**Installation Instructions for Windows Users**

We promote the use of Python through the Anaconda open data science platform. We are aware that other installation methods exist, but have solely included the Anaconda installation instructions below due to the ease of setup and use in a classroom environment:

1. In order to download Anaconda for Windows, navigate to the following webpage: <https://www.continuum.io/downloads>
2. In the section labeled “Anaconda for Windows”, there are installers for Python 2.7 and Python 3.5. The Schrodinger.py program is written for Python 2.7 and 3.5. *While you may want to install both versions of Python for personal use, the following instructions are provided for version 2.7 only.*
3. In the box labeled “Python 2.7”, click on the blue box labeled “WINDOWS 64-BIT GRAPHICAL INSTALLER.” *If you are using Windows 32-bit, the graphical installer is provided in smaller print below the 64-bit installer.*
4. Upon clicking the installer, you will notice a dialog box appear at the bottom of your web browser, indicating the download progress. Once finished, click the executable to begin the installation. If a dialog box does not appear, navigate to the downloads folder from the desktop or windows key, and double click the executable to begin installation.
5. Upon double clicking the executable, the Anaconda 64-bit Setup Wizard will open. Click “Next” to continue.
6. Click “I Agree” to accept the license agreement.
7. Select “Just Me” as the installation type. This will complete the installation without requiring administrative privileges.
8. Next, you will be prompted to select an installation location. Here, it is most likely that the default location is suitable. For example, the destination folder that we selected was **C:\Users\Username\Anaconda2**.
9. You will then be prompted for two installation options (add Anaconda to my PATH environment variable and Register Anaconda as my default Python 2.7). We advise that both these boxes are checked before proceeding.
10. Click “Install”. The installation process will take some time, please be patient.
11. Upon installation, several executables are generated. In order to find these executables, open Windows’ File Explorer and navigate to the installation location directory you specified in step 8 above. Upon locating this “Anaconda2” folder, you will find a subfolder called “Menu”. This folder contains all the executables that you will utilize for running Python programs or IPython notebooks. We advise copying the important executables as shortcuts to your desktop so that they are easier to access. The executables you will use most frequently are: IPython, Jupyter Notebook, Anaconda Prompt, and Spyder.
12. Once you have created shortcuts for the above executables, open the Anaconda Prompt. Upon opening, the prompt will appear similar to Windows Command Prompt. You will notice the path of your installation location from step 8 to the left of the Anaconda Prompt, followed by a cursor.
13. In the Anaconda prompt, type **conda update conda**.
14. A list of packages to be downloaded will appear and you will be asked to proceed [yes/no]. Select yes to begin the download.
15. Following the download, you will also need to manually install the numpy, scipy, matplotlib, and colorama packages. In order to install each of these, use the following example for formatting purposes: **conda install numpy.** After typing each install command once, type the same command a second time to assure that the package is correctly installed. If installed, you will receive the following message upon typing the install command a second time: “All requested packages already installed.”
16. Within the Python\_Files folder (where you found this installation instructions document), you will also find the Schrodinger.py, utils2.py, and utils3.py Python programs (for running in an Anaconda Prompt or via Windows Command Prompt), the Cases1-6.ipynb IPython notebooks (for instructor use in classrooms), and a file named **jupyter\_notebook\_config.py**
17. Using Windows File Explorer, navigate to the directory that contains the Anaconda2 folder from step 8 above. In the same directory as the Anaconda2 folder, you will find another folder named **.jupyter**. In this folder, you must place the **jupyter\_notebook\_config.py** file mentioned in step 16.
18. We also advise that you create a folder on your desktop called **Schrodinger** to place the Schrodinger.py, utils2.py, utils3.py Python programs as well as the Case1-6.ipynb IPython notebooks (for instructor use in classrooms).
19. Next, open an Anaconda Prompt and navigate to the Schrodinger desktop folder that you just created in step 18. In order to navigate directories using the Anaconda Prompt, the following Windows Command Prompt keystrokes should be utilized:

* **dir** = list files in your current directory
* **cd** = change directory (in order to use the **cd** command, you must first type **cd** followed by a **space**, followed by the **name** of the folder or directory you wish to navigate to)
* **cd ..** = move back one folder level

As an example, when you open your Anaconda Prompt, the default folder should be identical to what you declared in step 8 above (**C:\Users\Username\Anaconda2)**. If this is the case, you will simply type **cd Desktop\Schrodinger** to navigate to the Schrodinger folder on the desktop that you created in step 18.

