materials modeling workflows

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Sandia National Laboratories

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Integration and Analysis in Materials Engineering

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LAMMPS molecular dynamics code

- https://lammps.sandia.gov
- https://github.com/lammps/lammps

- Classical molecular dynamics for materials modeling
- Sub-atomic to atomic to CG to meso to continuum scales
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- Features that enable **code coupling** and **workflows**
  1. Build and call LAMMPS as a **library**
  2. Wrap with **Python** or call Python from LAMMPS or both
  3. Support for **MDI** (MolSSI Driver Interface) for code coupling
  4. Inter-operability with **OpenKIM** database of potentials
  5. **Machine-learning** capabilities

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- Enables coupled simulations: multiphysics, multiscale
- Enables use in a complex workflow
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- Enables coupled simulations: multiphysics, multiscale
- Enables use in a complex workflow
- Often just requires bit of **re-design** at highest level
- Allow **multiple instantiations** of your "simulator"
  - another code can call it (from any language)
  - can embed it multiple times within a higher-scale model
- **Code details**
  - no global variables
  - don't use MPI_COMM_WORLD (not using all processors)
- Provide a **library interface** (API) to basic functionality
  - C-style interface has maximum portability
  - callable from any language (C++,C,Fortran,etc)
  - enables scripting (from **Python**)
  - enables wrapping/connecting with a **GUI** or **visualizer**
  - API should be easily extensible, just add a new function

