

SiREM Fitting Python Code Quickstart Guide

Step 1: Download Anaconda

1. Follow the link to: <https://docs.anaconda.com/anaconda/install/index.html>

2. Click **Installing on Windows**

3. Click **Download the Anaconda Installer**

4. Click **Download** →



For Windows

Python 3.9 • 64-Bit Graphical Installer • 621 MB

Get Additional Installers

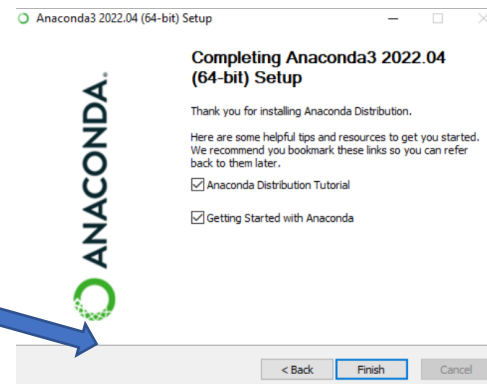
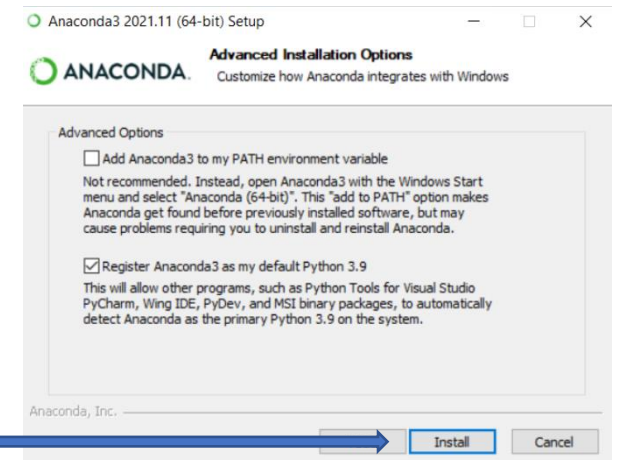
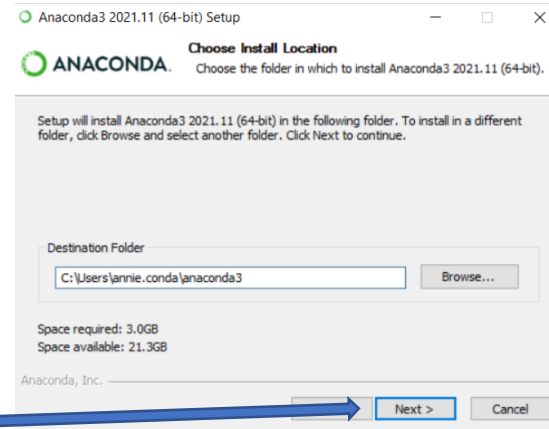


Step 2: Install Anaconda

1. Once the download is complete, navigate to your downloads folder and double-click the installer to launch
2. Install for **Just Me**
3. Click **Next**
4. Confirm that the destination folder matches this format:
C:\Users\{your username}\anaconda3
5. Click **Next**
6. Accept default advanced options and click **Install**
7. Click **Next**
8. After installation (may take a few minutes) click **Next** twice. You will see the following dialogue box. Select **Finish**

Anaconda is now installed! Move to Step 3

<input type="checkbox"/> Name	Date modified	Type	Size
Today (1)			
<input checked="" type="checkbox"/> Anaconda3-2022.10-Windows-x86_64 (1)	11/17/2022 9:38 AM	Application	636,133 KB




