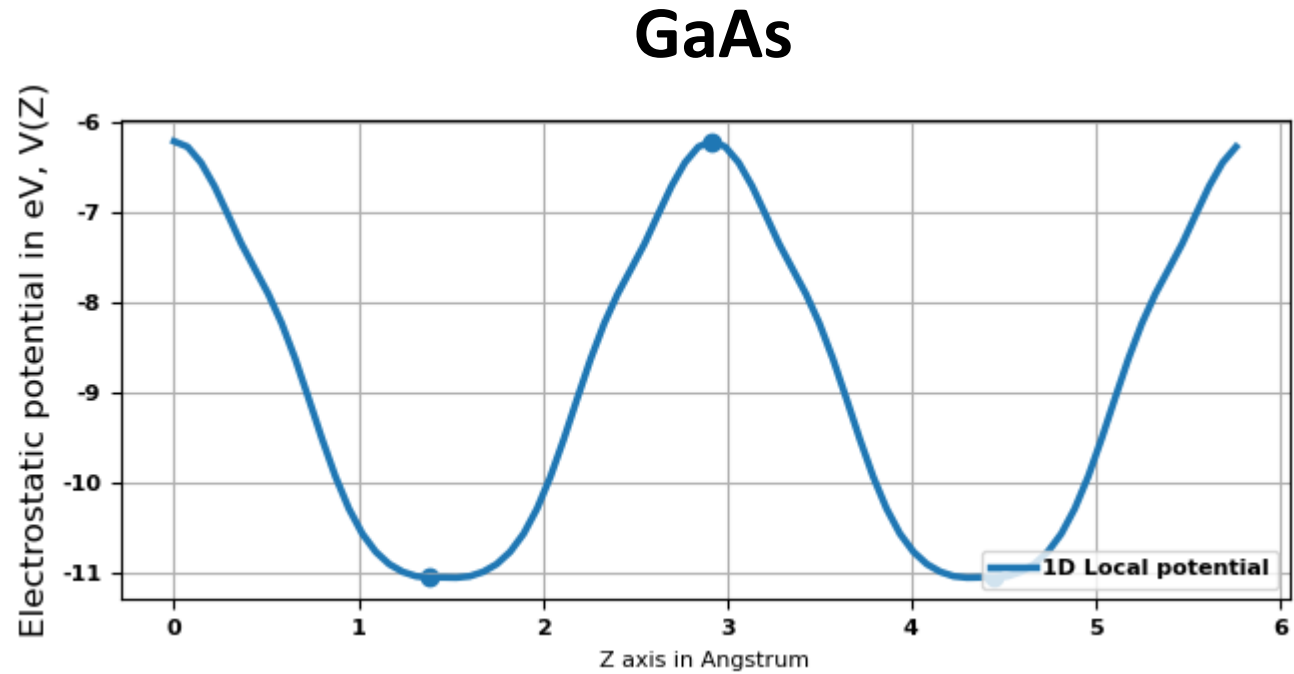
Import external bulk-locpot

Submit

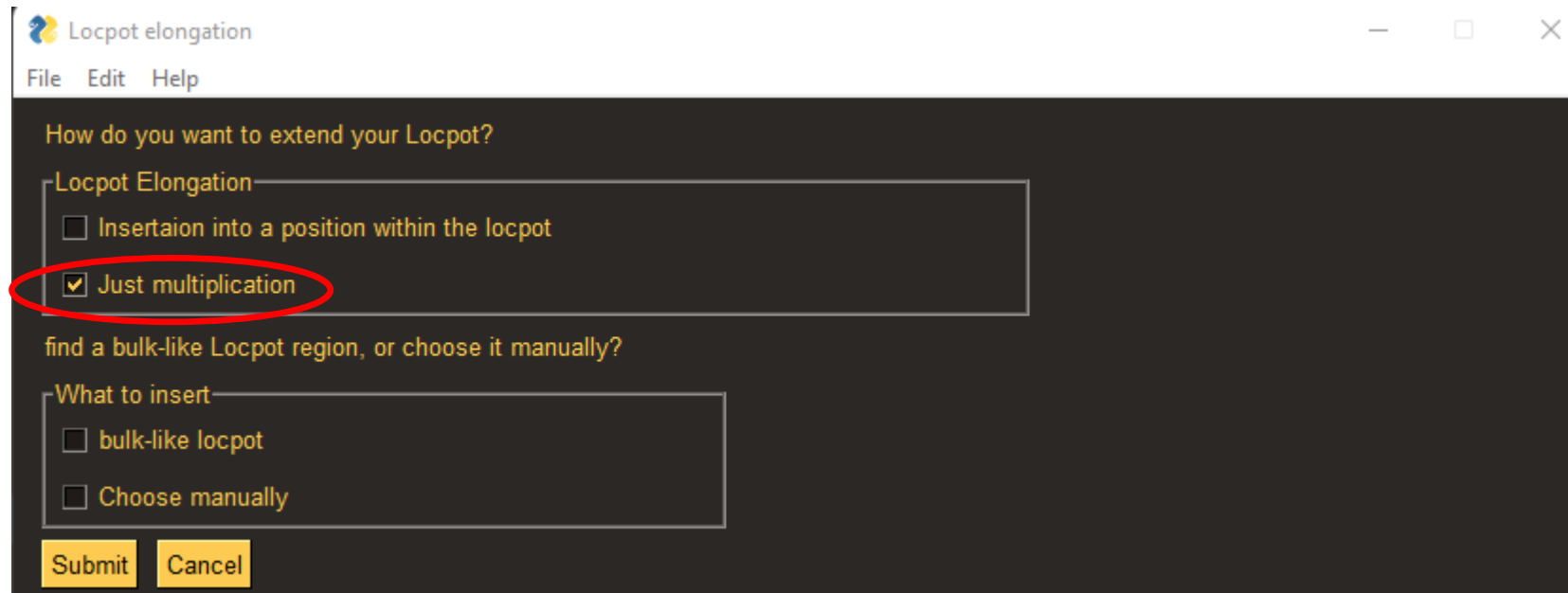
Cancel

# Printing potential

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



# Next GUI pop-ups: multiplying potential



Locpot elongation

File Edit Help

How do you want to extend your Locpot?

Locpot Elongation

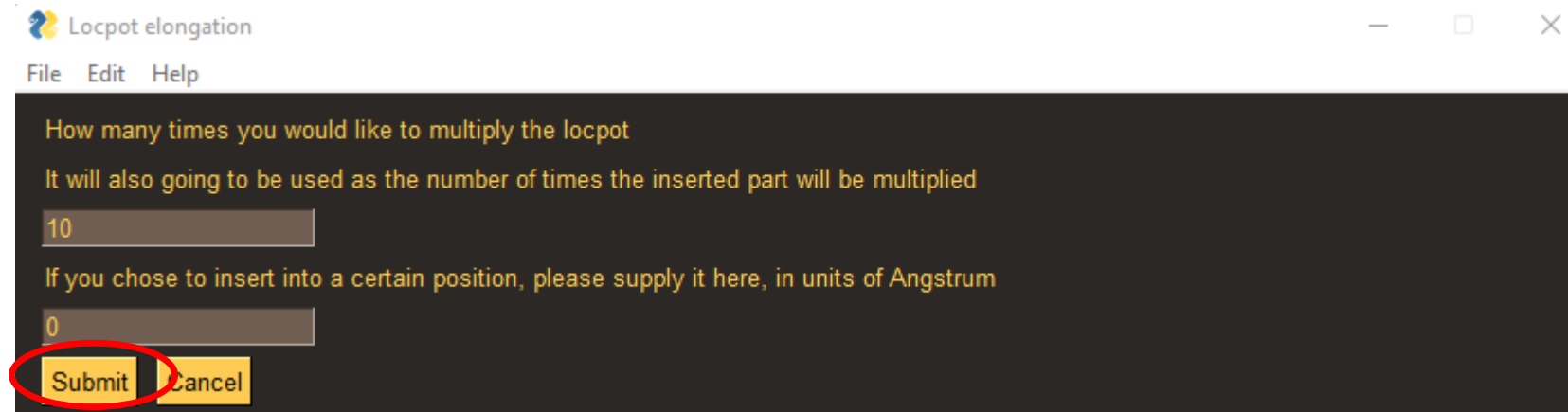
- Insertaion into a position within the locpot
- Just multiplication

find a bulk-like Locpot region, or choose it manually?