Main.cpp for LAMMPS

```
include "lammps.h"
int main(int argc, char **argv) {
  MPI_Init(&argc,&argv);
  LAMMPS *lammps =
    new LAMMPS(argc,argv,MPI_COMM_WORLD);
  lammps->input->file(); // read input script
  delete lammps;
  MPI_Finalize();
}
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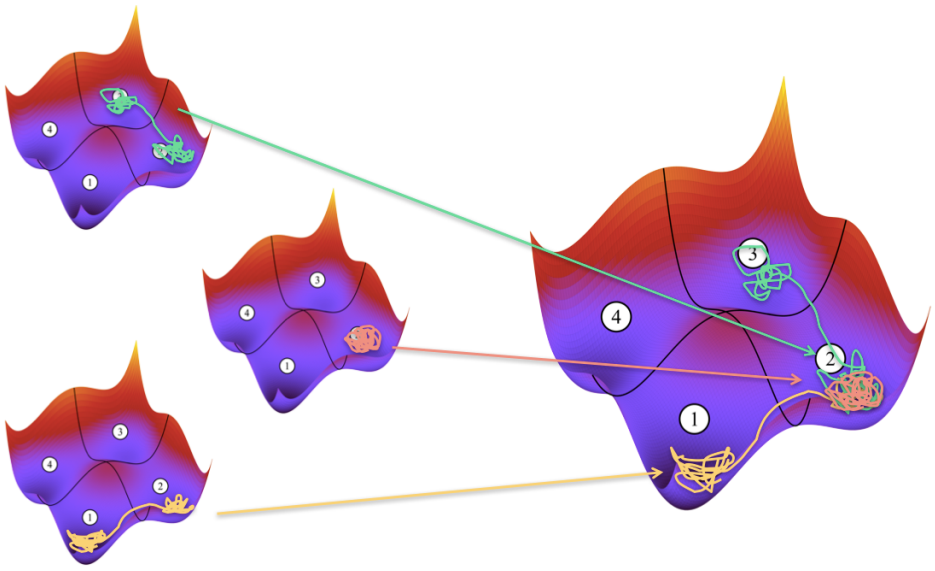
- Top-level LAMMPS is just a single class
- Just **remove main.cpp** to compile as a library
- Library call returns ptr to an instance of LAMMPS
  - C++ caller: use that ptr
  - anything else: include opaque ptr in other lib calls

ParSplice using LAMMPS as an MD engine

- Developed by Danny Perez (LANL) and collaborators
  Long-time dynamics through parallel trajectory splicing,
  D Perez, et. al., JCTC, 12, 18-28 (2016).



- Enables μs-ms time-accurate runs with 10^2-10^6 MD replicas
  - for rare-event systems (solid-state)
  - assigns configs to explore PE landscape, run each for few ps
  - detects and catalogs events in a distributed database
  - splices event sequence into long trajectories with correct stats
- Extended LAMMPS library API to facilitate this usage mode

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Example:

- QM code instantiates LAMMPS as a library
- QM code invokes MD run
  - uses **fix external**, sets a function pointer
  - triggers callback at appropriate point in timestep
- LAMMPS calls back to QM each step to get QM forces
- QM code can access LAMMPS data (coords, forces, etc)

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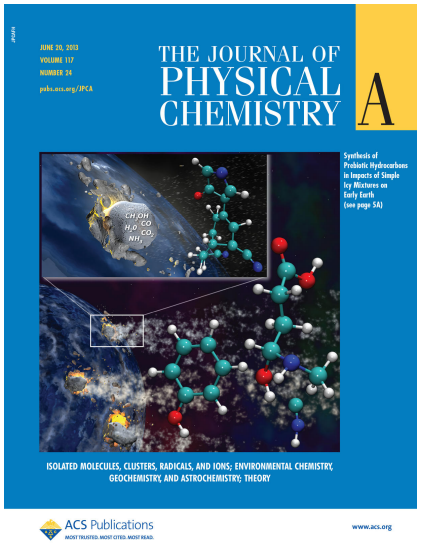
- Nir Goldman (LLNL) runs Fortran **DFTB+** with LAMMPS in this manner
- *Prebiotic Chemistry Within a Simple Impacting Icy Mixture*, N. Goldman and I. Tamblyn, J Phys Chem A, 117, 5124 (2013).



Other examples for using LAMMPS as a library

Tom Swinburne (CINaM Marseille, CNRS)

- TAMMBER: explore energy landscape to build kMC model
- 1000s of TAD runs, energy minimizations
- Phys Rev Materials 2018, DOI: 10.1103/PhysRevMaterials.2.053802

Noam Bernstein (NRL)

- Nested sampling for P-T-composition phase diagrams
- TE-HMC & GMC with LAMMPS lib as MD engine via ASE
- Phys Rev E 2017, DOI: 10.1103/PhysRevE.96.043311

ASE = Atomic Simulation Environment

- `https://wiki.fysik.dtu.dk/ase`
- simulation protocol (setup, run, analyze, viz) in Python
- supports dozens of QM and MD simulators as **calculators**
- can use LAMMPS either as a library or a stand-alone code

(2) LAMMPS with Python

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1. **Ctypes** module makes it easy to wrap any C-style API
   - every LAMMPS library function is exposed to Python
   - also allows callbacks to a Python function
2. **Multiprocessing** module to loop over 1000s of tasks
   $\Rightarrow$ each of which can instantiate LAMMPS as a lib
3. **Mpi4py** module enables parallel Python and split of MPI
   $\Rightarrow$ run one or more LAMMPS instances in parallel

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- LAMMPS data structs accessible by **Numpy** (no data copy)

