Location: /home/melissasanseverino/maceML

1. Install MACE on Palmetto

* Need to first create a conda for installing all the dependencies
* Upgrade the python to newest version
* Install Pytorch newest version
* Install MACE

1. Convert the dataset into the format required by MACE

* Example format can be found in their tutorial [T01\_MACE\_Practice\_I.ipynb](https://colab.research.google.com/drive/1ZrTuTvavXiCxTFyjBV4GqlARxgFwYAtX#scrollTo=JoYYvmRuDVln) data/solvent\_xtb.xyz
* write a script that converts ML\_AB into xyz format
  + Melissa: To get the final energies of each configuration in the ML\_AB file we need to extract the final energy without enthalpy value from each OUTCAR
  + Shirui: write a script to compile the ML\_AB and the energy file melissa provides into a xyz format, as the input for training the model → the name of the script is MakeInputFile.py
  + Now we have the input data file in the correct format
  + Consider adding charges

1. Understand the hyperparameters and try to train the model (learn from the tutorial)

* Installed all dependencies for training the model
* Wrote a config file for describing the training process

Reference page: <https://mace-docs.readthedocs.io/en/latest/guide/training.html#training-files>

* + E0 is reference energy of each atom (I just put in some random numbers I found on wiki, but later on we should calculate our own numbers)
  + Several things to change and try: batch size, num of epochs
* Wrote a .sh and a python script for training

1. Train the model

* Run train\_model.py to create train and test files
* Run .sh to train
* The .out file records the RMSE for every epoch and the final RMSE

After training, the models are stored in “MODEL\_mace” folder

1. Test the model

* Use the mace01\_run-123\_stagetwo.model to test
* Interface with LAMMPS to find minima and transition state

ERROR: facing memory issues