What to insert

- bulk-like locpot
- Choose manually

Submit Cancel



Locpot elongation

File Edit Help

How many times you would like to multiply the locpot

It will also going to be used as the number of times the inserted part will be multiplied

10

If you chose to insert into a certain position, please supply it here, in units of Angstrum

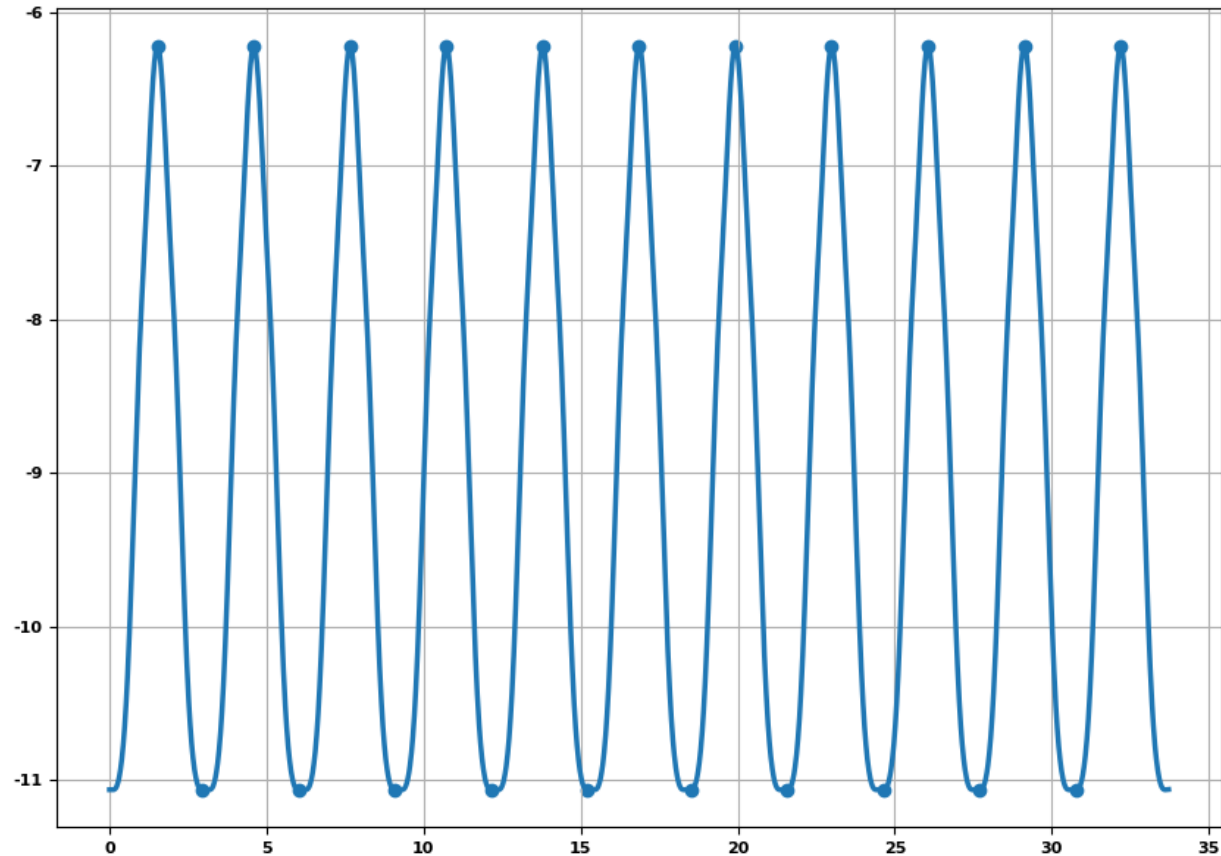
0

Submit Cancel

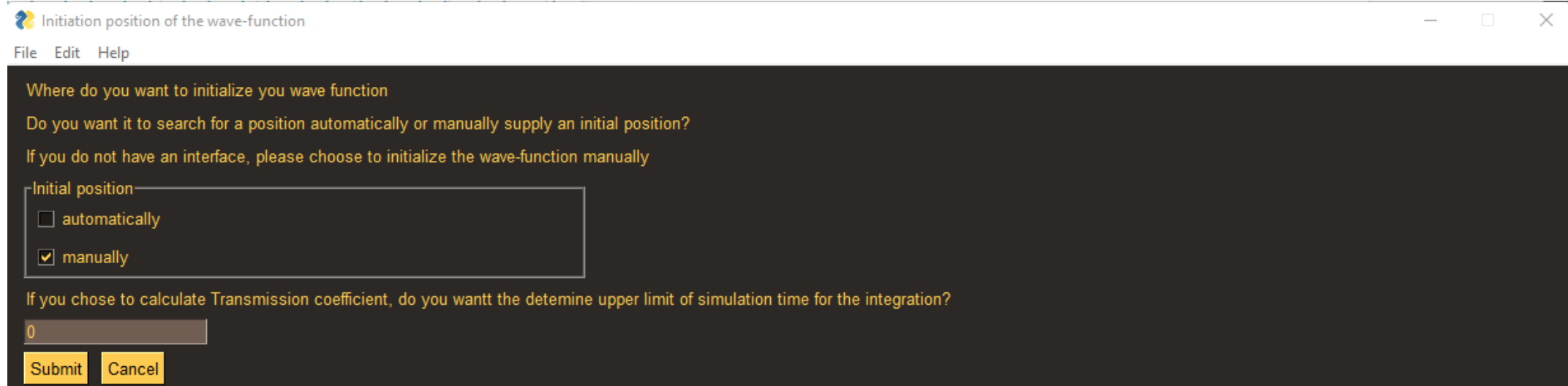
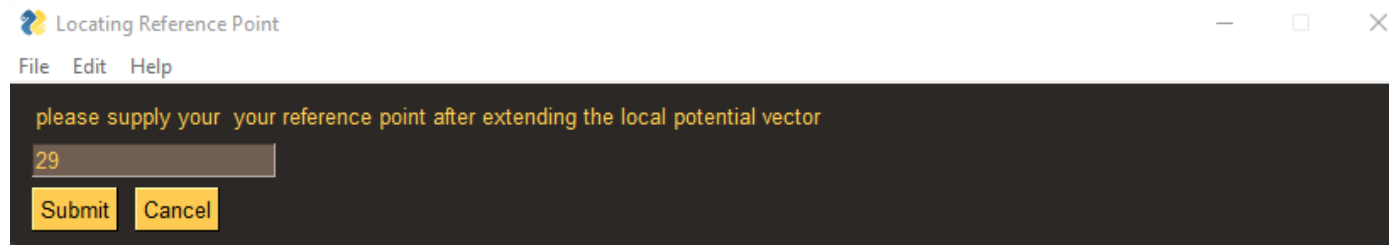
# Extending the potential

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

## GaAs



# Selections for flux position and initial wavefunction:

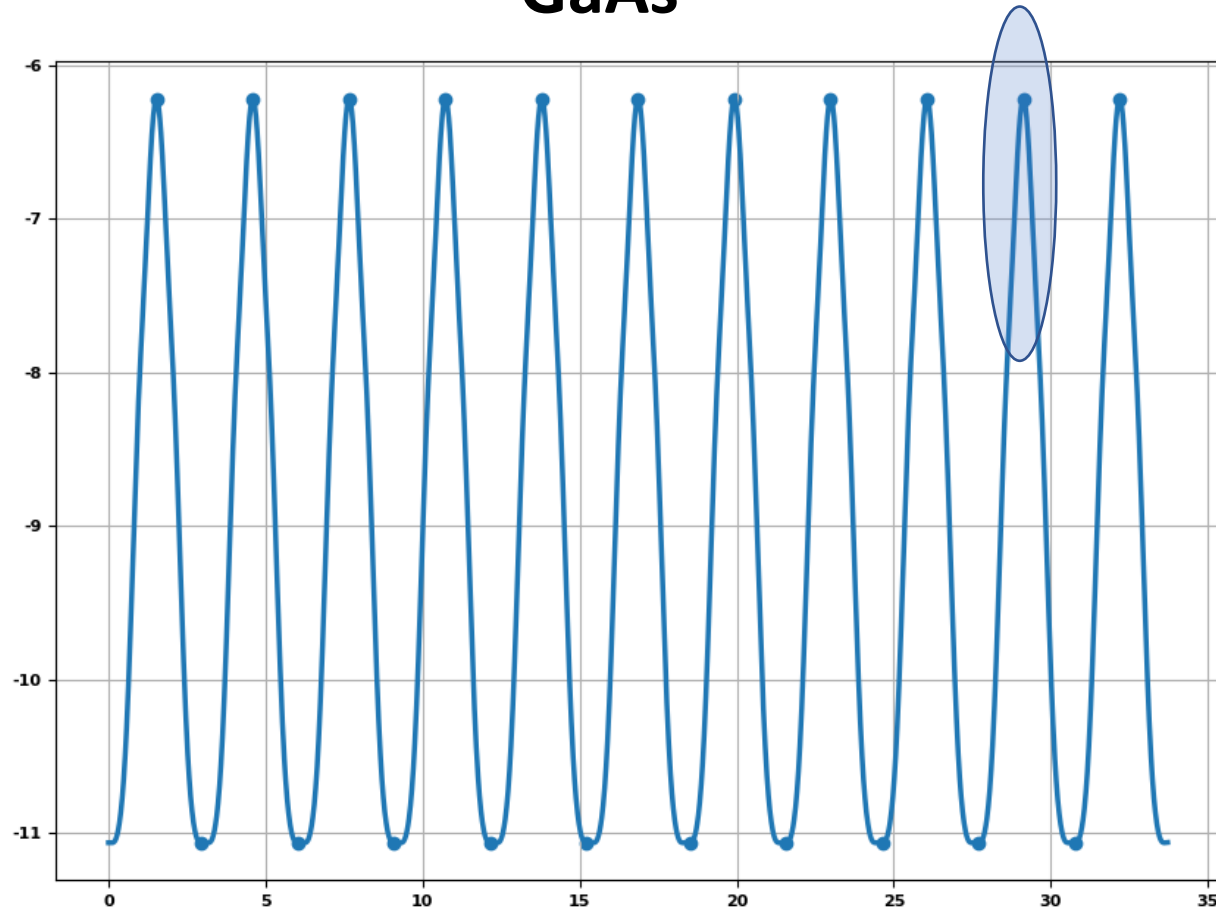


When asked where to **store the movie file**, you may select one of the LOCPOT files.