```
nlocal = lammps.extract_global("nlocal")
cptr = lammps.extract_atom("x")
coords = np.ctypeslib._array(cptr,shape=(nlocal,3))
```

- Python versions of LAMMPS **styles**: pair, fix, variable

(3) MolSSI Driver Interface (MDI) for code coupling

Goal: Enable scientific codes to easily exchange data (for materials modeling)

- **MDI** = library created by Taylor Barnes at MolSSI
- MolSSI = Molecular Sciences Software Institute (NSF funded)
  - https://molssi.org
  - https://molssi-mdi.github.io/MDI_Library
- Nice paper: TA Barnes et al, *The MolSSI Driver Interface Project: A framework for standardized, on-the-fly interoperability between computational molecular sciences codes*, Comp Phys Comm, 261, 107688 (2021).
- Standardized, high-level way to couple codes via **client/server** model (driver/engine in MDI lingo)

MDI in a nutshell for materials modeling

- Example #1: AIMD or QM/MM
  - **MD** = driver: sends coords to QM
  - **QM** = engine: computes and returns forces
  - QM/MM Python script is driver, MD and QM are both engines
- Example #2: Monte Carlo using MD as an engine
  - **MC** = driver: makes a complex move (configurational bias)
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- More examples: ML, NEB, sampling, PIMD, etc
- Driver can use **multiple instances** of multiple engines
- Umbrella drivers can be Python scripts

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- Driver can use **multiple instances** of multiple engines
- Umbrella drivers can be Python scripts
- Codes **exchange strings & data** via MDI calls (MPI-like)
  - ">COORDS" = here are my atom coords
  - "<COORDS" = send me your atom coords
  - under the hood: MPI or TCP/IP messaging (user choice)
  - MD can make MDI calls in middle of timestep

Advantages of client/server mode of code coupling

1. Two codes can be **stand alone** executables
2. Codes in **different languages**: C/C++, Fortran, Python
3. Easy to run codes on **different #s of processors**:
   - mpirun -np 4 driver -mdi ... -np 60 engine -mdi ...
   - sockets means 2 codes can run in different places
4. Use MDI-defined or custom **data exchange protocols**:
   - any MD code can work with any QM code

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- **LAMMPS** about to release MDI support (driver & engine)
- Other codes with some level of MDI support:
  - **MD**: Tinker, OpenMM
  - **QM**: Q Espresso, Molpro, MOPAC, GAMESS, NWChem, Q-Chem, Turbomole, CP2K, Siesta, ...
  - All except QE support MDI via **QCEngine** wrapper (files)
- **Key point**: any code can use MDI, not just MD & QM

(4) Interoperability with OpenKIM project

Open Knowledgebase of Interatomic Models (NSF funded)
https://openkim.org

- Goal: enable reliable, reproducible, portable atomistic sims
- Repository of interatomic potentials (tested, versioned)
- Material properties calculated for all potentials
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- LAMMPS has a **pair_style kim** command:
  - any KIM model can be used in a LAMMPS simulation
  - **model** = analytic potential plus material-specific parameters
  - KIM has ∼500 such models
  - also has ∼20 analytic potentials not natively in LAMMPS
- LAMMPS input scripts can **query KIM website** in real time
  - list of models that match criteria
  - model parameters: lattice type, lattice constant, α coeff, etc

Example workflow using LAMMPS + KIM repository

```
variable species index Ni        # grab list of Ni potentials
kim query model index get_available_models species=[${species}]

label loop
    log log.${model}
    kim init ${model} metal      # initialize for metal units
    kim query alat ...           # this potential's lattice constant
    lattice fcc ${alat}
    create_box ...
    create_atoms ...
    kim interactions ${species}  # invokes pair_style kim with model
    dump 1 all custom 1000 dump.${model}
    run 100000
    clear
    next model