Step 3: Download and Install Visual Studio Code

1. Follow the link to: <https://code.visualstudio.com/docs/setup/windows>

2. Click **Visual Studio Code installer**

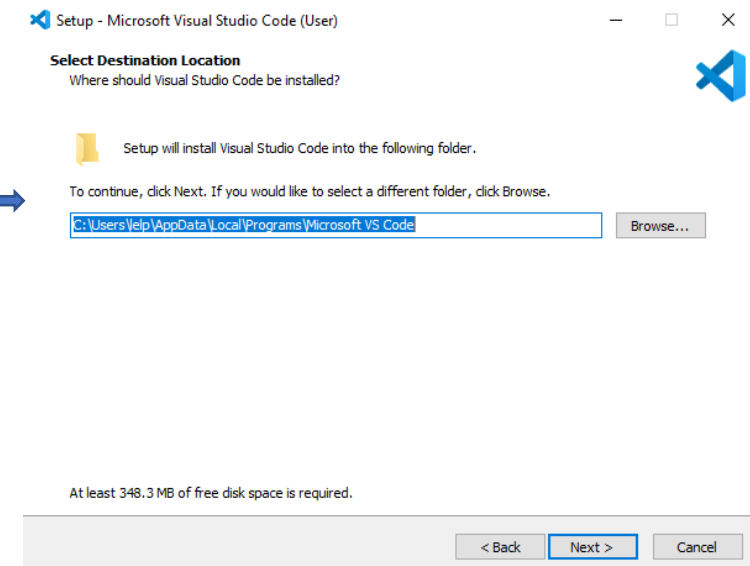
3. Navigate to your downloads folder and double-click the installer to launch



<input type="checkbox"/> Name	Date modified	Type	Size
▼ Today (1)			
<input checked="" type="checkbox"/> VSCodeUserSetup-x64-1.73.1 (3)	11/17/2022 10:22 AM	Application	90,429 KB

4. Accept the agreement and click **Next**

5. Accept default installation path
C:\Users\{yourusername}\AppData\Local\Programs\Microsoft VS Code
and click **Next**



6. Accept default Start Menu Folder setup and click **Next**

7. Accept default Additional Tasks and click **Next**

8. Click **Install**

9. Click **Finish**

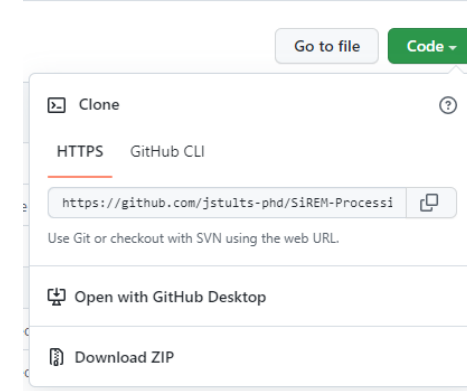
10. Visual Studio Code may open automatically after installation. We will return to this in Step 5

Step 4: Download and Extract SiremFitting Code

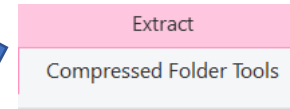
1. Follow the link to: <https://github.com/jstults-phd/SiREM-Processing>