# Charge time evolution

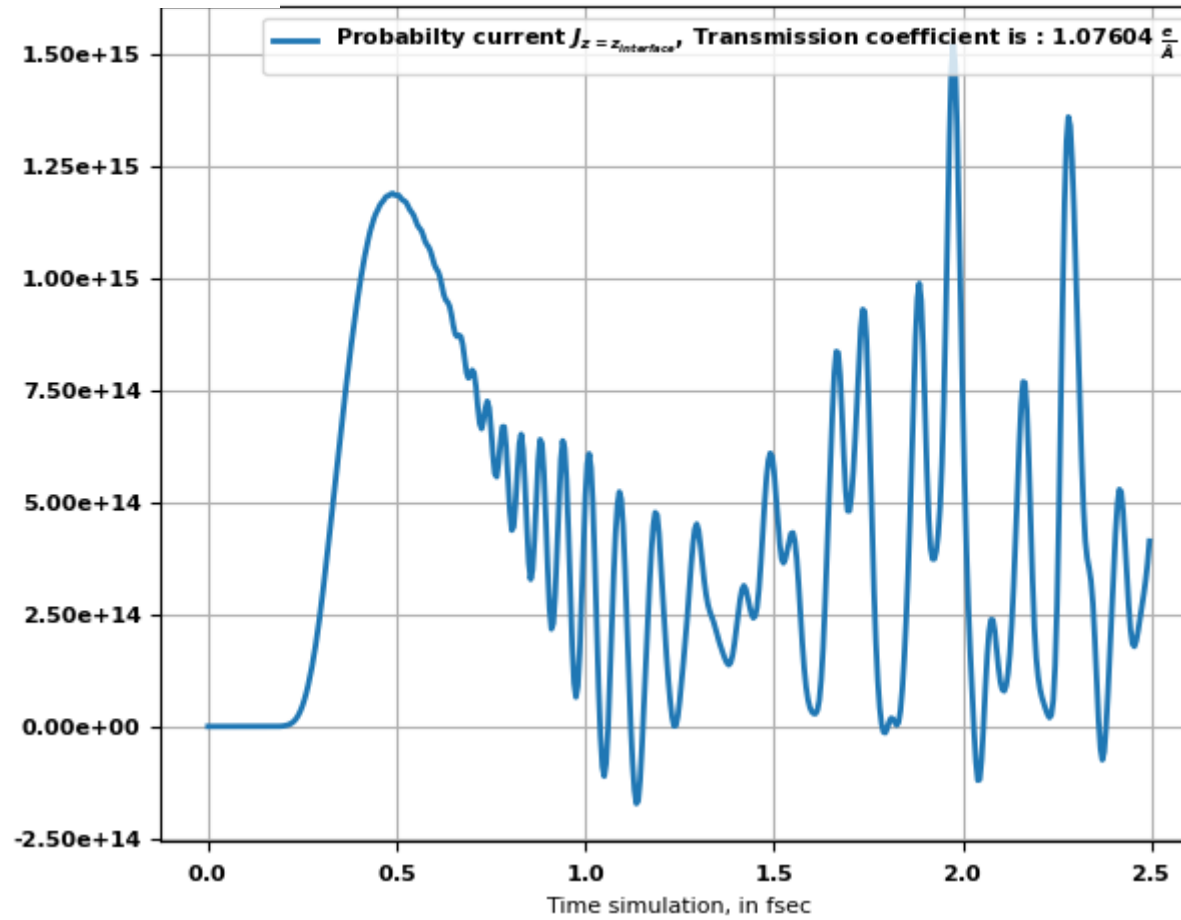
- \* Choose a reference location to calculate flux: write “29”.
- Manually select initial position: write “15” at the center of the grid.