1. Once you’ve navigated to the Schrodinger folder via the Anaconda Prompt, type **jupyter notebook** in the Anaconda Prompt. This will open jupyter in your default web browser. When the default web browser opens, you should see the Schrodinger.py (Python program) and the Cases1-6.ipynb (IPython notebook) documents. Double click on one of the Case.ipynb files to open the IPython notebook.
2. With the notebook open, users are encouraged to examine the options at the top of the web browser. Most importantly, the user should focus on the “play” button in the top panel, which can be used to run each cell in the IPython notebook. The IPython notebooks are broken down into sections of **markdown** (text that explains the Schrodinger program or theory/math behind the program) and **code** (Python commands that carry out the mathematics discussed in the manuscript). When using the notebook, users should progress through the cells of the notebook one-by-one and press the play button for each cell. This will update the screen of any changes and also prompt the user for any input that the program requires. In the edit tab of the top panel, users also have the option to **run all cells**. If the user updates markdown text or Python code, they must remember to press the play button to update the screen of those changes. In some instances, the user might need to begin at the beginning of the notebook and re-play all the cells again, or simply use the **run all cells** function.
3. When finished, the IPython notebook should be closed. However, the main jupyter web browser will remain open and the IPython notebook will show **Running** in green. Click on the green **Running** and an option will appear to **Shutdown** the notebook. Click **Shutdown** before closing the main jupyter notebook web browser. Last, press CTRL+C in the Anaconda Prompt to terminate the juptyer notebook process.
4. If users wish to simply run the Schrodinger.py program in the Anaconda Prompt (without the use of the IPython notebook), repeat step 19 above. Once you’ve navigated to the desktop folder containing the Schrodinger.py program, type **python** **Schrodinger.py**. Here, the program will run in the Anaconda window with various user input prompts. When running in the Anaconda prompt, users must first edit the **matplotlibrc** file in their working directory. Within this file, windows users should uncomment (remove the # symbol) the windows backend line and also comment out (add a # symbol at beginning of line) the macosx backend line.

**Installation Instructions for OSX Users**

1. In order to download Anaconda for OSX, navigate to the following webpage: <https://www.continuum.io/downloads>
2. In the section labeled “Anaconda for OSX”, there are installers for Python 2.7 and Python 3.5. The Schrodinger.py program is written for Python 2.7 and 3.5. *While you may want to install both versions of Python for personal use, the following instructions are provided for version 2.7 only.*
3. In the box labeled “Python 2.7”, click on the blue box labeled “MAC OSX 64-BIT GRAPHICAL INSTALLER.” *If you select the graphical installer, double-click on the downloaded .pkg file and follow the instructions in the installer window. These instructions will be very similar to those in steps 5-11 in the aforementioned Windows Installation Instructions.*
4. Below the blue graphical installer box, you will also notice a “MAC OSX 64-BIT COMMAND-LINE INSTALLER.” If you are more comfortable using MAC Terminal, select this download.
5. If using the COMMAND LINE INSTALLER, once the download completes, navigate to the downloads folder, type **bash Anaconda2-4.1.1-MacOSX-x86\_64.sh,** and follow the instructions printed to the MAC Terminal. *If you need a refresher on using MAC Terminal commands, please reference the following document:* [*https://ubuntudanmark.dk/filer/fwunixref.pdf*](https://ubuntudanmark.dk/filer/fwunixref.pdf)*. Some basic examples are as follows:*