2. Click the green **Code** button

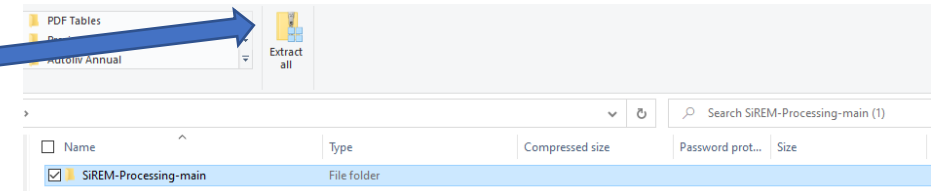
3. Click **Download ZIP**



4. Navigate to your downloads folder, select SiREM-Processing-main, click **Extract**

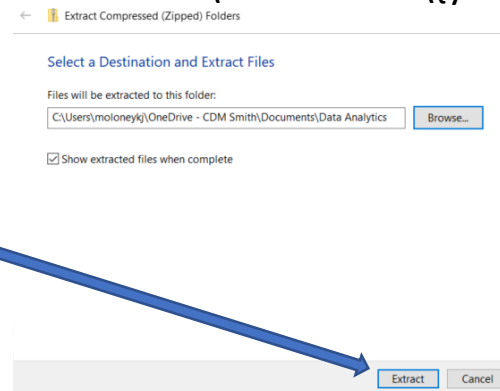


5. Click **Extract all**



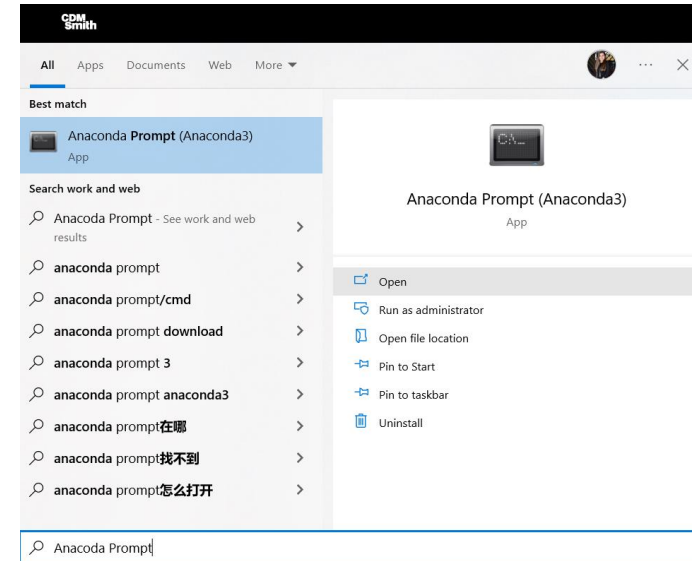
6. The default setting is to extract to your downloads. DO NOT select this. Instead, select the following folder destination
C:\Users\{your username}\OneDrive – CDM Smith\Documents\{your folder name}

7. Click **Extract**



Step 5. Install Required Packages

1. Open Anaconda Prompt by searching in taskbar and clicking **Open**



The following line of code will appear: (base)

C:\Users\{your username}












2. Type ">cd OneDrive – CDM Smith" and press enter
3. Type ">cd Documents" and press enter
4. Type ">cd {your folder name}" and press enter
5. Type ">cd SiREM-Processing-main" and press enter
6. Type >conda install - - yes - - file requirements.txt to install packages



A screenshot of the Anaconda Prompt terminal window. The window title is 'Anaconda Prompt (Anaconda3)'. The terminal shows the following commands and their output:



```
(base) C:\Users\{your username}>cd OneDrive - CDM Smith
(base) C:\Users\{your username}\OneDrive - CDM Smith>cd Documents
(base) C:\Users\{your username}\OneDrive - CDM Smith\Documents>cd {your folder name}
(base) C:\Users\{your username}\OneDrive - CDM Smith\Documents\{your folder name}>cd SiREM-Processing-main
(base) C:\Users\{your username}\OneDrive - CDM Smith\Documents\{your folder name}\SiREM-Processing-main>conda install - - yes - -file requirements.txt
```

Step 6. Open SiREM Fitting Code in Visual Studio Code

1. In file explorer, navigate to C:\Users\{your username}\OneDrive – CDM Smith\Documents\{your folder name}\SiREM-Processing-main
2. Click siremFitting Jupyter Source File and click Open