**GaAs**



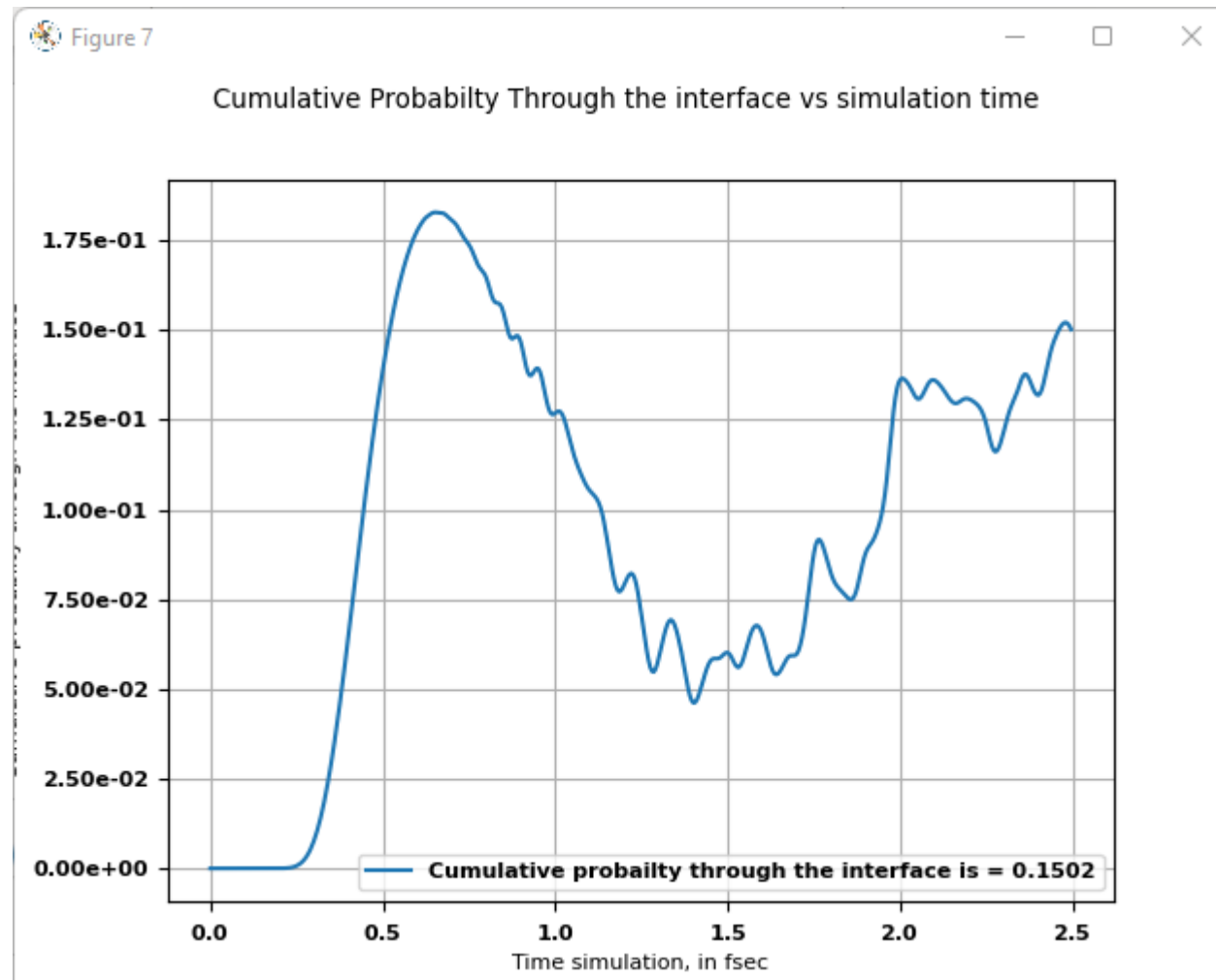
# Time-dependent flux

Cumulative Probability Through the interface and Transmission coefficient

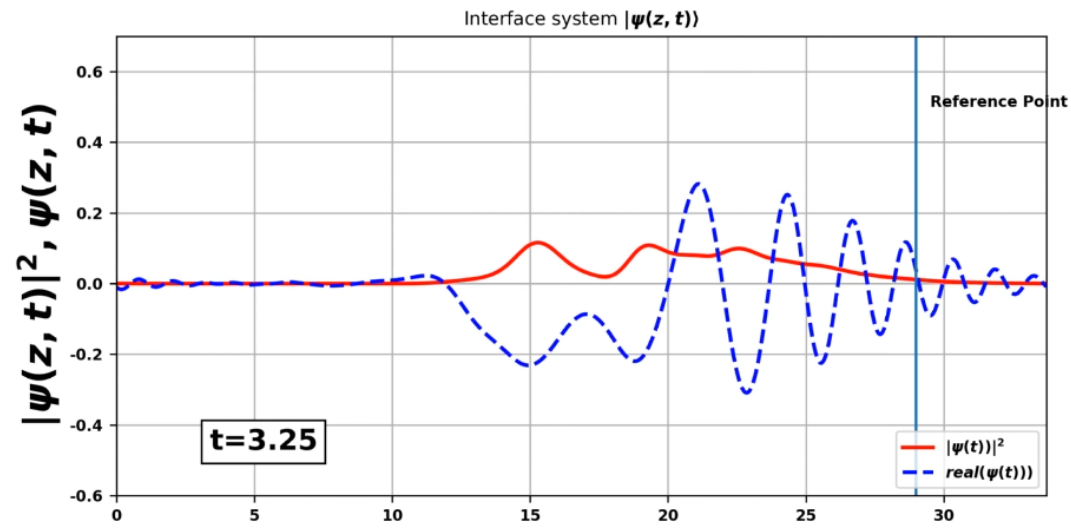
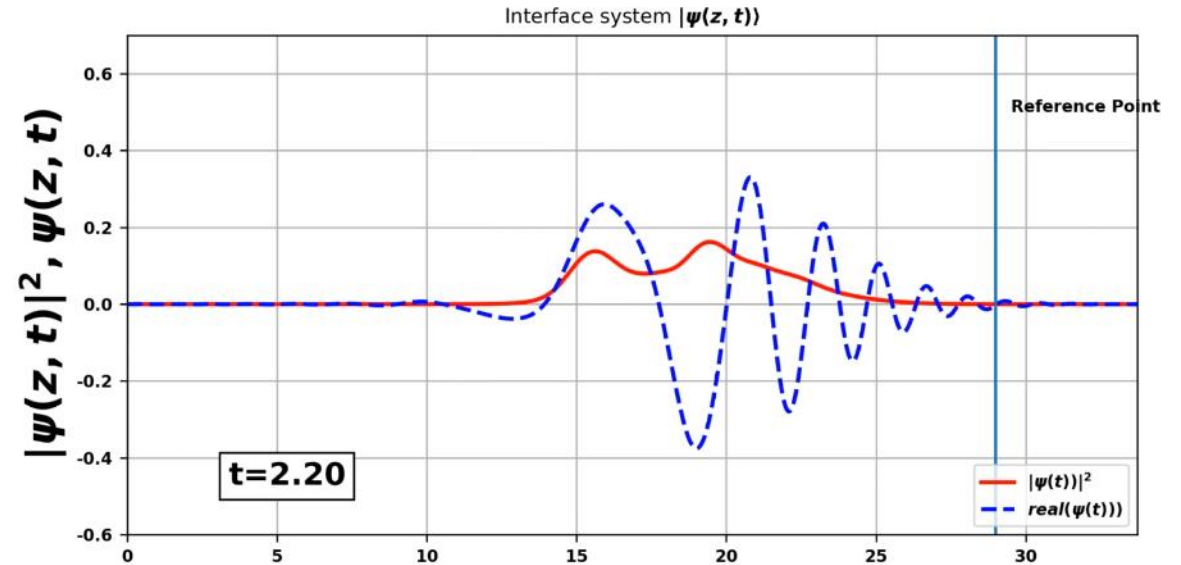
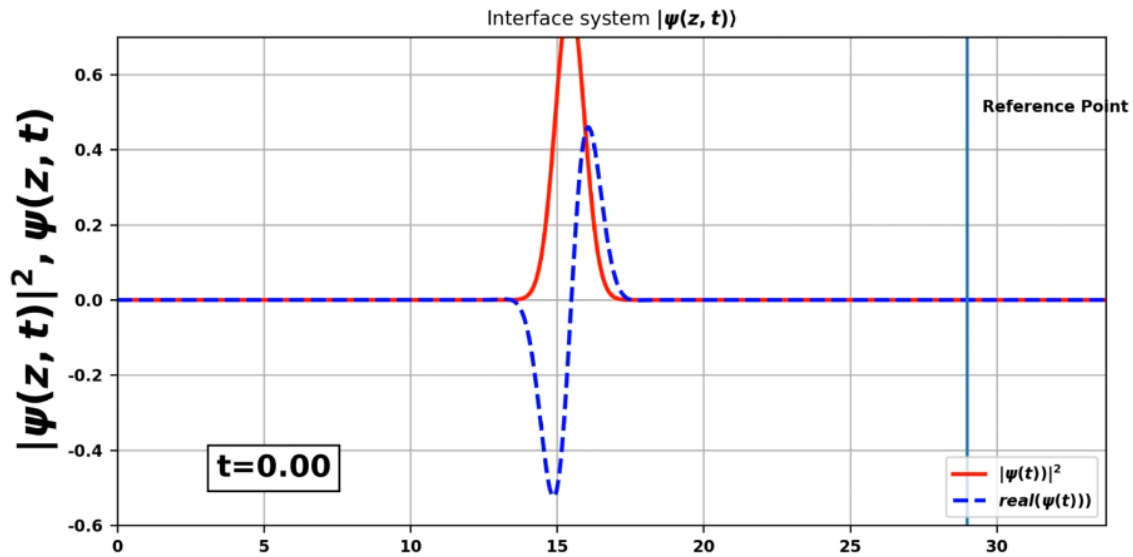




# Cumulative time-dependent Flux

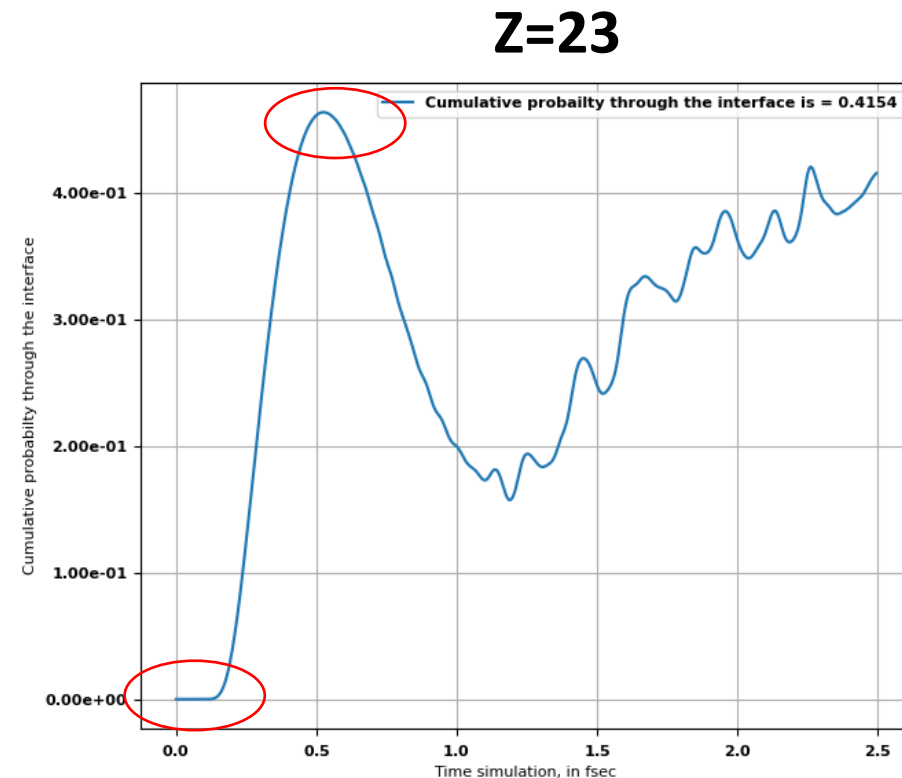
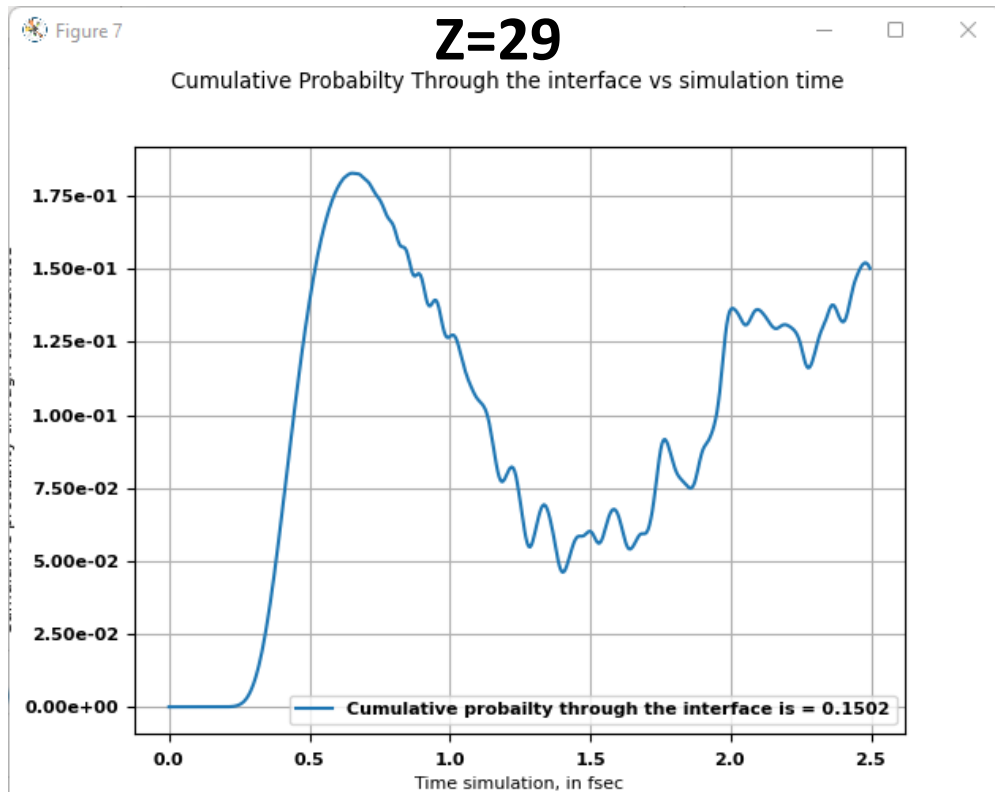
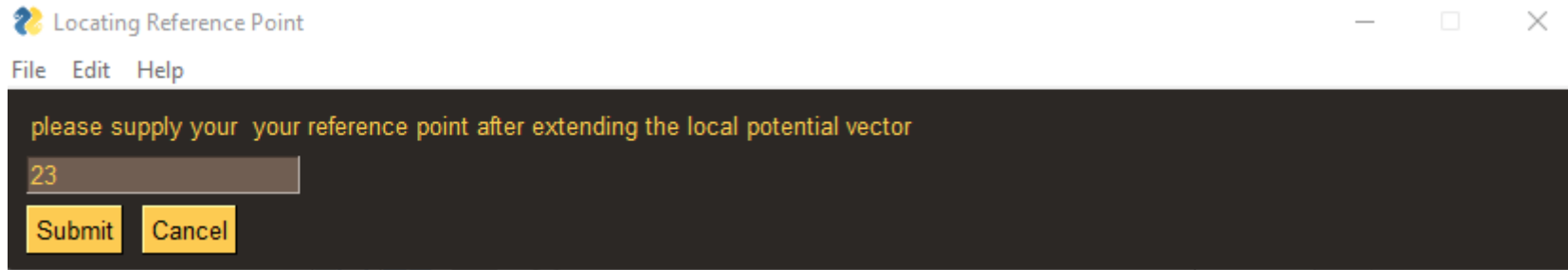


