Installation Documentation

Release 1.2.0rc2

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CONTENTS:

CHAPTER

ONE

INSTALLATION OF RSMAP3D ON LINUX HOST

These installation instructions assume the use of the Anaconda Python distribution. For these instructions, Anaconda 5.x (Images May be from 2.5) and the packages provided by Anaconda were used as much as possible. At this time, the current version available from anaconda.org is 2018.12.

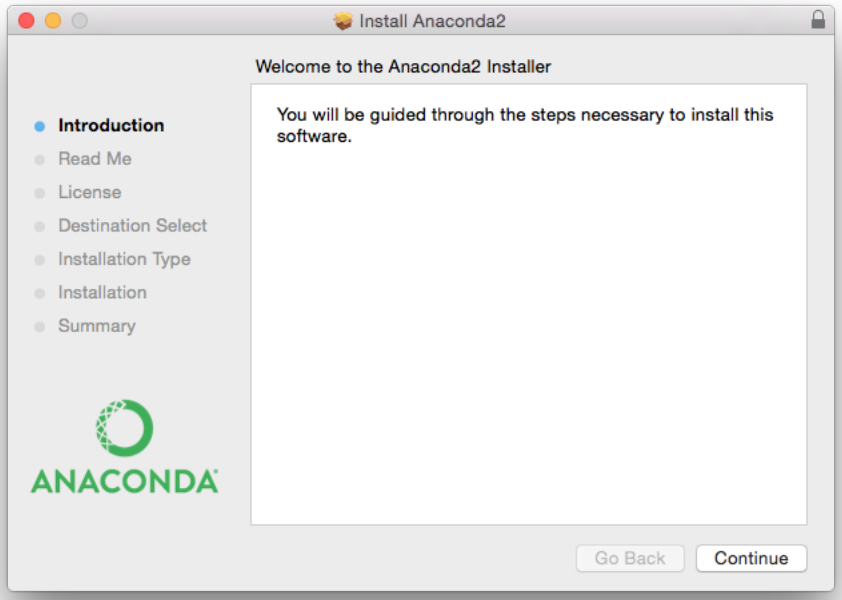
In order to install run rsmMap3D the user will need to install Anaconda, and install/check the install of a number of other python packages and then install:

- xrayutilities
- spec2nexus
- rsMap3D

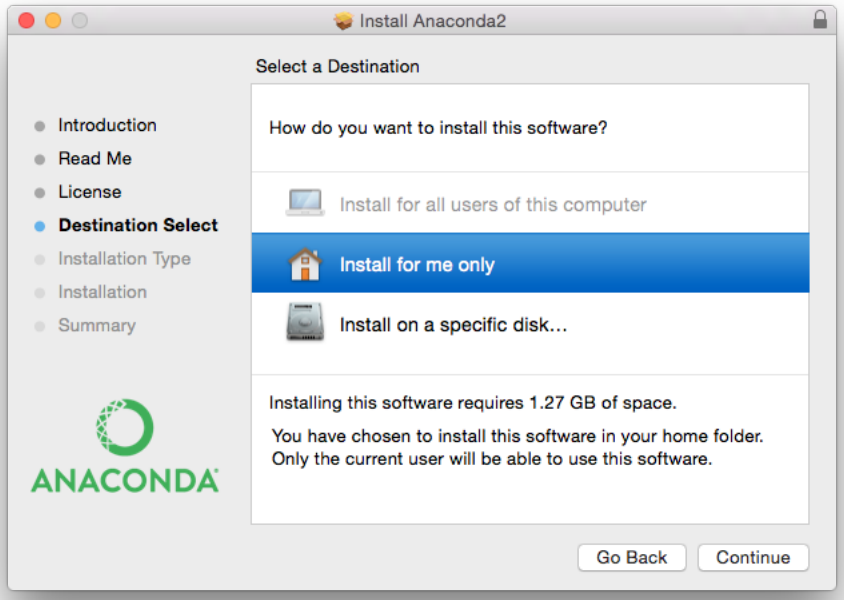
1.1 Installation and setup of Anaconda

Anaconda is a free bundling of Python and over 1500 open source Python packages. Support is available through open community or, for more advanced solutions, through paid support from Anaconda, Inc. Anaconda provides installers for both Python 2.7 and 3.x. Each has a different version of Python as a default. Note that although these installations are essentially the same, it is recommended that **if this your first install of Anaconda that you install the Python 3** version of Anaconda for more convenience since rsMap now requires Python 3. If you have already installed Python 2 version of Anaconda you can still use Python 3, but will need to create a *Python 3 environment,<https://docs.conda.io/projects/conda/en/latest/user-guide/tasks/manage-environments.html>*. Working in a python environment is suggested in either case since this will allow separation of the requirements of different Python applications.

