Setup on GreenPlanet and TSCC

Login to the remote clusters and then do the following:

Install Anaconda

While in your HOME directory

Download the Anaconda installation file

> wget https://repo.continuum.io/archive/Anaconda3-4.3.1-Linux-x86_64.sh

Install Anaconda (this may take 15-30mins)

> bash Anaconda3-4.3.1-Linux-x86_64.sh -b

When it asks you to add Anaconda to your bash shell PATH, select **YES**.

Check that Anaconda installed properly by running the command `python`. It's output should look something like:

```
Python 3.6.0 |Anaconda 4.3.0 (64-bit)| (default, Dec 23 2016
[GCC 4.4.7 20120313 (Red Hat 4.4.7-1)] on linux
Type "help", "copyright", "credits" or "license" for more in
>>>
```

Install some extra packages into a virtual

environment

All our software needs to be run on **Python 3.5** so we will create a virtual environment and install some extra packages we will need down the line.

Create a virtual environment called `py35` with:

> conda create -n py35 python=3.5

Activate the virtual environment with:

> source activate py35

The terminal will look like something below to indicate you're in the virtual environment:

```
[limn1@tscc-login2 ~]$ source activate py35
(py35) [limn1@tscc-login2 ~]$
```

Now, install the extra packages we will need down the line (this could take another 15mins):

```
conda install numpy matplotlib
conda install nb_conda -c conda-forge
conda install -c omnia -c omnia/label/dev -c mobleylab openm
```

Install OpenEye toolkits

While still in your py35 virtualenv

Make a license folder in your **HOME** directory:

> mkdir licenses

Your path should look like `/home/USERNAME/licenses`.

Upload/copy the `oe_license.txt` file into the `licenses` folder.

Add to your `~/.bash_profile` the following line:

> export OE_LICENSE='$HOME/licenses/oe_license.txt"'

Install the OpenEye toolkits with:

> pip install -i https://pypi.anaconda.org/OpenEye/simple OpenEye-toolkits

Verify the installation with:

> oecheminfo.py

The output should look something like:

```
Installed OEChem version: 2.1.1 platform: linux-g++4.x-x64 b

Examples: /home/limn1/anaconda3/envs/dev/lib/python3.5/site-
Doc Examples: /home/limn1/anaconda3/envs/dev/lib/python3.5/s

code| ext            | description                        |read
----+----------------+------------------------------------+----
  1 | smi            | Canonical stereo SMILES            | yes
  2 | mdl,mol,rxn    | MDL Mol                            | yes
  3 | pdb,ent        | PDB                                | yes
  4 | mol2,syb       | Tripos MOL2                        | yes
  5 | usm            | Non-Canonical non-stereo SMILES    | yes
  6 | ism,isosmi     | Canonical stereo SMILES            | yes
  7 | mol2h          | MOL2 with H                        | yes
  8 | sdf,sd         | MDL SDF                            | yes
  9 | can            | Canonical non-stereo SMILES        | yes
```

```
  10 | mf             | Molecular Formula                  | no
  11 | xyz            | XYZ                                | yes
  12 | fasta,seq      | FASTA                              | yes
  13 | mopac,pac      | MOPAC                              | no
  14 | oeb            | OEBinary v2                        | yes
  15 | dat,mmd,mmod   | Macromodel                         | yes
  16 | sln            | Tripos SLN                         | no
  17 | rdf,rd         | MDL RDF                            | yes
  18 | cdx            | ChemDraw CDX                       | yes
  19 | skc            | MDL ISIS Sketch File               | yes
  20 | inchi          | IUPAC InChI                        | no
  21 | inchikey       | IUPAC InChI Key                    | no
  22 | csv            | Comma Separated Values             | yes
  23 | json           | JavaScript Object Notation         | yes
 ----+----------------+------------------------------------+----
```

[Recommended] Install Bash on Windows (Locally)

On your local Windows laptop

Follow the guide linked here

If the BASH terminal guide works and you can successfully use BASH commands (i.e `cd`, `ls`). Do let me know, this is a pretty big deal and will help other people who aren't on MacOS/Linux. Now, try repeating the steps above to see if we can get Anaconda/OpenEye installed on your local machine too.

If you run into too many issues along the way and it's become a headache, don't worry about it. I'm not requiring you do this, but this may help alleviate some issues when running on a Windows machine

and prevent problems when trying to translate between running on different OS. This feature is still in BETA and I have not tried it out myself. So I'm really hoping it works out on your machine. This will replace PuTTY so that your terminal can more closely mimic the command terminal found on Linux/MacOS machines or when you login to remote clusters.