BE 240 - Open Source Tools for Biological Circuit Design
California Institute of Technology
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Week 1 - Software Setup

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These notes describe how to set up the basic software installation that we will use for the course. The notes are turned for Linux and Mac users. Suggestions for Windows are welcome (via comments in the Google Doc, for those with access).

Computer setup (Conda, Python, Git, Jupyter)

Access command line

- AWS: if you have created an Amazon instance, log in to the command line:
  ssh -i "be240.pem" ubuntu@ec2-18-236-147-16.us-west-2.compute.amazonaws.com

- Caltech HPC (run on interactive compute node with 120 min time limit):
  $ ssh murray@login.hpc.caltech.edu
  $ srun --pty -t 120 /bin/bash -l

- Mac: use Terminal

- Windows: ???

Install a C/C++ compiler + setup conda environment [following bioscrape]

1. Install C/C++ (for Cython, used by bioscrape)

- Linux/MacOS:

  $ sudo apt-get update
  $ sudo apt-get install build-essential

- Windows 10: see bioscrape instructions.

Install anaconda

2. Google "anaconda download"; find the version you need
   - Note: better not to use miniconda, since you need a lot of the packages

3. Run the following on the command line to download

- ○ Linux/MacOS: from the command line, type

  $ wget https://repo.anaconda.com/archive/Anaconda3-2020.02-Linux-x86_64.sh

- ○ Windows 10

4. Execute the anaconda script to install

- ○ Linux/MacOS:

  $ bash Anaconda3-2020.02-Linux-x86_64.sh

  - ● Follow the prompts, using default settings unless you know what you are doing
  - ● You can say 'yes' to running 'conda init' or run 'conda init' after installation finishes:

    /home/ubuntu/anaconda3/bin/conda init

- ○ Windows 10

5. Log out of your shell and back in, to make sure initialization is set up. Alternatively, you can just re-run your shell initialization script

  $ source .bashrc

2. Set up conda environment

  $ conda update conda
  $ conda update anaconda

  $ conda create -n python3.7-bioscrape python=3.7
  $ conda activate python3.7-bioscrape

Bioscrape setup

Instructions for installing bioscrape can be found on the bioscrape wiki:
https://github.com/ananswam/bioscrape/wiki

The directions here largely parallel the information on that page.

Install pre-requisites for running bioscrape

  $ conda install -c SBMLTeam -c anaconda python-libsbml lxml beautifulsoup4 numpy scipy cython jupyter matplotlib sympy pandas

  $ pip install emcee

Install bioscrape

> $ git clone https://github.com/biocircuits/bioscrape.git

> $ cd bioscrape
> $ python setup.py install

Run basic example using Jupyter

> $ jupyter notebook --no-browser

> Basic Examples - START HERE.ipynb

Access Jupyter via a web browser

- Local host (Mac, Linux): no additional actions required
- AWS: complicated (need to open firewall)
- Caltech HPC: *after* you start the Jupyter server, run the following in a *separate* terminal window (yy = some digit until it works)

> ssh -L localhost:8888:localhost:88yy murray@login.hpc.caltech.edu
> ssh -L localhost:88yy:localhost:8888 murray@hpc-xx-xx

Running bioscrape in Google Colab

It is also possible to run bioscrape within Google Colab. To do so, you should add the following code to your notebook:

```
# Install emcee
!pip install emcee

# Install bioscrape
!git clone https://github.com/biocircuits/bioscrape.git
!(cd bioscrape; python setup.py install)

# Make sure it worked
import bioscrape
```

An example test file that runs the above code on Google Colab is available on BE240 Google drive here (open with Google Colab).