AMPL (version 1.4.1) was successfully installed on the Andes system at ORNL by Sean Black

The below steps are taken from the github page (https://github.com/ATOMScience-org/AMPL) and only modified to

1. removed the git clone step as I have already cloned the AMPL repository into this shared space
2. added the "module load gcc" and "module load python" steps which is ORNL specific to activate python/conda/other tools

Running the below list of commands within a terminal connected to the Andes system should result in a functioning conda environment to utilize AMPL components. The test section (below the install steps) will run one set of tests called delaney_RF. If all goes well after the provided install steps, then you should be able to get started using AMPL.

Install steps to use AMPL:

$ module load gcc
$ module load python
$ cd <ampl_directory_location>/AMPL/conda
$ conda create -y -n atomsci --file conda_package_list.txt
$ conda activate atomsci
$ pip install -r pip_requirements.txt
$ pip uninstall -y keras
$ pip install -U tensorflow==2.8.0 keras==2.8.0
$ conda activate atomsci
$ cd ..
$ ./build.sh && ./install.sh system

Add an environmental variable for deepchem to create temporary files:

This step is only necessary if you are accessing a ***shared*** AMPL install. This step can be skipped if you are installing AMPL for your own use that will not be accessed by anyone other than yourself.

$ vim ~/.bashrc
Add the following line:

```
export DEEPCHEM_DATA_DIR=/var/tmp/
```

Test:

$ conda activate atomsci
$ cd atomsci/ddm/test/integrative/delaney_RF
$ pytest

If the above pytest gives errors, send me the errors. It is not unusual for there to be warnings output from these tests. Everything should work at this point! If you want to start running

hyper parameter optimization, then we may need to add some parameters in the code for you to use the provided HPO scripts.

Tutorials:

The tutorials provided at

AMPL/atomsci/ddm/example/tutorials

are intended to be ran on Google Colab in a web browser as they have code at the beginning to install AMPL into the cloud environment and have lines to connect to google drive. While you are exploring the capabilities of AMPL before you begin implementing AMPL into your workflow, it is recommended to use Google Colab. In each of the tutorial files, there is a button at the top that will connect you to a Google Colab environment (free to use).

You do not need to execute these tutorials to see their output since the output of each cell is saved in the notebook files, but it can be helpful to follow along the code and make changes to explore features and options.