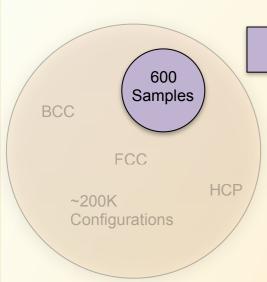
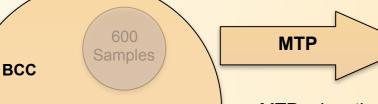
MTP steps



Catalog

DFT

600 samples. randomly chosen between a pool of ~200K samples of bcc, fcc, and hcp crystalline structures, are taken as a training set. MTP generates a fit for the interatomic potential.



FCC HCP ~200K **Configurations**

MTP relaxation of the ~200K configurations

600 Samples Configurations

Pick additional configurations that will best benefit the training set.

+training set

Training



- First, verify you can run 600 jobs at Maryland supercomputer:
 - squeue -r -A glh43 | wc -l
- Script1.sh randomly selects 600 configurations, creates 600 folders, each with a POSCAR, and send them to gueue to run static DFT calculations using VASP.



/script2.sh

- In each folder created in the previous step, script2.sh creates a diff.cfg file:
 - ./mlp convert-cfg OUTCAR diff.cfg --input-format=vasp-outcar >> outcar.txt
- create the train.cfg file. Script2.sh will send to gueue a job to do the following:

Training: ./mlp train pot.mtp train.cfg > training.txt

Updating pot.mtp: mv Trained.mtp_ pot.mtp

Generate state.mvs file: ./mlp calc-grade pot.mtp train.cfg train.cfg temp1.cfg

After fixing diff.cfg format (fixing cfgFiles.cpp), script2.sh will concatenate the diff.cfg files to

Relaxation



- Script3.sh will send a job to relax ~200K configurations using mlp instead
 - ./mlp relax relax.ini --cfq-filename=to relax.cfq -save-

relaxed=relaxed.cfg

 The previous step generated a group of files selected.cfg n, with n = {1,2,..., #processors}. Script3.sh will concatenate them:

cat selected.cfg * > selected.cfg

Active Learning



- To avoid MTP errors, selected.cfg is renamed to new.cfg
- MTP will choose the best candidates to be added to the training set. ./mlp select-add pot.mtp train.cfg new.cfg diff.cfg

/script4.sh

./script7.sh

/script6.sh

./script5.sh

- Getting POSCARs from the diff.cfg: ./mlp convert-cfg diff.cfg POSCAR --output-format=vasp-poscar
- After fixing POSCARs format (fixing POSCARs.cpp), script5.sh will send to queue the additional configurations to run on VASP.

The previous step creates a diff.cfg file containing new configurations to run on VASP.

/script8.sh