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(U) ATCC-10 LSCI: Active learning for atomic plutonium potentials.

Ben Nebgen, Justin Smith,
Kipton Barros

5/5/2021

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Scale Bridging for Materials Properties

s

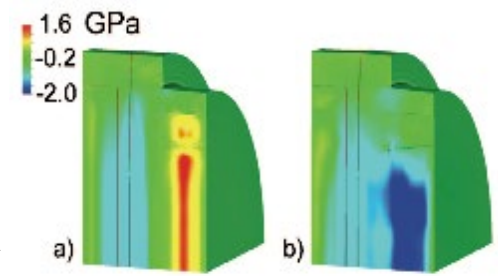
ms

µs

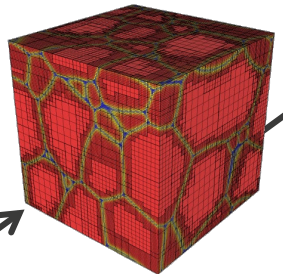
ns

ps

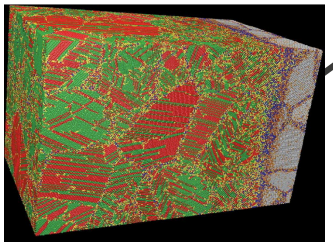
Continuum Methods



Phase-Field Modeling

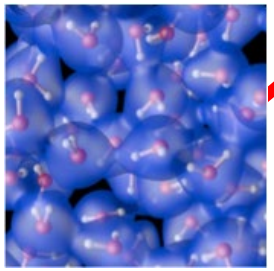


Molecular Dynamics



100s Atoms

Ab-initio Methods



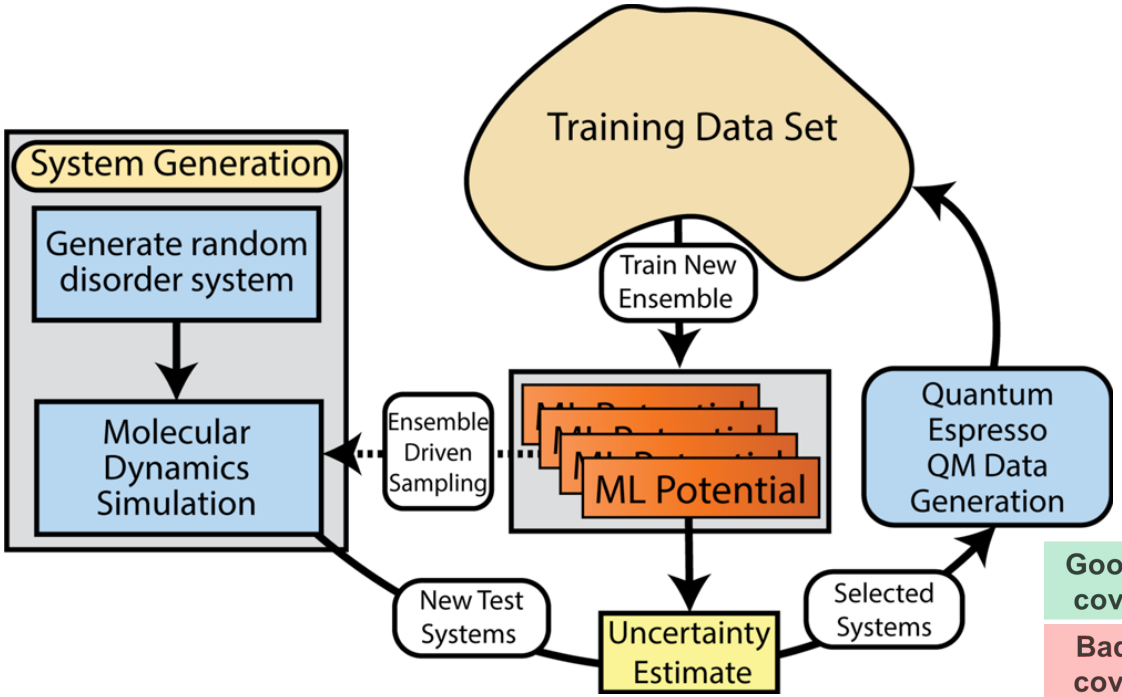
The goal: predict macroscopic materials properties (specifically, Pu alloys) from first principles physics.

