Installation and Requirements of Demeter-W (Version 1.0)

Li, Xinya Xinya.Li@pnnl.gov

Vernon, Chris R Chris. Vernon@pnnl.gov

September 09, 2017

Installing Required Packages

Demeter-W is written in Python 2.7 (version 2.7.11 is used in testing) with dependencies (packages). The user is required to install all the packages as follows:

- NumPy (version 1.13.1) http://www.numpy.org/
- SciPy (version 0.18.1) https://www.scipy.org/
- Matplotlib (version 2.0.2) https://matplotlib.org/
- pandas (version 0.19.2) http://pandas.pydata.org/
- ConfigObj (version 5.0.6) http://www.voidspace.org.uk/python/configobj.html

The versions of the packages are used in testing. Lower version for each of the package is not recommended. Higher versions of the packages should be compatible.

It is strongly recommended that all the listed dependencies can be obtained by using the Python's tool for installing packages called pip (https://pypi.python.org/pypi/pip). The basics of how to install Python packages are described at https://packaging.python.org/tutorials/installing-packages/. A simple example of installing a needed packages with the latest version is:

```
pip install numpy
```

To install a certain version of the package:

```
pip install numpy==1.13
```

To install all the packages:

```
pip install numpy scipy matplotlib pandas configobj
```

The installation of scipy, may require numpy+mkl (numpy with Intel Math Kernel Library). Thus, the user needs to install numpy+mkl from a wheel file again after the installation of all the other packages. The wheel file of numpy+mkl can be downloaded from the site http://www.lfd.uci.edu/~gohlke/pythonlibs/ for Windows. Then use pip to install the wheel package, for example:

```
pip install numpy-1.13.1+mkl-cp27-cp27m-win32.whl
```

For use with the conda package manager for a fresh Python 2.7 environment, the user can use the following command to install required packages:

```
conda install numpy scipy matplotlib pandas configobj
```

To install a certain version of the package:

```
conda install numpy==1.11
```

Download and Install Demeter-W

Demeter-W can be cloned from https://github.com/JGCRI/demeter-w

All the source codes are in "demeter-w". "example" folder contains inputs, outputs and configuration file of example cases. The documents are included in "docs".

The user is able to install Demeter-W as a Python package by running "setup.py" from terminal or command line:

```
python setup.py install
```

After installation, Demeter-W is able to be imported as follows in a Python script:

```
from demeter w.model import DemeterW
```

If a permissions error is encountered either run the command sudo or on Windows open cmd as an administrator. For more information, please refer to https://docs.python.org/2/install/

How to use Demeter-W

Step 1 Create a configuration file

The user needs to create a configuration file (*.ini) for a model simulation. The INI format is described at https://en.wikipedia.org/wiki/INI_file#Format.

The example configuration files are: "example\config.ini". The user needs to define the controlling parameters, select the simulation options and indicate the input files.

```
Step 2 Run a script
```

An example script is included in "example". A model simulation can be executed with a simple single command:

System Requirements

Demeter-W has been tested on Linux (64-bit), Windows 7 and Mac OS X.

The core modules are designed to process large data sets. Thus, a minimum memory size of 8GB is recommended to run the model and memory capacity also determines how fast the model can run according to the large size of the data sets.