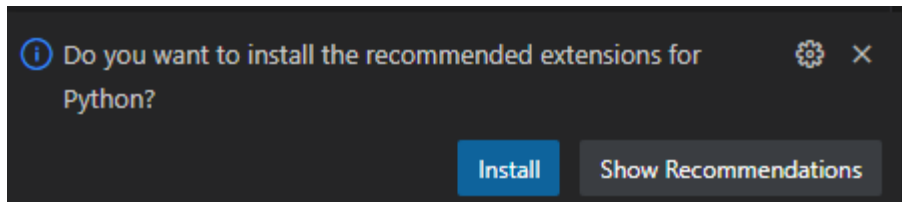
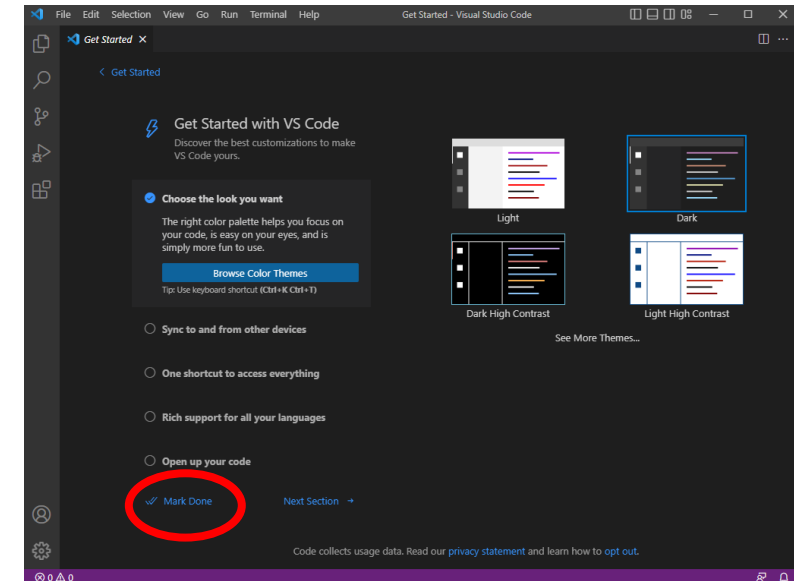
	input		11/17/2022 11:40 AM	File folder	
	output		11/17/2022 11:40 AM	File folder	
	LICENSE		11/17/2022 11:40 AM	File	7 KB
	README		11/17/2022 11:40 AM	Markdown Source File	3 KB
	requirements		11/17/2022 11:40 AM	Text Document	1 KB
	siremFitting		11/17/2022 11:40 AM	Jupyter Source File	58 KB

 siremFitting

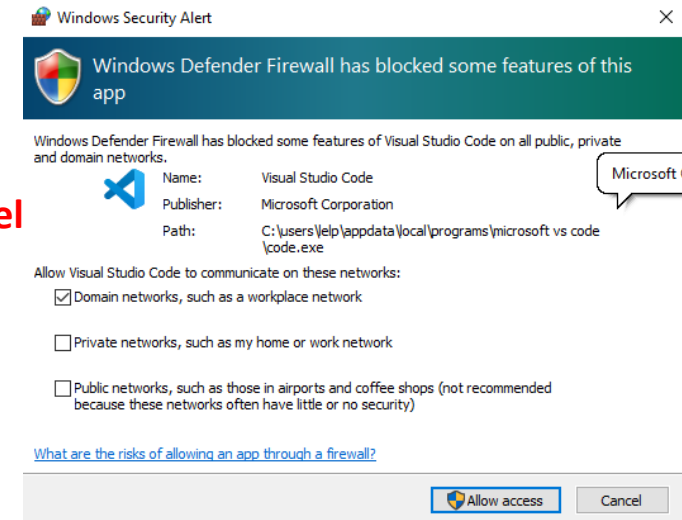
 Open
 Open with Code

Step 7: Set up Visual Studio Code

1. Visual Studio Code should open automatically
2. Complete “Get Started with VS Code” walkthrough and click **Mark Done**
3. A pop-up will appear asking to install the recommended extensions for Python. Click **Install**

