Setting up pysrim on Windows

Installing SRIM (1)

- Download SRIM-2013 from the official website (http://www.srim.org/SRIM/SRIMLEGL.htm)

DOWNLOAD SRIM-2013

SRIM-2013 or SRIM-2013 (Professional)

SRIM(Standard) is 10 MB   SRIM(Pro) is 34 MB

SRIM-2013 contains all of the SRIM calculation software. SRIM(Pro) also has about 500 plots of (Experiment/Theory) stopping that shows the accuracy of SRIM. These extra plots are not needed for SRIM calculations.
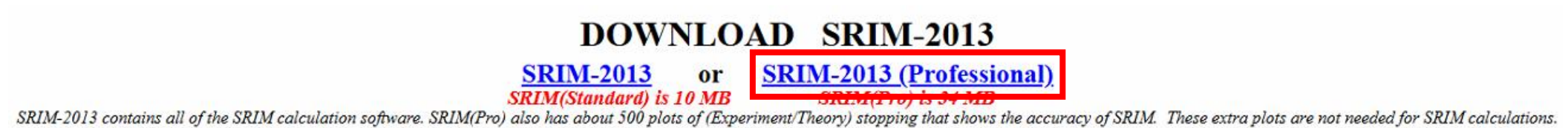
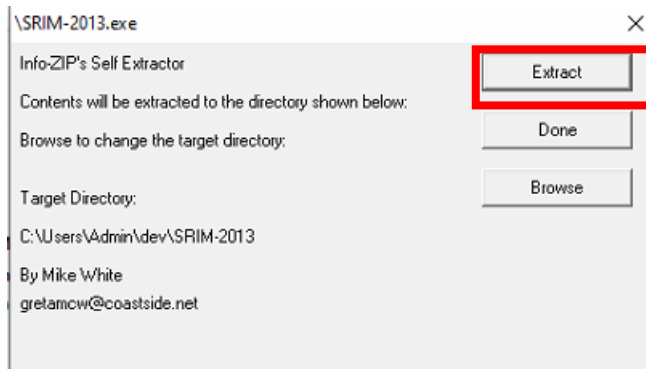- The downloaded file is called SRIM-2013.e

Installing SRIM (2)

- Create a new directory called SRIM-2013
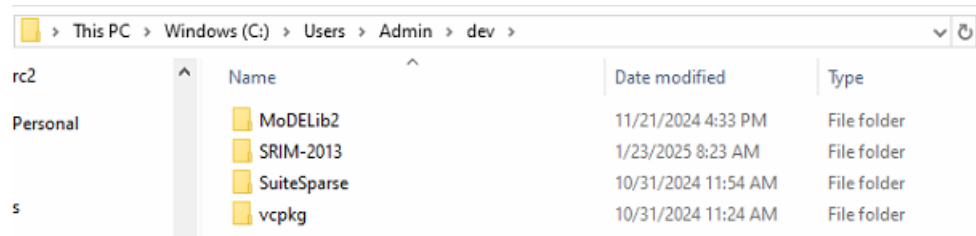
Folder SRIM-2013 has been created in C:/Users/Admin/dev

- Move the previously downloaded .e file to the new directory SRIM-2013

- Change the file name of the .e file to SRIM-2013.exe

- Double click on the .exe file to begin extraction

Extract -> Done

Installing SRIM (3)

- After extracting all files, if installing SRIM for the first time, some additional steps must be taken.