These instructions assume that you will install the Python 3.x, 64-bit graphical installer. Launching this installer should present a window like:

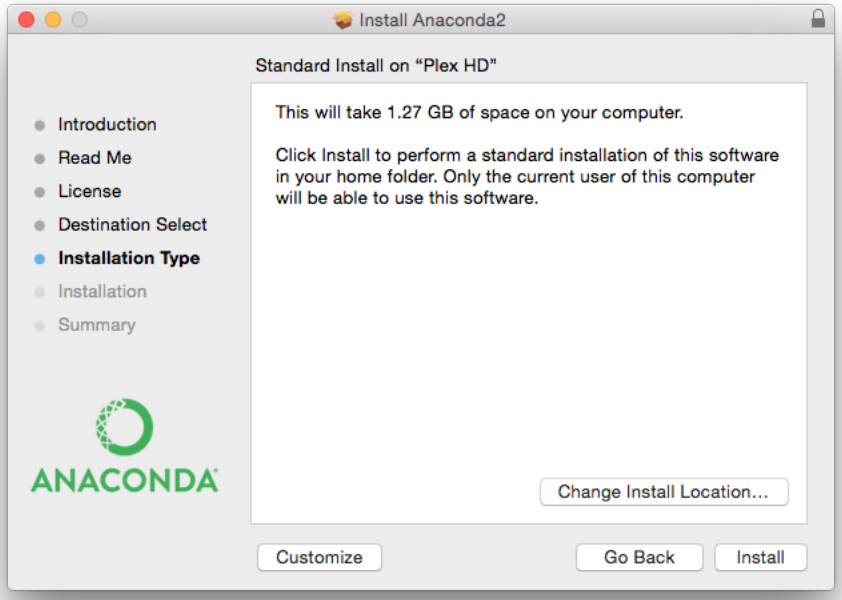


Clicking next you will be asked to accept the license agreement. You will then be prompted to select an installation type see image below. Anaconda allows installation on a per user basis ("Install for me only") or for all users (requires admin privilege).



This installation assumes selection of "Install for me only" which requires only normal user privilege. In this case anaconda will be installed in the user's home directory by default. Before final installation the user will be prompted for installation type (see image). This allows customization of installed packages and location. It is recommended to

accept the defaults here. Accepting defaults should add python executables to the user's PATH environment variable. It will take some time to complete the installation since Anaconda provides many common packages by default.



For rsMap3D we need to make sure that the following packages are installed: numpy, vtk,scypy pillow and pyqt. Installation can be verified by launching an Anaconda prompt from Start->All Programs->Anaconda2 (64-bit). We can verify package installation with

```
conda search <packagename> at the prompt.
```

If you previously installed Anaconda (you see older versions of packages than listed here) you may need to update your distribution. At this time, Anaconda 5.x is being used and the following packages are available and those not installed by default can be installed with the command.

```
conda install <packagename>
```

As mentioned earlier, it is suggested to run rsMap3D using a *Python environment*. *Python environments* allow creating a separate space for an application to run, separating it's package requirements from other applications. An example of this is the ability to run one application using Python 2 and another in Python 3. Anaconda and it's conda package manager allow creation of a *Python environment*. More information on managing environments in python can be found here: https://docs.conda.io/projects/conda/en/latest/user-guide/tasks/manage-environments.html

After installing Python 3 and optionally creating a *Python environment* ensure that the following packages are installed. If not, use the conda install command listed above.

Required packages

- numpy 1.16.2
- pyqt 5.9.2
- vtk 8.2.0
- h5py 2.5.0
- pillow 5.4.1

- scipy 1.2.1

Make sure to install these packages now. Note that we will also need xrayutilities and spec2nexus (described below).