# Watching the movie (checking the file MP4)



# 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.



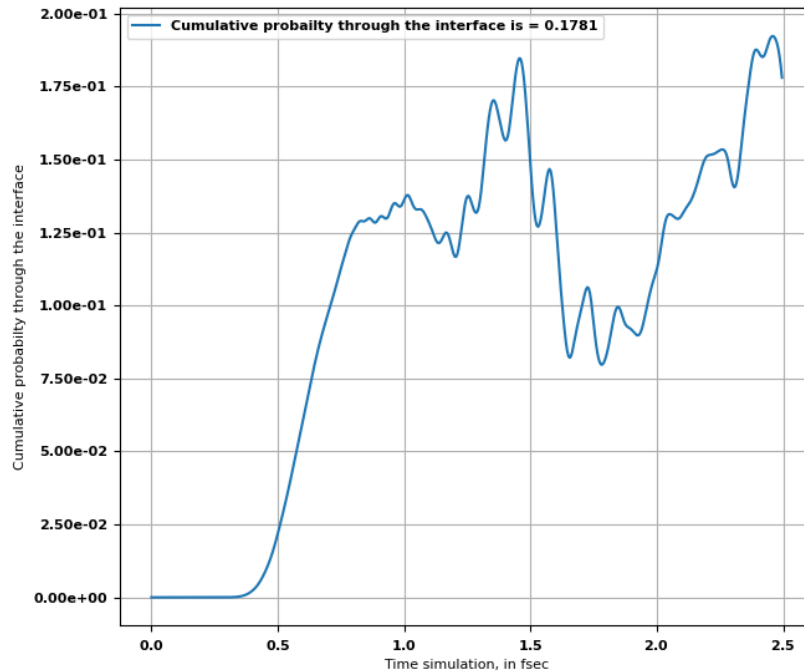
# Comparing between different initial positions

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

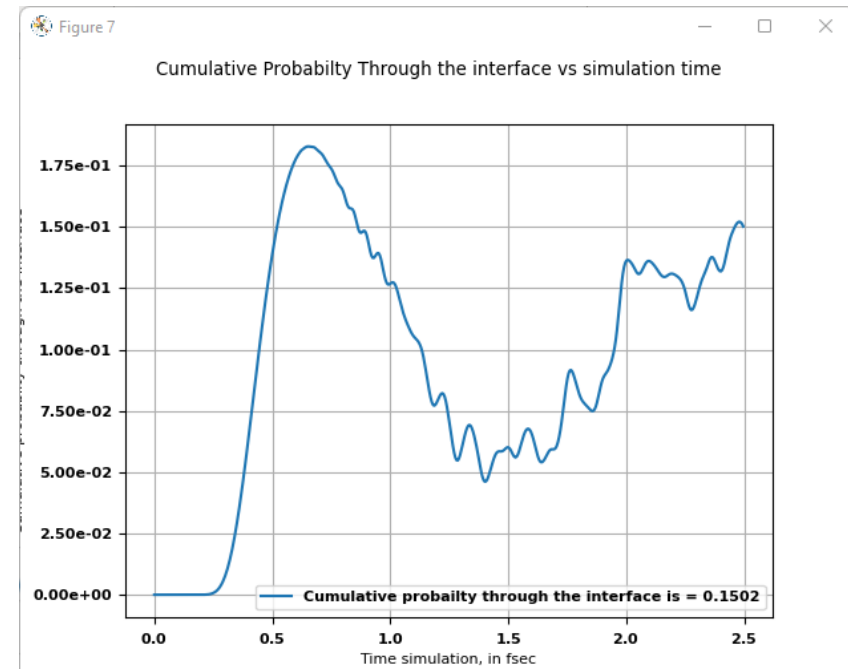
Late and less sharp rise.



$Z_0=9$



$Z_0=15$



# 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

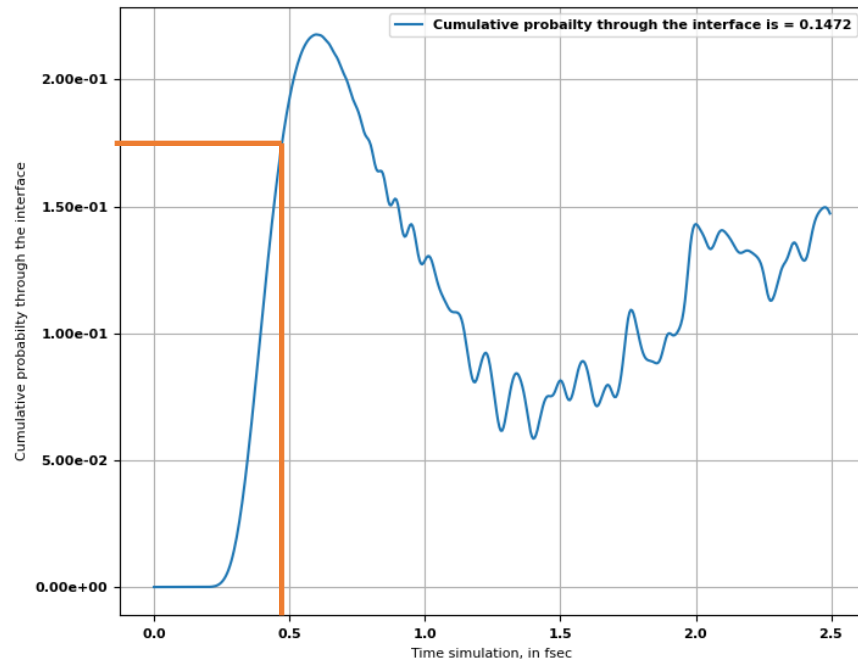
5e-19

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

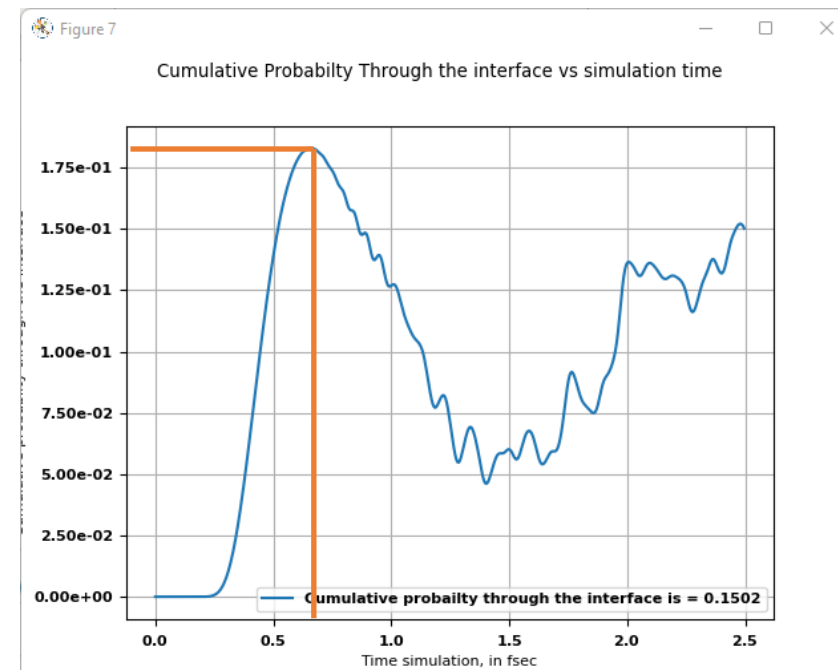
10e-19

- More and faster transmission.