- Go to SRIM-Setup. There should be a file named _SRIM-Setup (Right-Click).bat

- Right click on this file, and "Run as Admistrator". This should open a Command Window. Follow onscreen instructions
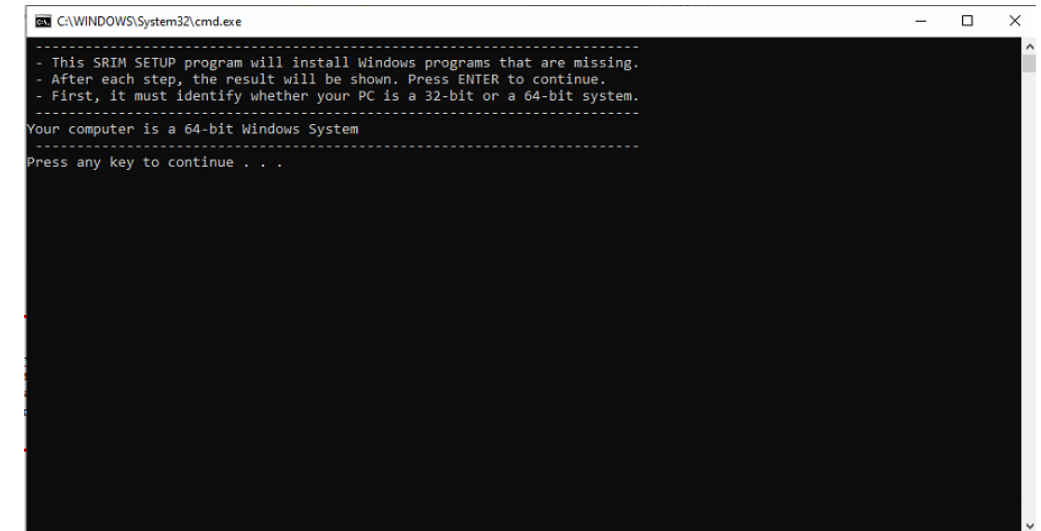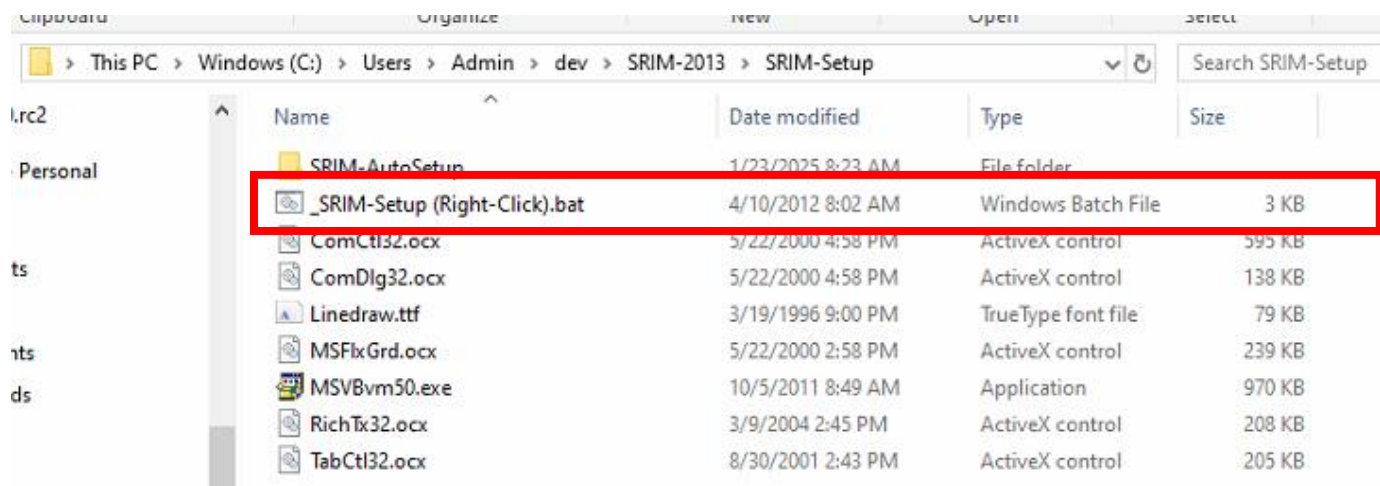
* Instructions are available in _SRIM Setup Message.pdf in the SRIM-2013 directory

Installing PySRIM

- Clone the pysrim repository (https://gitlab.com/costrouc/pysrim/-/tree/master)

- Extract the zipped file
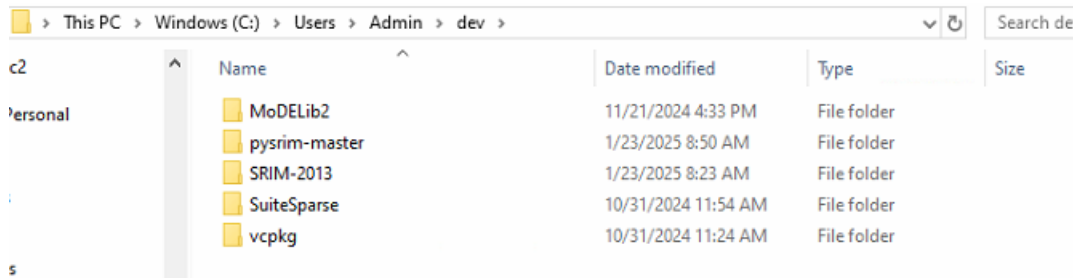
- In the root directory of the repository, open a terminal and run pip install .

Running PySRIM (1)

- Open the pysrim directory using Visual Studio Code

- We will test if everything is working by running a tutorial notebook

- Open the notebook   pysrim-master > examples > notebooks > 📓 Analysis.ipynb

- Specify the path to SRIM in the second code cell

```python
# Construct a 3MeV Nickel ion
ion = Ion('Ni', energy=3.0e6)

# Construct a layer of nick 20um thick with a displacement energy of 30 eV
layer = Layer({
        'Ni': {
            'stoich': 1.0,
            'E_d': 30.0,
            'lattice': 0.0,
            'surface': 3.0
        },
}, density=8.9, width=20000.0)

# Construct a target of a single layer of Nickel
target = Target([layer])

# Initialize a TRIM calculation with given target and ion for 25 ions, quick calculation
trim = TRIM(target, ion, number_ions=500, calculation=1)

# Specify the directory of SRIM.exe
# For windows users the path will include C://...
# The directory must have SRIM 2013 installed. TRIM.exe should be in this folder
srim_executable_directory = 'C:/Users/Admin/dev/SRIM-2013'

# takes about 10 seconds on my laptop
results = trim.run(srim_executable_directory)
# If all went successfull you should have seen a TRIM window popup and run 25 ions!
```

Tutorial

Make sure that you have done a proper installation of pysrim and SRIM

This means that you have SRIM 2013 installed. **NOT 2018**.

In this tutorial we will cover:

- running a TRIM calcualtion
- running a SR calculation
- analyzing TRIM calculation output files

Most emphasis will be put on what is possible for analysis of SRIM calcualtions.

We will assume **python3** for this notebook.

```python
%matplotlib inline

import os
from pprint import pprint

# Only needed to embed the images in notebook
from IPython.display import Image

import numpy as np
import matplotlib.pyplot as plt

from srim import TRIM, SR, Ion, Layer, Target
from srim.output import Results
```

[3]   ✓ 0.5s

Run a SRIM Calculation

Running a srim calculation is much like the gui that SRIM provides.

Running PySRIM (2)

- If everything has been installed correctly, we should see a pop up TRIM window when the second code cell is executed