1.2 Installing xrayutilities

Xrayutilities is a package written by Dominik Kriegner and Eugen Wintersberger. We are presently using version 1.5.1 of xrayutilities. This package can be downloaded as a tar.gz file from http://sourceforge.net/projects/xrayutilities/.

To unbundle the package in /local/xrayutilities-1.5.1:

```
cd /local
tar -xzvf 'path to file'/xrayutilities-1.5.1.tar.gz
```

This package includes a setup.py file to help with the install. To install xrayutilities run:

```
cd /local/xrayutilities-1.5.1
~/Enthought/Canopy_64bit/User/bin/python setup.py install
```

1.3 Installing spec2nexus

spec2nexus is a python package written by Pete Jemian at the APS. This package provides a subpackage that enables parsing spec files in python. This package has been used in places to read spec files as input for the rsMap3D. Note that rsMap3D requires at least version 2016.216.0.

```
pip install spec2nexus
```

1.4 Installing rsMap3D

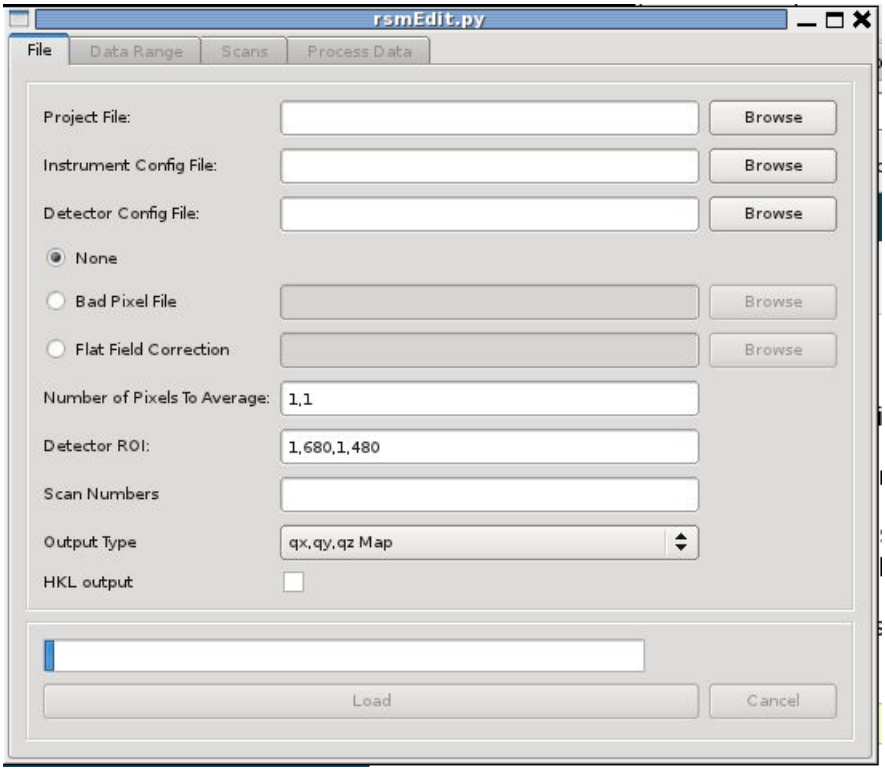
rsMap3D is now available as a package on the Python Package Index. This allows installation of rsMap3D using the python pip installer

```
pip install rsMap3D
```

A windows .bat file is installed in the path defined by the python installation (the Scripts subdirectory for the Anaconda distribution). The application can be launched by running

```
python -m rsMap3D.rsmEdit
```

You will then see a window like the following:



You are now ready to start using rsMap3D.

CHAPTER

TWO

INSTALLATION OF RSMAP3D ON MAC/OSX HOST

These installation instructions assume the use of the Anaconda Python distribution. For these instructions, Anaconda 5.x (Images May be from 2.5) and the packages provided by Anaconda were used as much as possible. At this time, the current version available from anaconda.org is 2018.12.