Initial energy 10e-19J



Initial energy 5e-19J

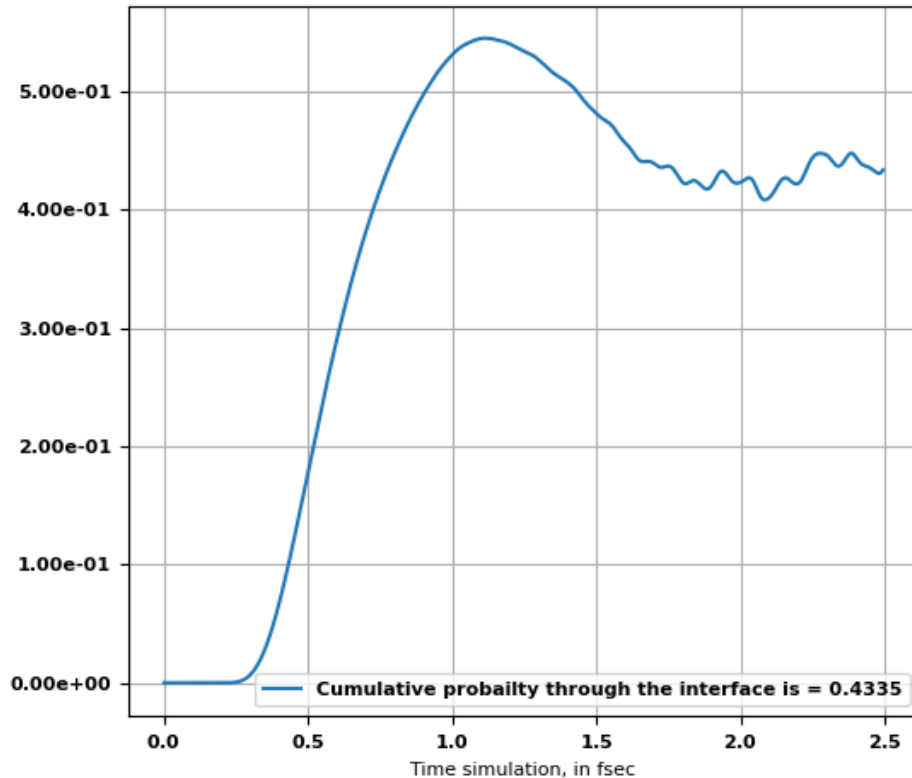


# Comparing between different sizes of potential multiplications

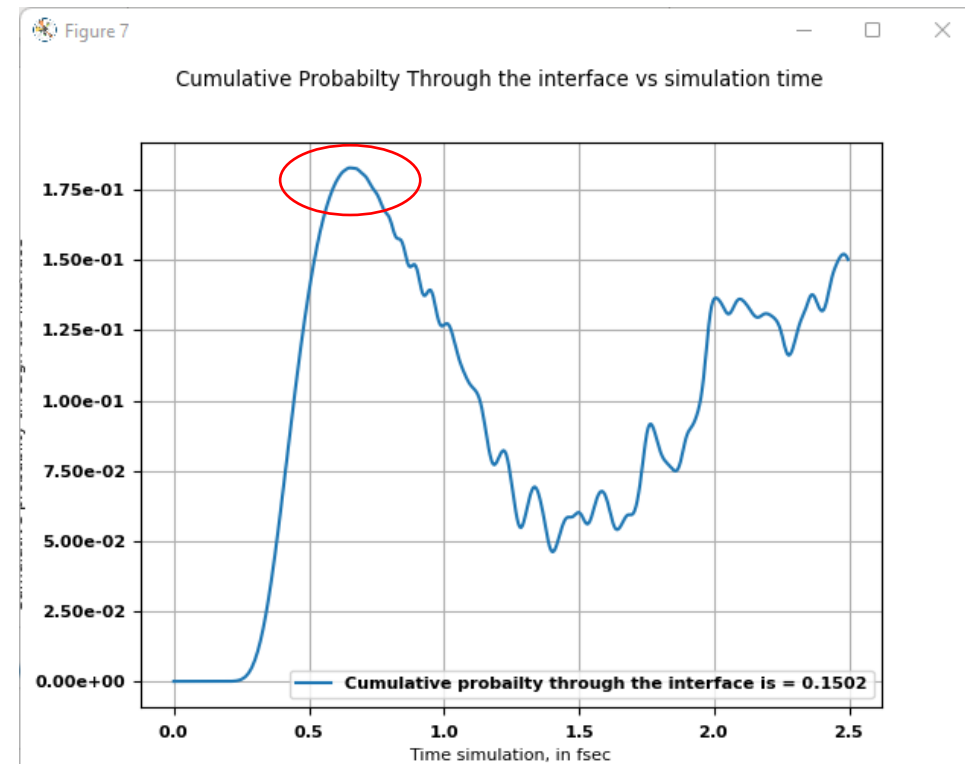
- Multiply the potential 20 times (instead of 10).

Not converged yet, noise scattering from grid edges.

### Multiplied 20



### Multiplied 10

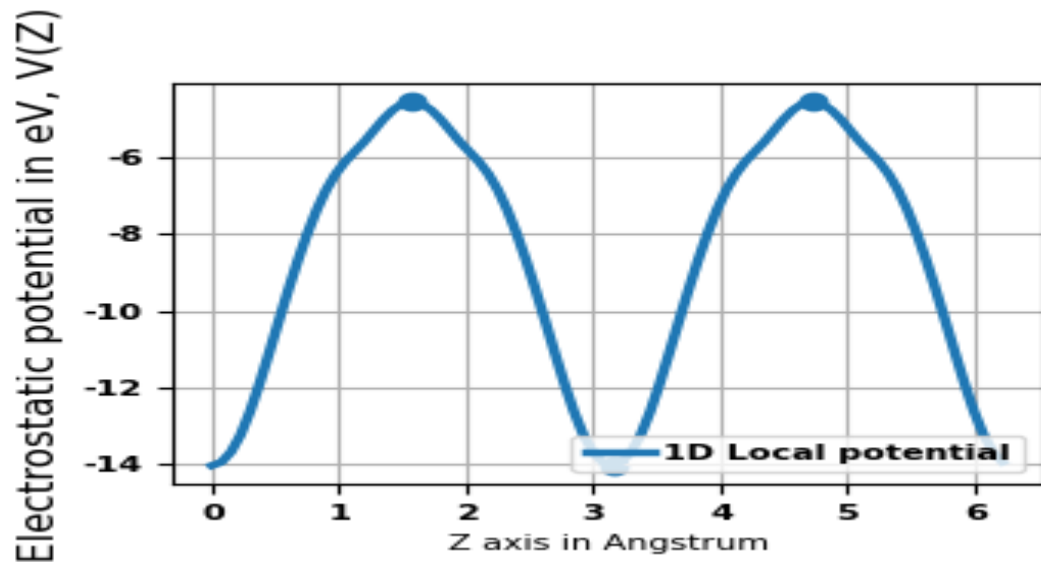


# Comparing between materials

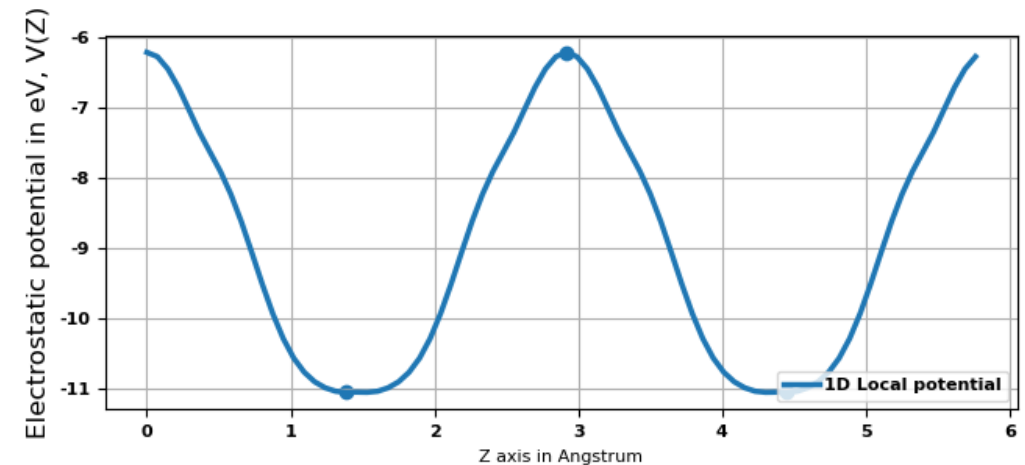
experiment	<a href="http://www.ioffe.ru/SVA/NSM/Semicond/GaAs/electric.html">http://www.ioffe.ru/SVA/NSM/Semicond/GaAs/electric.html</a>	
GaAs	$\leq 8500 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$	
GaSb	$3000 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$	

- 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).