* **ls** = list files in your current directory
* **cd** = change directory (in order to use the **cd** command, you must first type **cd** followed by a **space**, followed by the name of the folder or directory you wish to navigate to)
* **cd ..** = move back one folder level

1. Regardless of your installation method (graphical or command line installer), you must now open a MAC Terminal and follow the instructions below:
2. In the MAC Terminal, type **conda update conda**
3. A list of packages to be downloaded will appear and you will be asked to proceed [yes/no]. Select yes to begin the download.
4. Following the download, you will also need to manually install the numpy, scipy, matplotlib, and colorama packages. In order to install each of these, use the following example for formatting: **conda install numpy.** After typing each install command once, type the same command a second time to assure that the package is correctly installed. If installed, you will receive the following message upon typing the install command a second time: “All requested packages already installed.”
5. Within the Python\_Files folder (where you found this installation instructions document), you will also find the Schrodinger.py, utils2.py, and utils3.py Python programs (for running in an Anaconda Prompt or via Windows Command Prompt), the Cases1-6.ipynb IPython notebooks (for instructor use in classrooms), and a file named **jupyter\_notebook\_config.py**
6. Using the MAC Terminal, navigate to the directory that contains the Anaconda2 folder from the installation in step 4/5. In the same directory as the Anaconda2 folder, you will find another folder named **.jupyter**. In this directory, you must place the **jupyter\_notebook\_config.py** file mentioned in step 10.
7. We also advise that you create a folder on your desktop called **Schrodinger** to place the Schrodinger.py, utils2.py, utils3.py Python programs as well as the Case1-6.ipynb IPython notebooks (for instructor use in classrooms).
8. Using MAC Terminal, navigate to the Schrodinger directory you just created in step 12. Once there, type **jupyter notebook** in the Terminal. This will open jupyter in your default web browser. When the default web browser opens, you should see the Schrodinger.py (Python program) and the Cases1-6.ipynb (IPython notebook) documents. Double click on one of the Case.ipynb files to open the IPython notebook.
9. With the notebook open, users are encouraged to examine the options at the top of the web browser. Most importantly, the user should focus on the “play” button in the top panel, which can be used to run each cell in the IPython notebook. The IPython notebooks are broken down into sections of **markdown** (text that explains the Schrodinger program or theory/math behind the program) and **code** (Python commands that carry out the mathematics discussed in the manuscript). When using the notebook, users should progress through the cells of the notebook one-by-one and press the play button for each cell. This will update the screen of any changes and also prompt the user for any input that the program requires. In the edit tab of the top panel, users also have the option to **run all cells**. If the user updates markdown text or Python code, they must remember to press the play button to update the screen of those changes. In some instances, the user might need to begin at the beginning of the notebook and re-play all the cells again, or simply use the **run all cells** function.
10. When finished, the IPython notebook should be closed. However, the main jupyter web browser will remain open and the IPython notebook will show **Running** in green. Click on the green **Running** and an option will appear to **Shutdown** the notebook. Click **Shutdown** before closing the main jupyter notebook web browser. Last, press CTRL+C in the Terminal to terminate the juptyer notebook process.
11. If users wish to simply run the Schrodinger.py program in the MAC Terminal (without the use of the IPython notebook), navigate to the Schrodinger folder on the desktop again. Once you’ve navigated to the desktop folder containing the Schrodinger.py program, type **python** **Schrodinger.py**. Here, the program will run in the terminal window with user input prompts. When running in the terminal window, users must first edit the **matplotlibrc** file in their working directory. Within this file, mac or linux users should uncomment (remove the # symbol) the macosx or linux backend line and also comment out (add a # symbol at beginning of line) the Windows backend line.

**Links for Getting Started with Markdown**

<https://sourceforge.net/p/jupiter/wiki/markdown_syntax/>

<http://jupyternotebook.readthedocs.io/en/latest/examples/Notebook/Working%20With%20Markdown%20Cells.html>