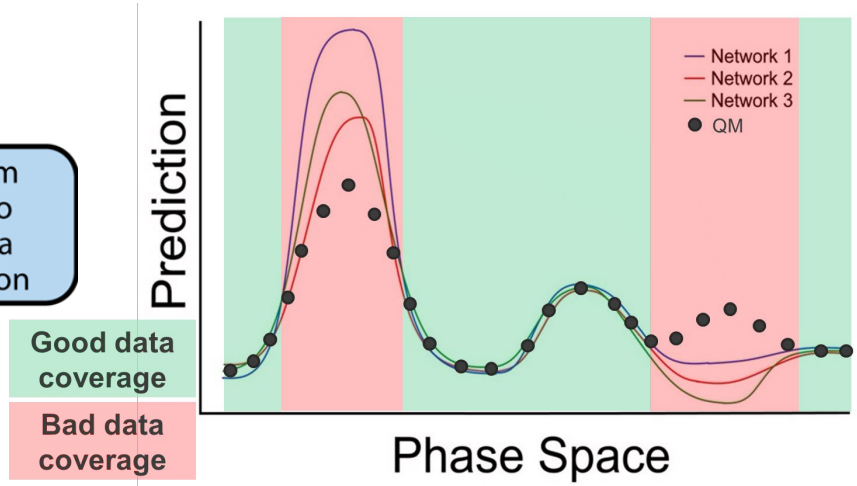
Breakthrough for understanding materials when experiments are difficult or impossible.