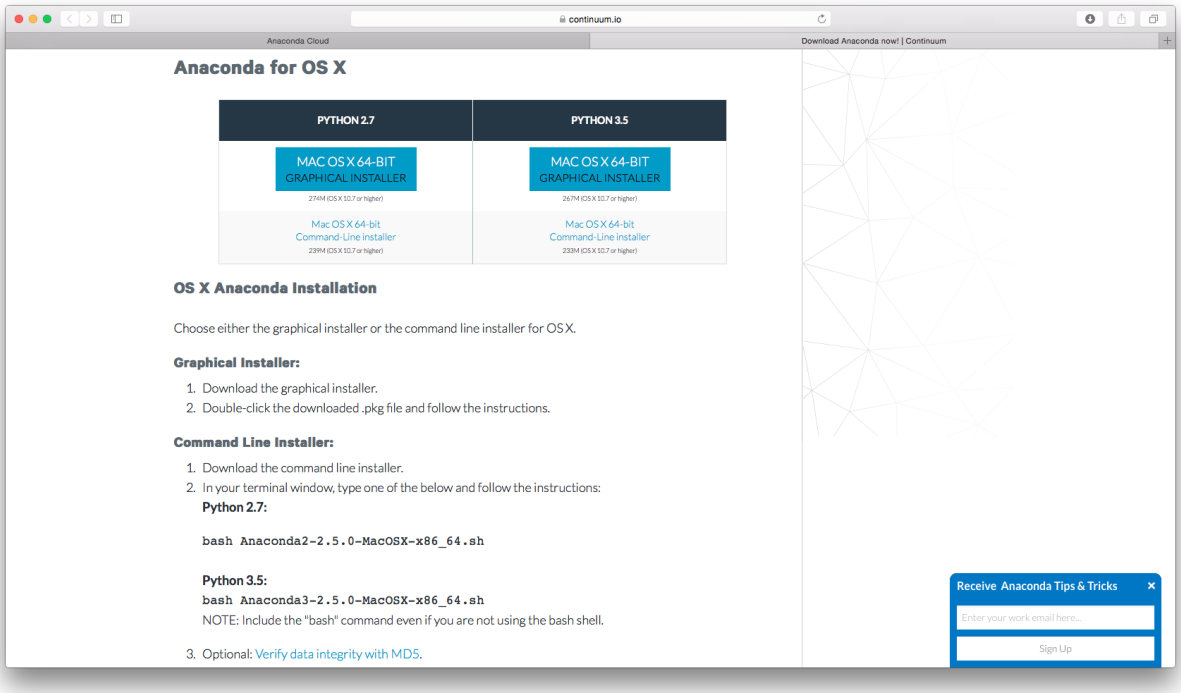
In order to install run rsmMap3D the user will need to install Anaconda, and install/check the install of a number of other python packages and then install:

- xrayutilities
- spec2nexus
- rsMap3D

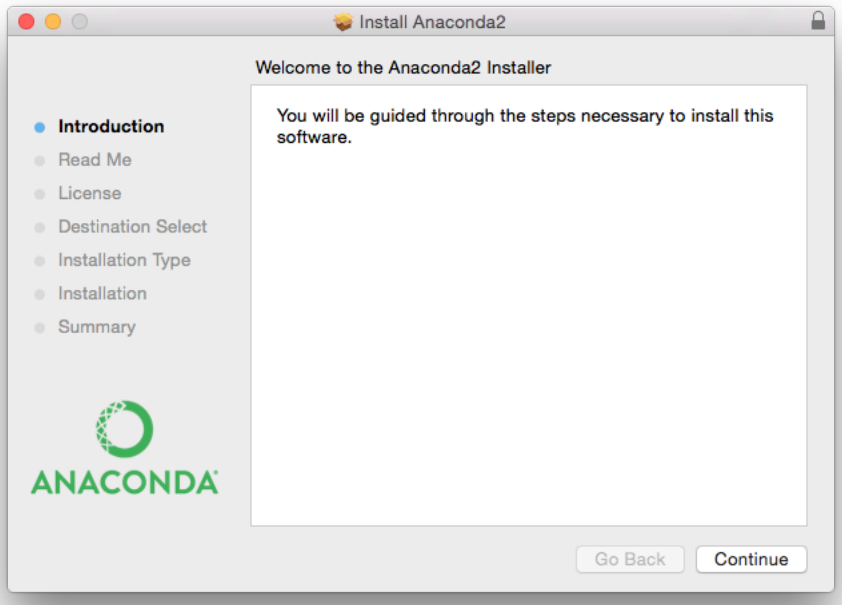
2.1 Installation and setup of Anaconda

Anaconda is a free bundling of Python and over 1500 open source Python packages. Support is available through open community or, for more advanced solutions, through paid support from Anaconda, Inc. Anaconda provides installers for both Python 2.7 and 3.x. Each has a different version of Python as a default. Note that although these installations are essentially the same, it is recommended that **if this your first install of Anaconda that you install the Python 3** version of Anaconda for more convenience since rsMap now requires Python 3. If you have already installed Python 2 version of Anaconda you can still use Python 3, but will need to create a *Python 3 environment,<https://docs.conda.io/projects/conda/en/latest/user-guide/tasks/manage-environments.html>*. Working in a python environment is suggested in either case since this will allow separation of the requirements of different Python applications.

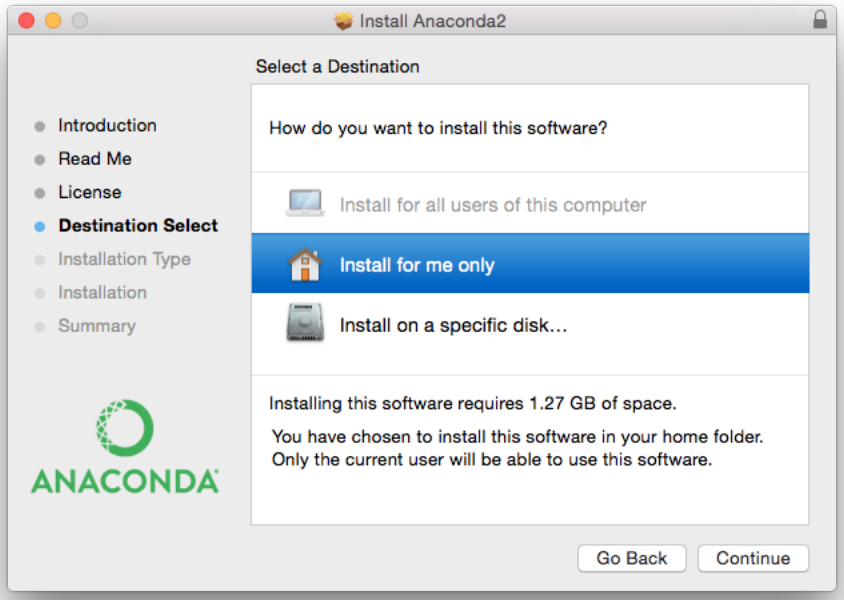
To install Anaconda Python, go to the download site mentioned above you should see a web page with a section that looks like



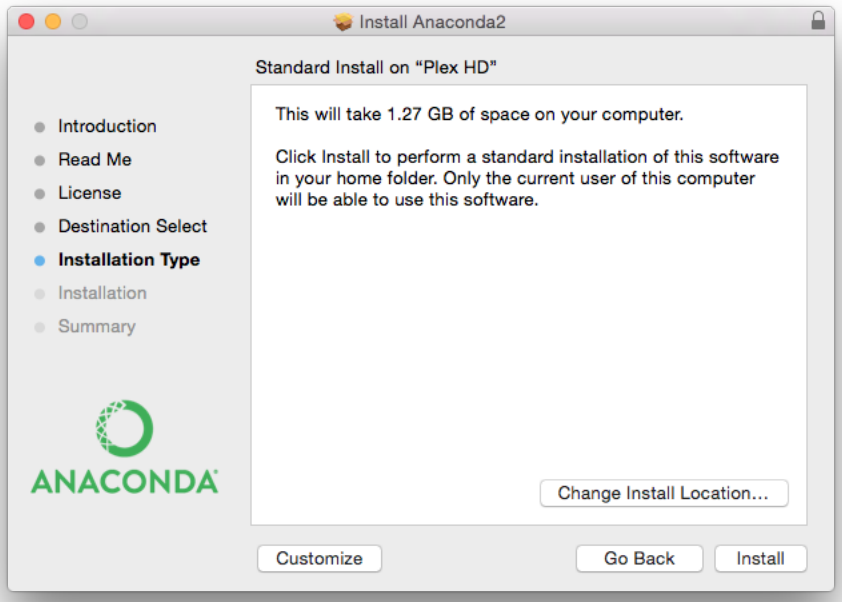
These instructions assume that you will install the Python 2.7, 64-bit graphical installer. Launching this installer should present a window like:



Clicking next you will be asked to accept the license agreement. You will then be prompted to select an installation type see image below. Anaconda allows installation on a per user basis ("Install for me only") or for all users (requires admin privilege).



