NANO266 Lab General Instructions

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1 Introduction

Welcome to the lab sessions for NANO266. Before you begin, you should read this carefully and follow all instructions to make sure that your computer /computing resource is set up properly. Your instructors are on hand to help you if you run into any problems.

2 First Principles Modeling Codes

In the labs, we will be using two open-source first principles modeling codes:

1. NWchem (http://www.nwchem-sw.org) is a computational chemistry code that aims to be scalable both in their ability to treat large scientific computational chemistry problems efficiently.
2. QuantumEspresso (http://www.quantum-espresso.org/) is an integrated suite of computer codes for electronic-structure calculations and materials modeling at the nanoscale. It is based on density-functional theory, plane waves, and pseudopotentials.

Before you start any of the labs, make sure that you have the software installed and in your path. You have four options:

1. We have secured an XSEDE allocation for this course. Please go the the XSEDE portal (https://portal.xsede.org) and create an account as shown above. After you have done so, email your username to one of the TAs to be added to the allocation for this course. You can then login to the allocations with

   ```
   ssh <your_username>@trestles.sdsc.edu
   ```

   Once you are logged in, immediately run

   ```
   module load qe nwchem
   ```

   to make sure that QuantumEspresso and NWChem are loaded for you.
2. If you have your own Mac, you can use the executables already included in this repo (see cloning the repo section). Run the following command to add the bin directory to your path as follows (assuming you are on bash):

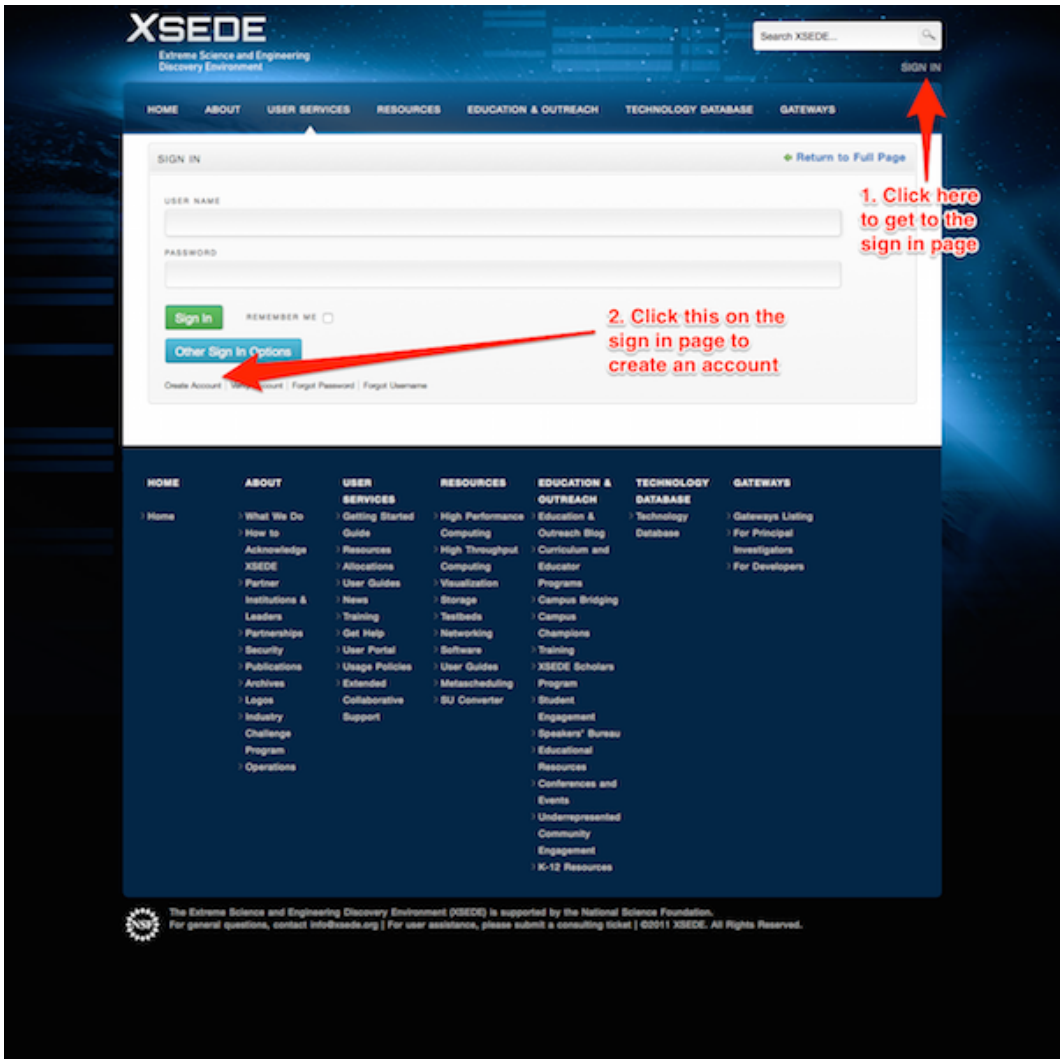

Figure 1: XSEDE user portal

```
export PATH=$PATH:<path/to/repo>/bin/Mac
# The following is to set the NWChem basis sets used in lab1. Be careful
# that the ending slash is needed!
export NWCHEM_BASIS_LIBRARY = <path/to/repo>/resources/nwchem_basis/
```

3. You can download VirtualBox (https://www.virtualbox.org/), and a pre-configured Ubuntu virtual machine at this link[1]. Note that it is a hefty 3 Gb download, so you will want to download this on a fast connection. After launching VirtualBox, do File->Import Appliance and then select the downloaded `nano266.ova` file. You can then start the virtual machine. You should be able to login to the virtual machine without a password. If one is ever needed, it is simply "nano266fun". Start a terminal by clicking on the icon on the left. By typing `ls`, you should see that a nano266 directory is already cloned for you. Simply `cd nano266` and you are ready to begin to do the labs.

4. You can download the source code for QuantumEspresso or NWChem and install it yourself. *Attempt this only if you have a fairly good familiarity with compiling things on Unix-based OSes, or are willing to spend the time to figure it out!* If you foresee you will be working on such calculations extensively in future, it is generally useful for you to learn how to do this. Start with the QuantumEspresso code as it is more straightforward to compile.

In general, it is not recommended that you run on a native Windows OS for these labs. Most first principles codes are designed to run primarily on supercomputing clusters that have Unix-based OSes. If you have a Windows machine, you should try option 1 or 3 above.

3 Cloning the repo

On wherever you are performing the calculations for the lab, you should clone this repo by doing:

```
git clone https://github.com/materialsvirtuallab/nano266.git
```

This assumes you already have git installed, which comes by default in XSEDE and Mac and can easily be installed in Unix-based OSes. To update your repo to the latest version at any time, you can do:

```
git pull
```

from within the repo.

4 Programming code

A lot of the labs use Python as a scripting language for automating calculations and analysis. You should ensure that you have Python 2.7.x installed with numpy. If you have a Mac, this should be already the case. If you use the virtual machine, it is also already set up.

[1] https://s3.amazonaws.com/mavrl-web/nano266.ova

If you don't know Python, get a quick primer from the official Python documentation at https://docs.python.org/2.7/. You don't really need to know much more than that for the purposes of the labs. Learning how to use a scripting language like Python can save you loads of time in automating calculations.