## GaSb

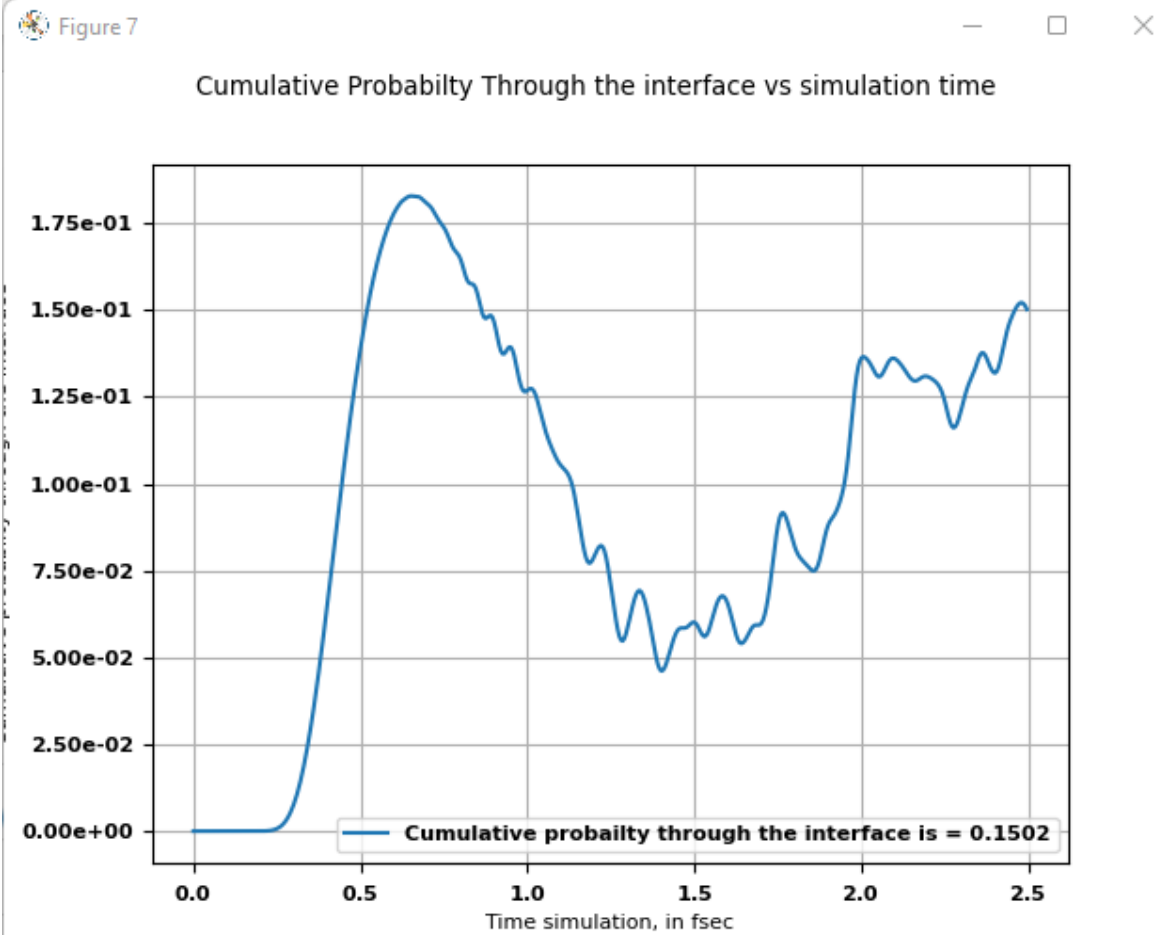
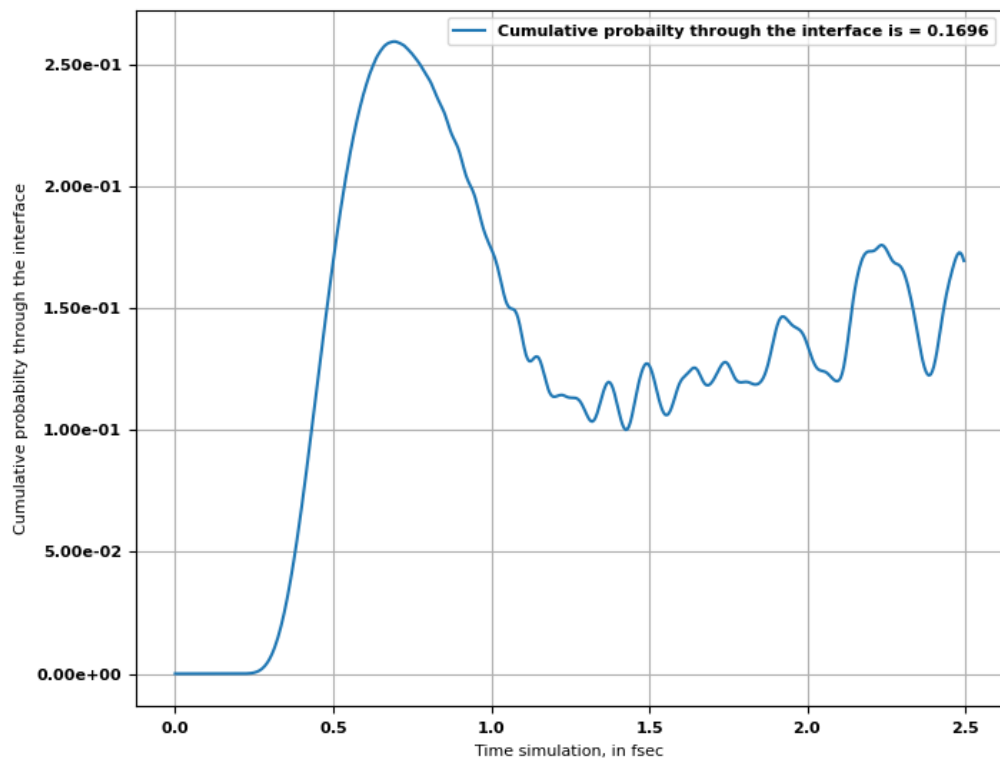