This installation assumes selection of "Install for me only" which requires only normal user privilege. In this case anaconda will be installed in the user's home directory by default. Before final installation the user will be prompted for installation type (see image). This allows customization of installed packages and location. It is recommended to accept the defaults here. Accepting defaults should add python executables to the user's PATH environment variable. It will take some time to complete the installation since Anaconda provides many common packages by default.



For rsMap3D we need to make sure that the following packages are installed: numpy, vtk, scipy, pillow and pyqt.

Installation can be verified by launching Terminal (Applications->Utilities->Terminal) and running

```
conda search <packagename> at the prompt.
```

At this time, Anaconda 5.x is being used and the following packages are available and those not installed by default can be installed with the command

```
conda install <packagename>
```

As mentioned earlier, it is suggested to run rsMap3D using a *Python environment*. *Python environments* allow creating a separate space for an application to run, separating it's package requirements from other applications. An example of this is the ability to run one application using Python 2 and another in Python 3. Anaconda and it's conda package manager allow creation of a *Python environment*. More information on managing environments in python can be found here: https://docs.conda.io/projects/conda/en/latest/user-guide/tasks/manage-environments.html

After installing Python 3 and optionally creating a *Python environment* ensure that the following packages are installed. If not, use the conda install command listed above.

Required packages

- numpy 1.16.2
- pyqt 5.9.2
- vtk 8.2.0
- h5py 2.5.0
- pillow 5.4.1
- scipy 1.2.1

Make sure to install these packages now. Note that we will also need xrayutilities and spec2nexus (described below).

2.2 Installing xrayutilities

Xrayutilities is a package written by Dominik Kriegner and Eugen Wintersberger. We are presently using version 1.5.1 of xrayutilities. This package can be downloaded as a tar.gz file from http://sourceforge.net/projects/xrayutilities/.

To unbundle the package in the user's home directory (i.e ~/xrayutilities-1.5.1):

```

```

To install directly with pip: – code-block:: none

pip install –global-option="–without-openmp" xrayutilities

if the compiler that you are using supports openmp then you can omit –global-option="–without-openmp"

2.3 Installing spec2nexus

spec2nexus is a python package written by Pete Jemian at the APS. This package provides a subpackage that enables parsing spec files in python. This package has been used in places to read spec files as input for the rsMap3D. Note that rsMap3D requires at least version 2019.321.0.

```
pip install spec2nexus
```

2.4 Installing rsMap3D

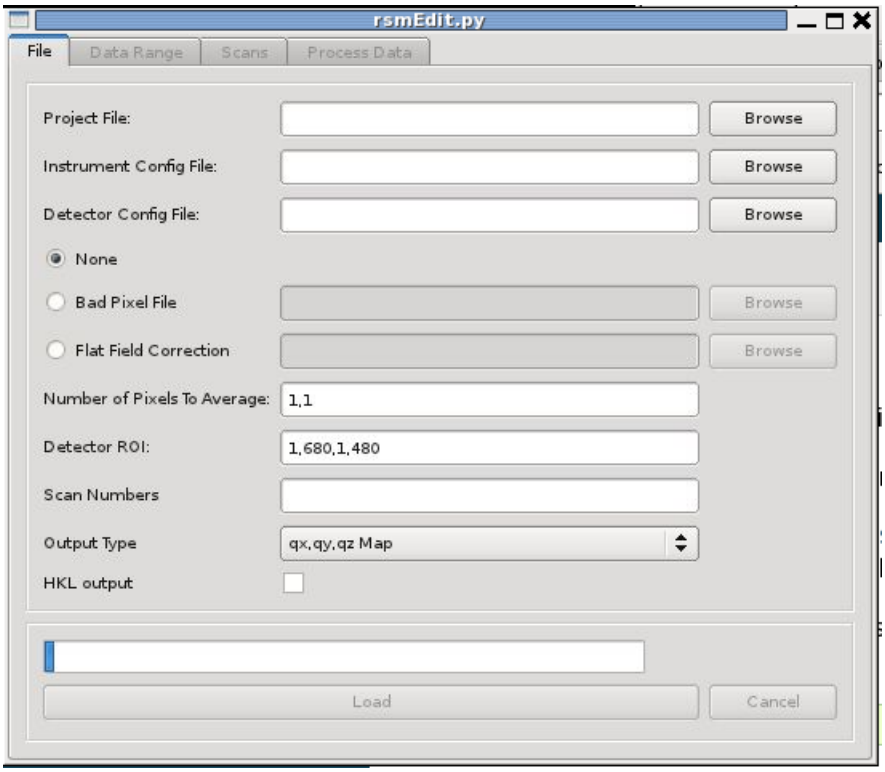
rsMap3D is now available as a package on the Python Package Index. This allows installation of rsMap3D using pip

```
pip install rsMap3D
```