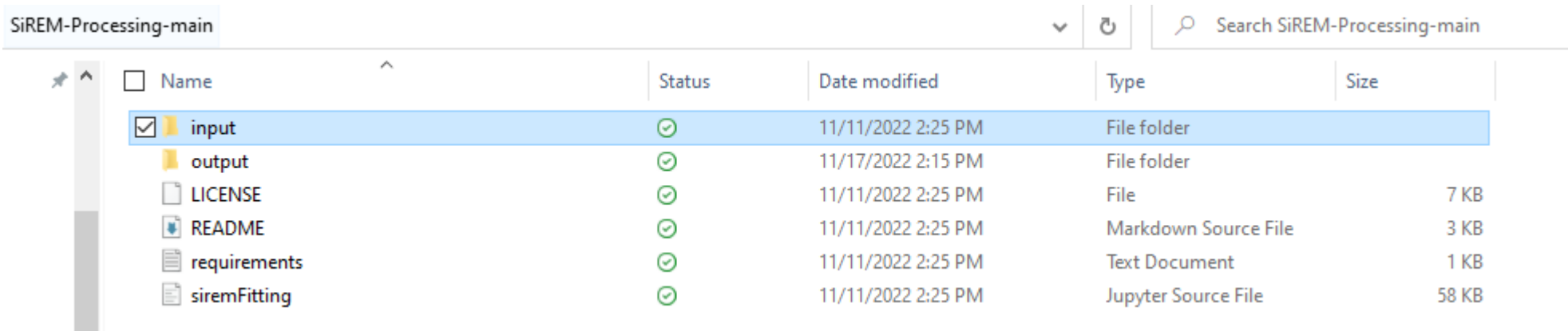


4. A Windows Defender Firewall pop-up may appear. If so, click **Cancel**



Step 8. Check input folder files

1. Check input folder for test Data excel file
2. If using different data, save input data into the input folder as an .xlsx excel file at file path
C:\Users\{your username}\OneDrive – CDM Smith\Documents\{your folder name}\SiREM-Processing-main\input



Name	Status	Date modified	Type	Size
<input checked="" type="checkbox"/> input	✓	11/11/2022 2:25 PM	File folder	
<input type="checkbox"/> output	✓	11/17/2022 2:15 PM	File folder	
<input type="checkbox"/> LICENSE	✓	11/11/2022 2:25 PM	File	7 KB
<input type="checkbox"/> README	✓	11/11/2022 2:25 PM	Markdown Source File	3 KB
<input type="checkbox"/> requirements	✓	11/11/2022 2:25 PM	Text Document	1 KB
<input type="checkbox"/> siremFitting	✓	11/11/2022 2:25 PM	Jupyter Source File	58 KB

Step 9. Check input/output files

1. Check second block of code, change folder or file names as needed to match your input naming scheme

```
# *** Specify directories files for input and output *** #
openDir = 'input'
saveDir = 'output\\'

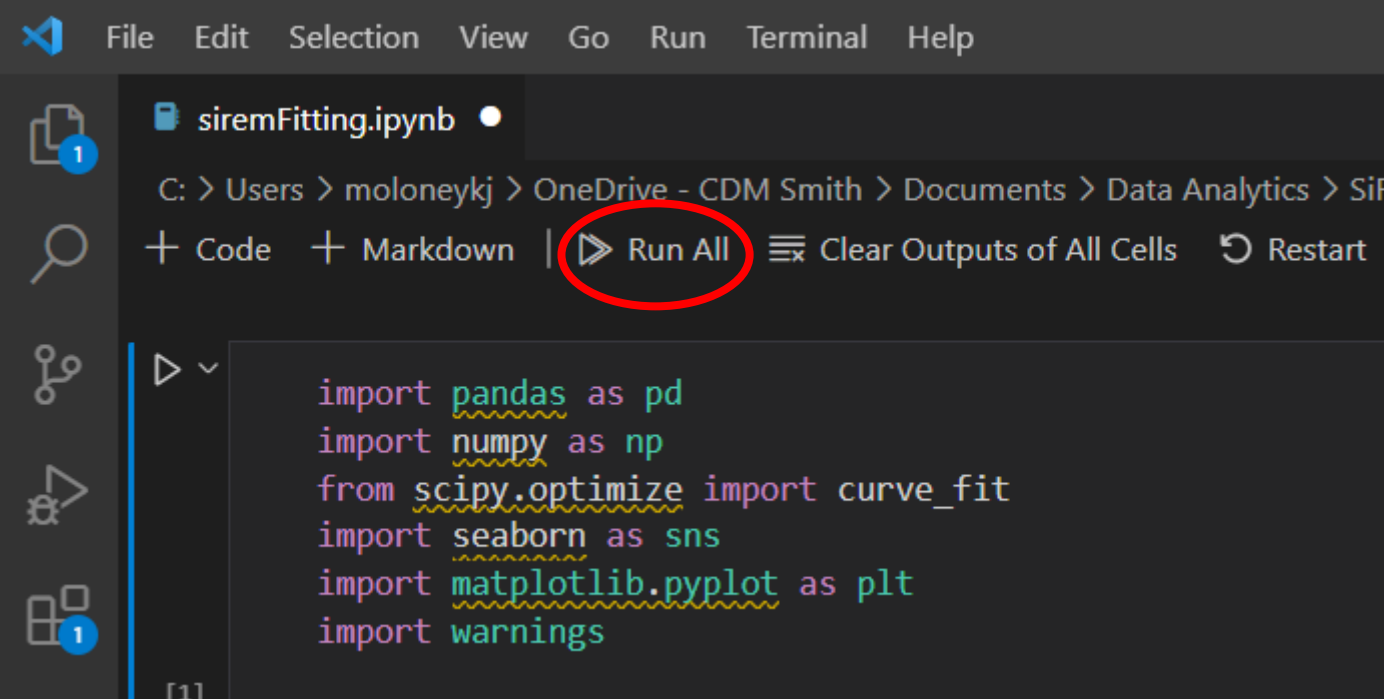
saveCal = 'testCalCurve.xlsx'
saveStds = 'testStandardsCalc.xlsx'
saveSam = 'testSamplesCalc.xlsx'
# *** End directories /files for input and output *** #
```