LENGTH

nm µm mm m

Active Learning for Dataset Generation



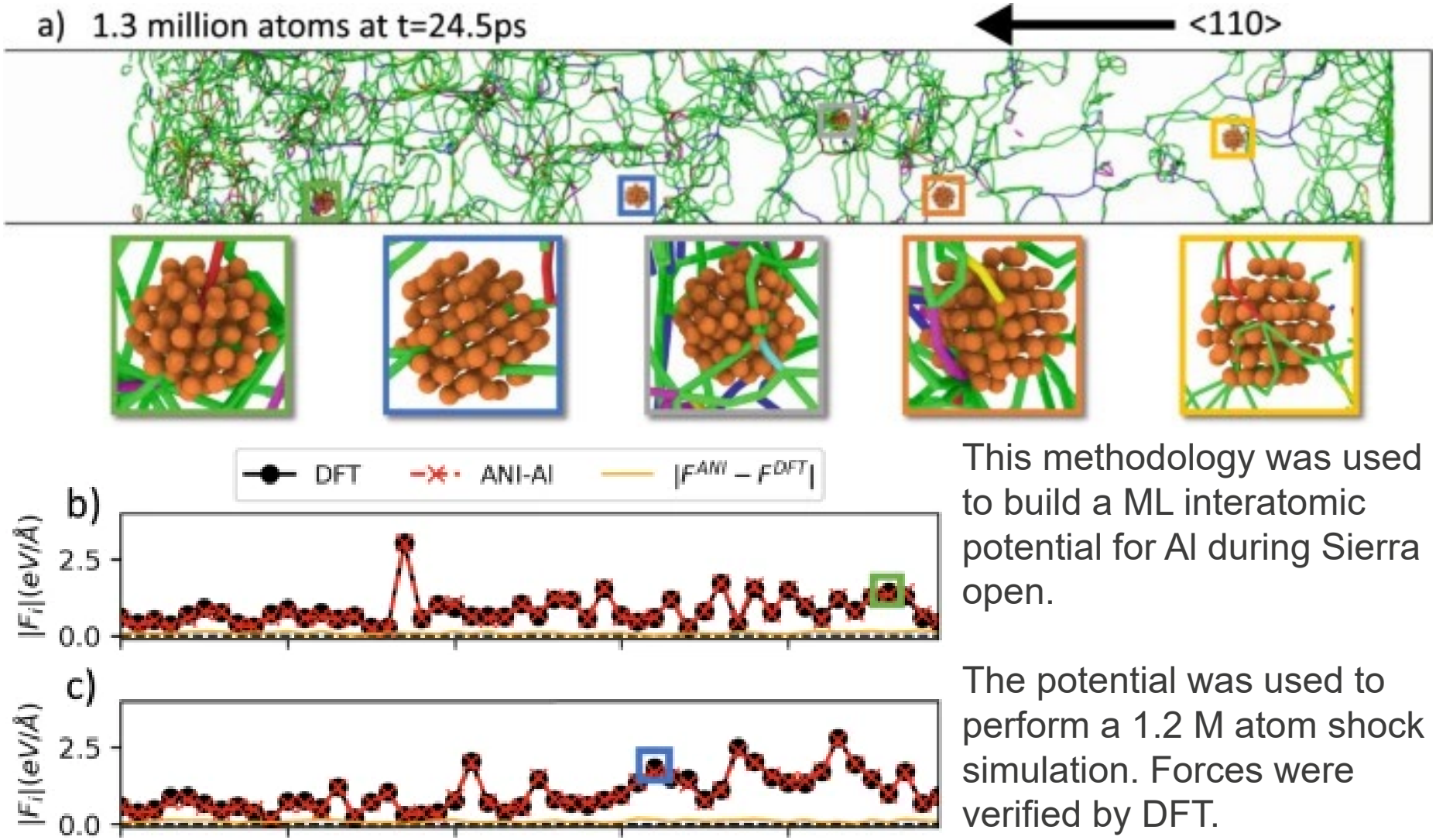


An Active Learning system was developed for the automated exploration of phase space. This system builds a training dataset for an Machine Learned interatomic potential with little to no human intervention.

Using Query by Committee (a UQ method), we intelligently select configurations to augment the ML training set intelligently.

Smith, J. S.; Nebgen, B.; Mathew, N.; Chen, J.; Lubbers, N.; Burakovsky, L.; Tretiak, S.; Nam, H. A.; Germann, T.; Fensin, S.; Barros, K., Automated discovery of a robust interatomic potential for aluminum. *Nature Comm.* **2021,** *12.*