A windows .bat file is installed in the path defined by the python installation (the Scripts subdirectory for the Anaconda distribution). The application can be launched by running

```
python -m rsMap3D.rsmEdit
```

You will then see a window like the following:



You are now ready to start using rsMap3D.

CHAPTER

THREE

INSTALLATION OF RSMAP3D ON WINDOWS HOST

These installation instructions assume the use of the Anaconda Python distribution. For these instructions, Anaconda 5.x (Images May be from 2.5) and the packages provided by Anaconda were used as much as possible. At this time, the current version available from anaconda.org is 2018.12.

In order to install run rsmMap3D the user will need to install Anaconda, and install/check the install of a number of other python packages and then install:

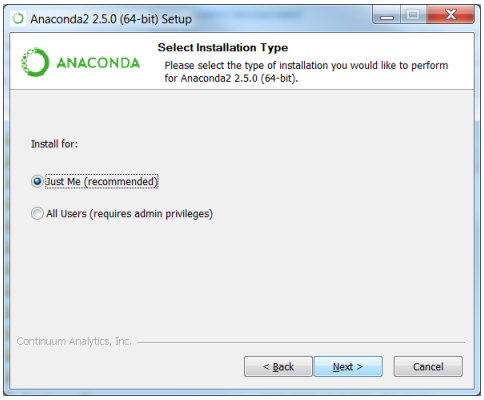
- xrayutilities
- spec2nexus
- rsMap3D

3.1 Installation and setup of Anaconda

Anaconda is a free bundling of Python and over 1500 open source Python packages. Support is available through open community or, for more advanced solutions, through paid support from Anaconda, Inc. Anaconda provides installers for both Python 2.7 and 3.x. Each has a different version of Python as a default. Note that although these installations are essentially the same, it is recommended that **if this your first install of Anaconda that you install the Python 3** version of Anaconda for more convenience since rsMap now requires Python 3. If you have already installed Python 2 version of Anaconda you can still use Python 3, but will need to create a *Python 3 environment,<https://docs.conda.io/projects/conda/en/latest/user-guide/tasks/manage-environments.html>*. Working in a python environment is suggested in either case since this will allow separation of the requirements of different Python applications.

These instructions assume that you will install the Python 2.7, 64-bit graphical installer. Launching this installer should present a window like:

Clicking next you will be asked to accept the license agreement. You will then be prompted to select an installation type see image below. Anaconda allows installation on a per user basis ("Just Me") or for all users (requires admin privilege).



This installation assumes selection of "Just Me" which requires only normal user privilege. Before final installation the user will be prompted for installation location and permission to modify the path to include path to installed executables. It is recommended to accept the defaults here. It will take some time to complete the installation since Anaconda provides many common packages by default.