## GaAs



# GaSb

Cumulative Probability Through the interface vs simulation time

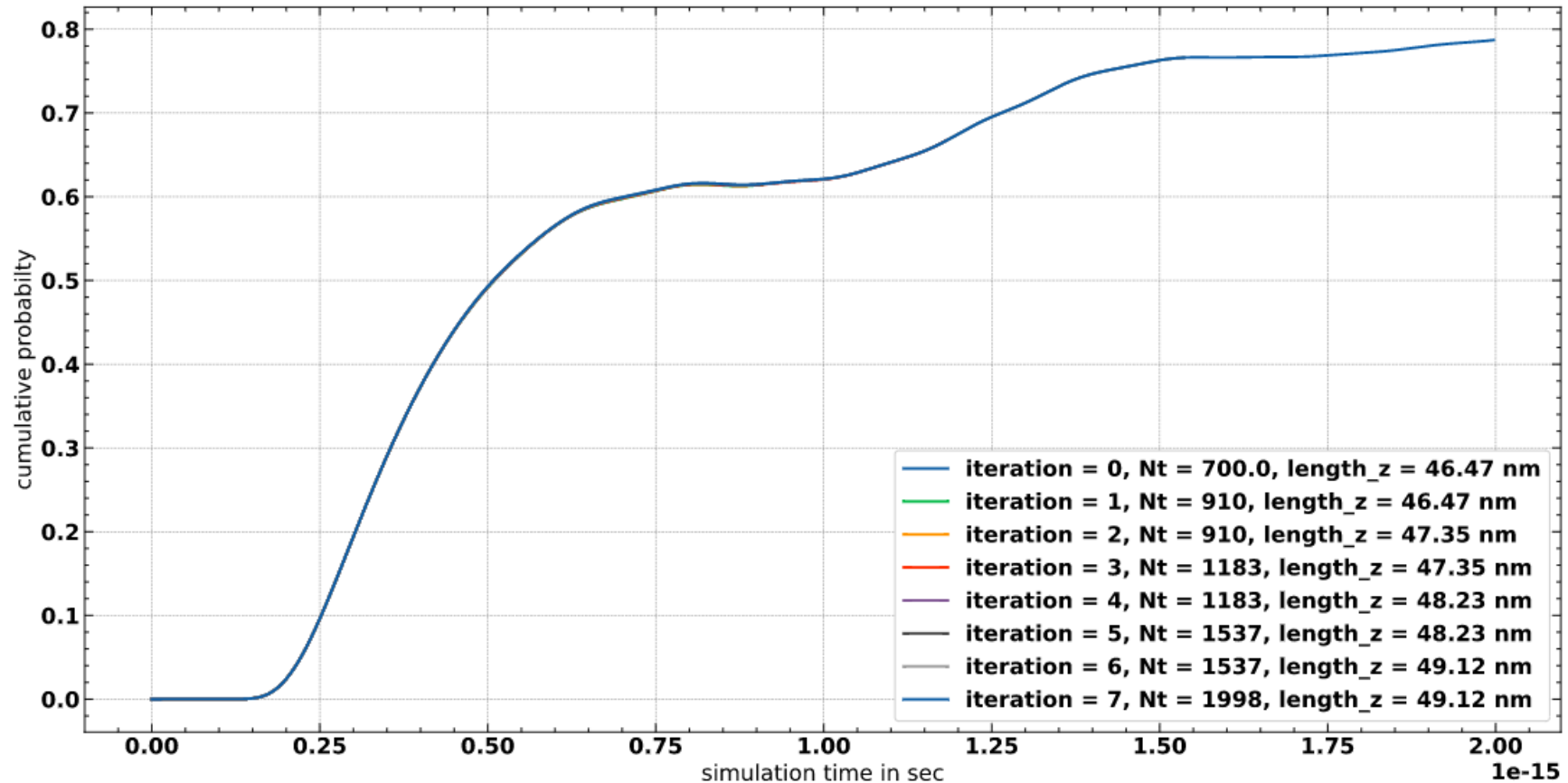




# Examples for convergence tests

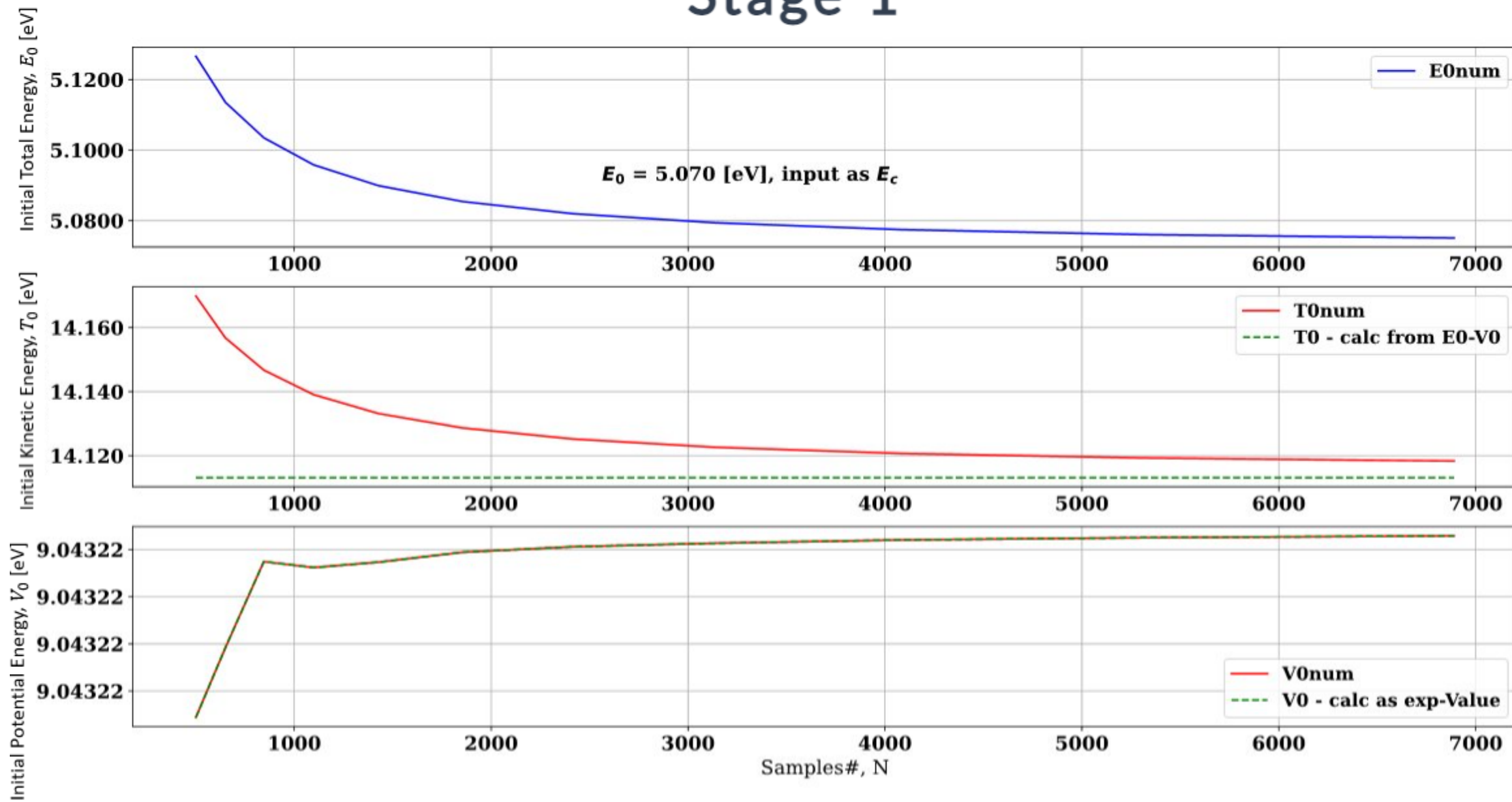
python library implementation

Stage 2 - Simulation time Convergence test



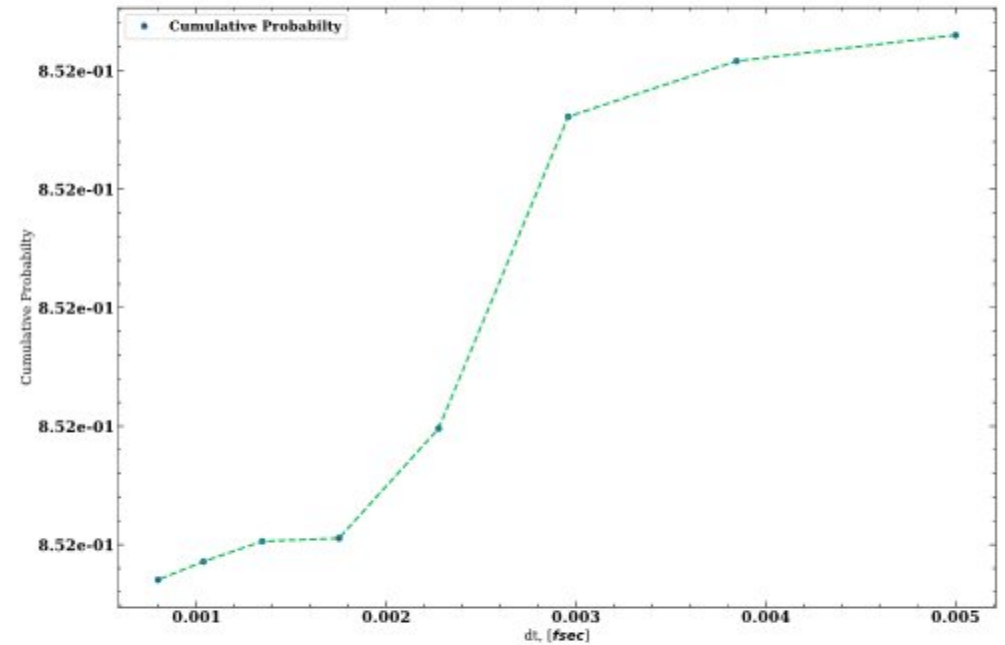
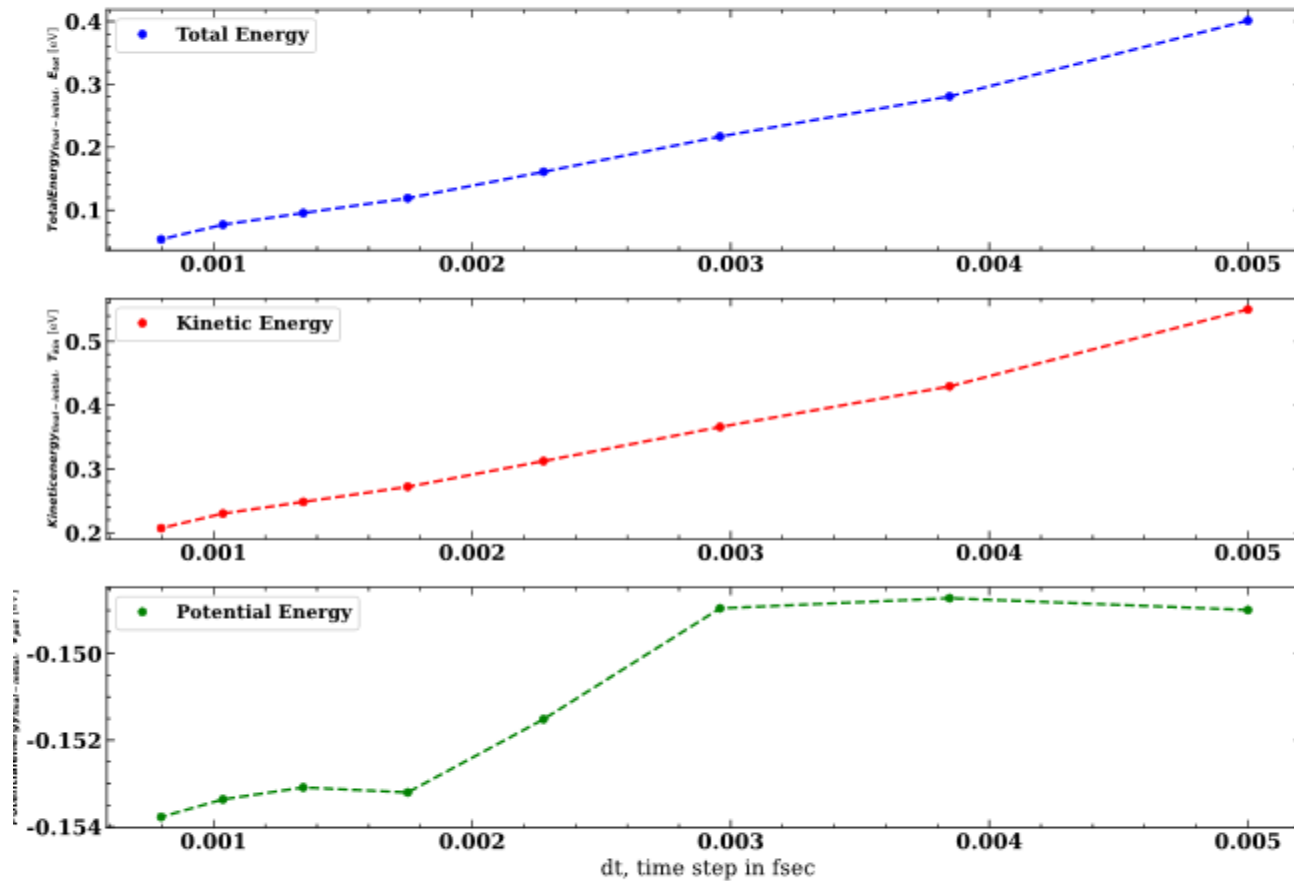
# python library implementation

## Stage 1



# python library implementation

## Stage 2 – time step convergence tests



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

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