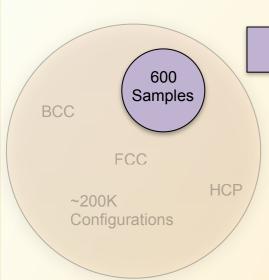
MTP steps



Catalog

FCC

Configurations

~200K

BCC

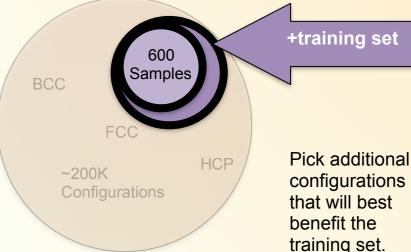
600

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.



MTP relaxation of the ~200K configurations



HCP

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.



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

/script2.sh

- After fixing diff.cfg format (fixing cfgFiles.cpp), script2.sh will concatenate the diff.cfg files to create the train.cfg file. /script6.sh
- 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

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

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



- 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.

/script8.sh

/script4.sh

./script7.sh