For rsMap3D we need to make sure that the following packages are installed: numpy, vtk, scipy, pillow and pyqt. We can verify package installation with

```
conda search <packagename> at the prompt.
```

If you previously installed Anaconda (you see older versions of packages than listed here) you may need to update your distribution. At this time, Anaconda 5.x is being used and the following packages are available and those not installed by default can be installed with the command.

```
conda install <packagename>
```

As mentioned earlier, it is suggested to run rsMap3D using a *Python environment*. *Python environments* allow creating a separate space for an application to run, separating it's package requirements from other applications. An example of this is the ability to run one application using Python 2 and another in Python 3. Anaconda and it's conda package manager allow creation of a *Python environment*. More information on managing environments in python can be found here: https://docs.conda.io/projects/conda/en/latest/user-guide/tasks/manage-environments.html

After installing Python 3 and optionally creating a *Python environment* ensure that the following packages are installed. If not, use the conda install command listed above.

Required packages

- numpy 1.16.2
- pyqt 5.9.2
- vtk 8.2.0
- h5py 2.5.0
- pillow 5.4.1
- scipy 1.2.1

Make sure to install these packages now. Note that we will also need xrayutilities and spec2nexus (described below).

3.2 Installing xrayutilities

Xrayutilities is a package written by Dominik Kriegner and Eugen Wintersberger. We are presently using version 1.2.1 of xrayutilities. This package is available for install from the pypi distribution site and can be installed using the pip command

```
pip install xrayutilities
```

3.3 Installing spec2nexus

spec2nexus is a python package written by Pete Jemian at the APS. This package provides a subpackage that enables parsing spec files in python. This package has been used in places to read spec files as input for the rsMap3D. Note that rsMap3D requires at least version 2016.216.0. Although the installation instructions suggest this can be installed with the conda installer, this method currently installs an older version. To install the correct version use:

```
pip install spec2nexus
```

3.4 Installing rsMap3D

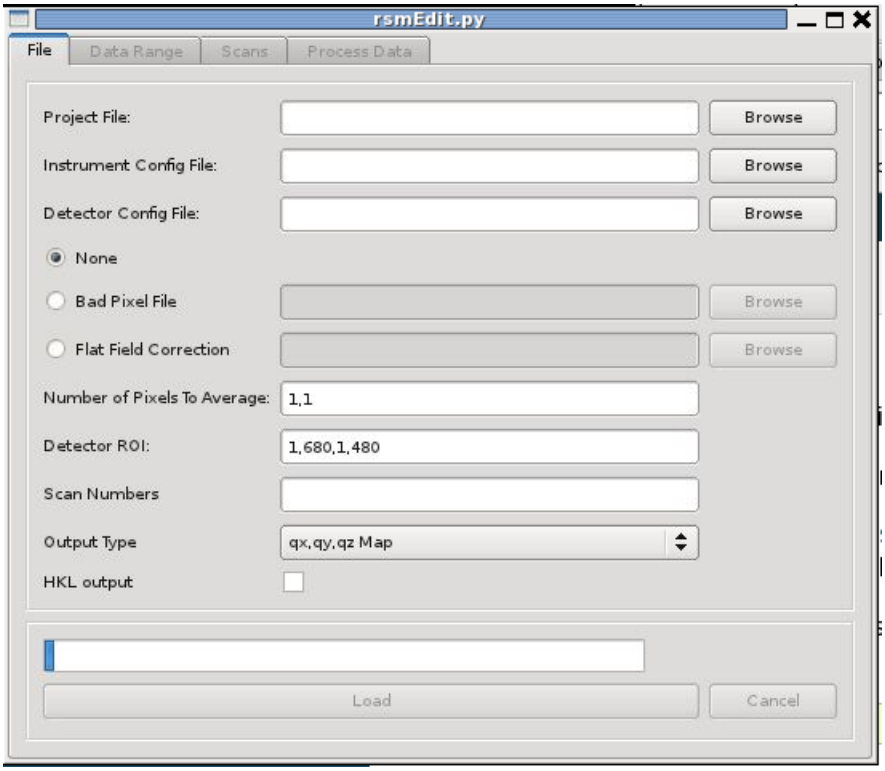
rsMap3D is now available as a package on the Python Package Index. This allows installation of rsMap3D using pip

```
pip install rsMap3D
```

A windows .bat file is installed in the path defined by the python installation (the Scripts subdirectory for the Anaconda distribution). The application can be launched by running

```
rsMap3D.bat
```

You will then see a window like the following:



You are now ready to start using rsMap3D.

CHAPTER

FOUR

INDICES AND TABLES

- genindex
- modindex
- search