2. Check excel file names in third block of code, change file or sheet names as needed to match your input data .xlsx file

```
# *** Specify excel for input *** #
refs = pd.read_excel(openDir + '\\testInputData.xlsx', sheet_name='sampleRef')
stds = pd.read_excel(openDir + '\\testInputData.xlsx', sheet_name='standards')
samples = pd.read_excel(openDir + '\\testInputData.xlsx', sheet_name='samples')
chemRef = pd.read_excel(openDir + '\\testInputData.xlsx', sheet_name='chemRef')
# *** End Specify excel for input *** #
```

Step 10. Run Code

1. Click **Run All** at top left of screen
2. This will take a few seconds to process



The screenshot shows a Jupyter Notebook interface with a dark theme. The top menu bar includes 'File', 'Edit', 'Selection', 'View', 'Go', 'Run', 'Terminal', and 'Help'. Below the menu, the file name 'siremFitting.ipynb' is displayed. The file path is shown as 'C: > Users > moloneykj > OneDrive - CDM Smith > Documents > Data Analytics > Si'. The toolbar contains icons for '+ Code', '+ Markdown', a 'Run All' button (a right-pointing triangle), 'Clear Outputs of All Cells', and 'Restart'. The 'Run All' button is circled in red. Below the toolbar, a code cell is visible with the following Python code:

```
import pandas as pd
import numpy as np
from scipy.optimize import curve_fit
import seaborn as sns
import matplotlib.pyplot as plt
import warnings
```

The cell is labeled '[1]' at the bottom left.

Step 11. Check output folder for results

1. In file explorer, navigate to
C:\Users\{your username}\OneDrive – CDM Smith\Documents\{your folder name}\SiREM-Processing-main\output

:essing-main					
Search SiREM-Processing-main					
<input type="checkbox"/>	Name	Status	Date modified	Type	Size
<input type="checkbox"/>	input	✓	11/11/2022 2:25 PM	File folder	
<input checked="" type="checkbox"/>	output	✓	11/17/2022 2:01 PM	File folder	
<input type="checkbox"/>	LICENSE	✓	11/11/2022 2:25 PM	File	7 KB
<input type="checkbox"/>	README	✓	11/11/2022 2:25 PM	Markdown Source File	3 KB
<input type="checkbox"/>	requirements	✓	11/11/2022 2:25 PM	Text Document	1 KB
<input type="checkbox"/>	siremFitting	✓	11/11/2022 2:25 PM	Jupyter Source File	58 KB

2. Click output subfolder
3. See results as shown below



	S1_calibration	✓	11/17/2022 2:15 PM	PNG File	79 KB
	S2_calibration	✓	11/17/2022 2:15 PM	PNG File	70 KB
	S3_calibration	✓	11/17/2022 2:15 PM	PNG File	72 KB
	testCalCurve	✓	11/17/2022 2:15 PM	Microsoft Excel Worksh...	6 KB
	testSamplesCalc	✓	11/17/2022 2:15 PM	Microsoft Excel Worksh...	8 KB
	testStandardsCalc	✓	11/17/2022 2:15 PM	Microsoft Excel Worksh...	9 KB