User Guide for Particle Velocity and Trajectory Calculator

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4. Overview and Software

This software is a GUI built in Python 3.8.5 meant for calculating the trajectory and velocity of nano/micro-particles.

An installation of python is needed to run the program (<https://www.anaconda.com/products/individual>). I recommend getting the most recent version of python and letting me (Stephen) know if there is anything that doesn’t work, so that I can update it to the newest version.

To run the GUI, I recommend using the Spyder IDE. This comes as part of the Anaconda installation package and will be installed when you install Python, but is not the default. The GUI should still run if you use a different IDE, but I won’t know how to help troubleshoot it if something goes wrong.

1. Operating Procedure

Two things are needed to run the code.

1. The python code (file ending in .py)
2. Gas data from COMSOL (text file)

Once you have these, take the following steps:

1. Open the file in the Spyder IDE and hit run

Graphical user interface, application

Description automatically generated

A GUI will open. Sometimes it will be minimized, and will just show up on the taskbar next to the Spyder icon.



1. In the GUI fill in the your particle and gas properties

Graphical user interface, application

Description automatically generated

NP Diameter: The diameter of your particle or agglomerate.

Material Density: Material density

Agglomerate Density: A fraction used to calculate the density of agglomerates. Set to 100 if measuring speeds for non-agglomerated particles.

File explorer: Click on this to choose the COMSOL gas data file

NP initial axial velocity: Initial velocity of the particle in the direction perpendicular to the substrate

NP initial radial velocity: Initial velocity of the particle in the direction horizontal to the substrate

NP initial axial position: Initial position of the particle in the direction perpendicular to the substrate (NOTE: this is dependent on the geometry set in COMSOL)

NP initial radial position: Initial position of the particle in the direction perpendicular to the substrate

Gas Type: Select He, N2, or Ar

# of timesteps for ODE solver output: Number of individual points used in the output graph. Should be fine to leave as the default.

Total time for ODE solver: Use a short initial guess (.0001 s) and update depending on the result.

Interpolation method: Nearest (fastest, less accurate), linear (fast, good accuracy), cubic (best accuracy, slowest). I usually use linear.

1. Choose an initial guess for ODE solver time and hit ‘Run’

A choose a small initial guess (0.0001 s) and work upwards. You will see the following output on the console in Spyder:

Text

Description automatically generated

Slightly longer than the time given that the particle hits the substrate should be used as the ODE solver time.

If no message is given that the particle hits the substrate, increase the ODE solver time and run again.

1. Output

Once the solver is finished, three windows will appear with the trajectory, radial velocity, and axial velocity.

If you wish to run another particle, close these windows before hitting ‘Run’ in the GUI a second time.

1. Troubleshooting

This will be updated as users run into problems.

If the GUI does not open when you initially run the code:

Go to Tools>Preferences>IPython Consol>Graphics>Graphics backend: Choose Qt4

Re-run the code