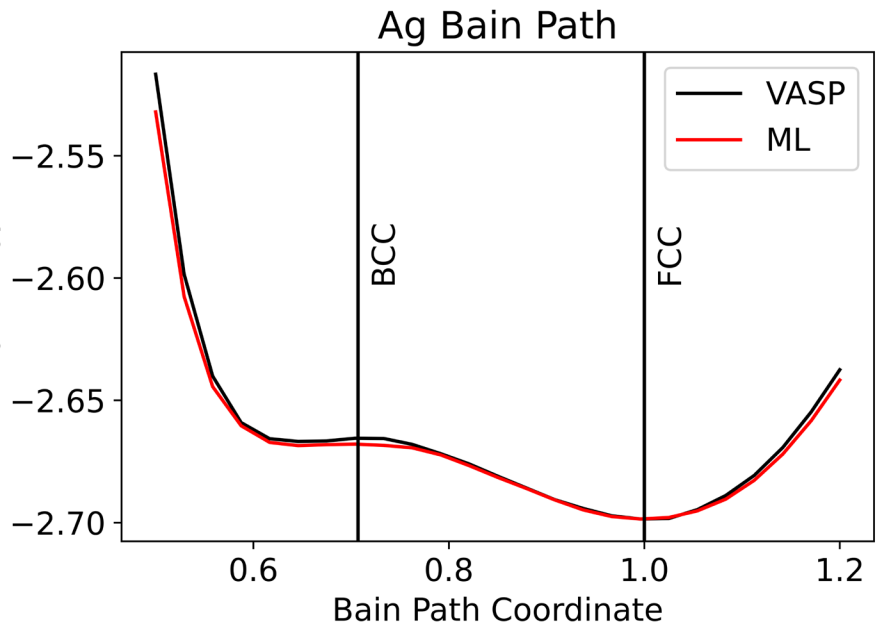
Aluminum Shock

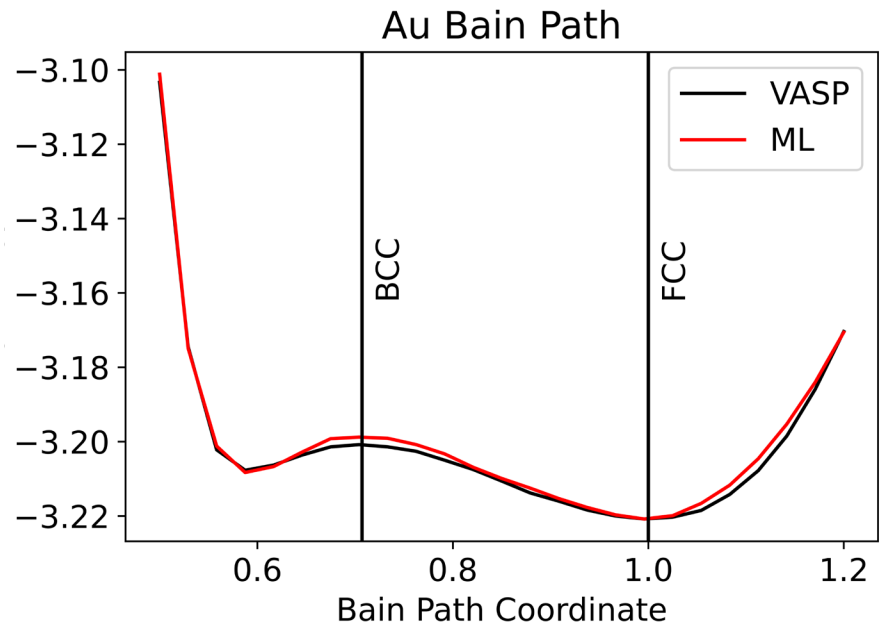


This methodology was used to build a ML interatomic potential for Al during Sierra open.

The potential was used to perform a 1.2 M atom shock simulation. Forces were verified by DFT.

Potentials Developed in ATCC-10: Au, Ag, and Pu





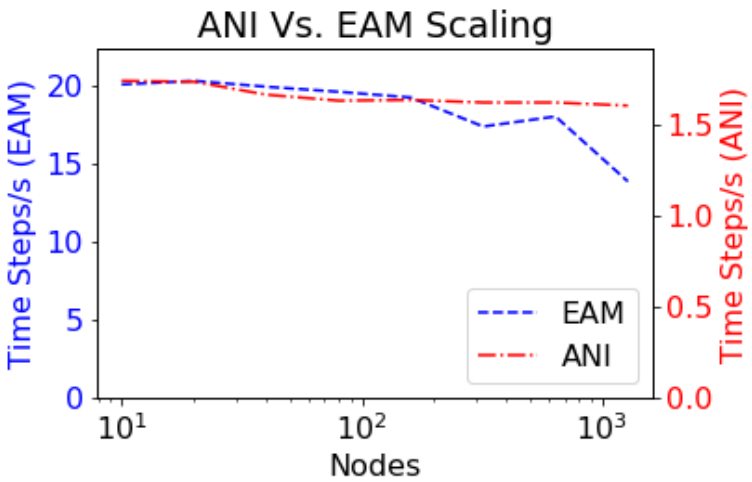
Au, Ag, and Pu ML potentials developed during ATCC-10 show good agreement with Density Functional Theory (DFT) properties.

Ag-ML potential melting point computed to be ~980 ºC, experimental is 962 ºC (very good agreement).

Pu in good agreement with DFT properties, ATCC-11 will further refine with higher accuracy methods.

Outlook and Lessons Learned

- **ML potentials represent about a x10,000,000 speedup over Quantum Mechanical Methods**
  - ML potential (ANI+LAMMPS) can run on 1280 Sierra nodes efficiently.
- **Sierra is an incredibly powerful resource.**
  - Development of Pu potential is computationally ~100 times more difficult than development of Au/Ag. **Only possible on a computer like Sierra.**
  - Distributed GPU architecture (Sierra) works extremely well for both Active Learning and domain decomposition (small regions of space on each GPU node).



- **Difficult to estimate time until completed and validated Pu-alloy potential. Between end of 2021 to end of 2022.**
  - Pu requires transfer learning. Collaboration with Gabi Kotliar (Rutgers).
    - Smith et al "Approaching coupled cluster accuracy with a general-purpose neural network potential through transfer learning" *Nat. Comm.* 2019, 10, 2903.
- **Future Work**
  - Incorporating experimental data in ML potential training (ongoing LDRD-DR project building capability).