jump SELF loop
```

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- Could loop on species, query alloy models, run N sims at once, each in parallel

(5) Machine learning: workflows for fitting ML potentials

- Machine learning interatomic potentials for classical MD:
  - trained on **large volumes** of QM data
  - forces via **geometry-based** eqs or NN, not physics-based eqs
  - **goal**: QM accuracy in an MD simulation for cheap O(N) cost

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- Typical training procedure is a workflow:
  - DFT data for small configs: energy, forces, virial = **QM truth**
  - Each atom + neighborhood $\Rightarrow$ geometric **descriptors**
  - Descriptors used in **big matrix** eq or as input to **NN**
  - Solve big matrix (e.g. least squares) or iteratively train NN
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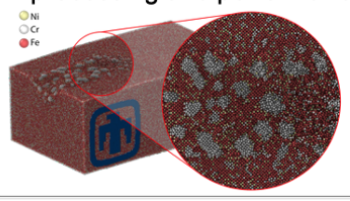
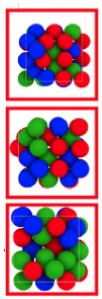
- **fitSNAP.py** $\Rightarrow$ `https://github.com/FitSNAP/FitSNAP`
  - used to train **SNAP** (spectral neighbor analysis potential)
  - calls LAMMPS as library to compute bispectrum descriptors
  - parallelism: **multiple LAMMPS instances**, large LSQ solve
  - output = vector of dozens or a few 100 bispectrum coeffs

Applications of SNAP via fitSNAP.py

High Entropy Alloys

- Complex chemical composition space limits accuracy of MD predictions
- Massive training spaces needed to generate a ML-IAP
- Predictive modeling of AM processing and performance

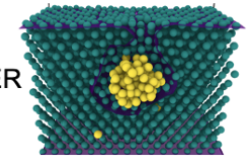


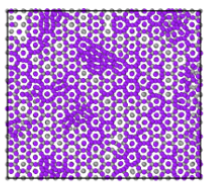


Plasma-Facing Materials

Office of Science

- Multiscale effort to predict lifetime and failure modes of ITER
- SNAP potentials generated for W/Be/N/H/He
- Bubble bursting at tungsten surface
- Beryllium deposition on tungsten leading to bimetallic ordering

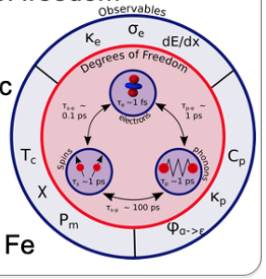




OAK RIDGE National Laboratory

Coupled-Physics Modeling

- REHEDS LDRD FY20 (A. Cangi)
- Integrated software tools for strongly coupled magnetic, phononic and electronic degrees of freedom
- Actively learned ML-IAP for phononic sub-system
- Targeting magneto-structural phase transitions in Fe



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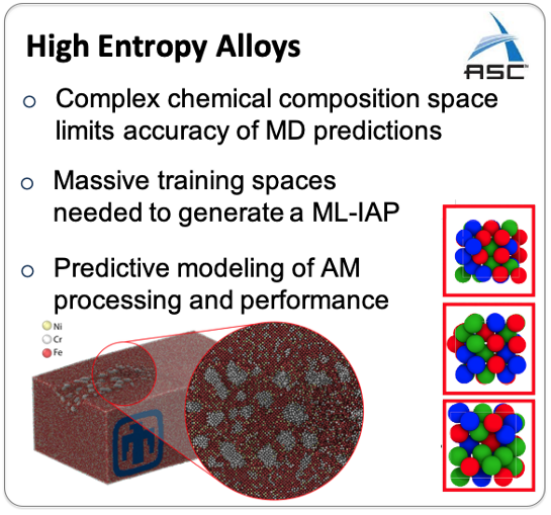

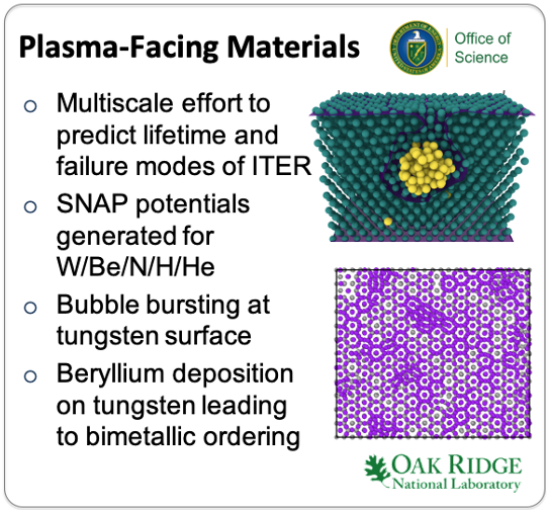

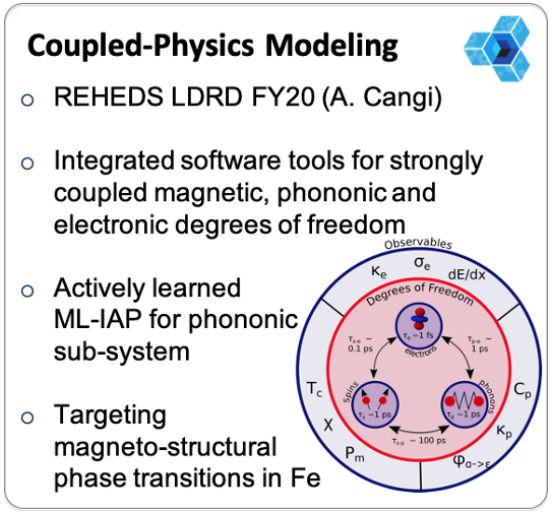

- Dislocation motion (Ta)
- Radiation damage (InP)
- Shock phase transitions (actinides)
- Super-ionic condutors (LiN)
- Vitrification (GeSe)
- Lithium-ion batteries (LiMoS)
- Thermoelectric materials (SiGeSnPb)

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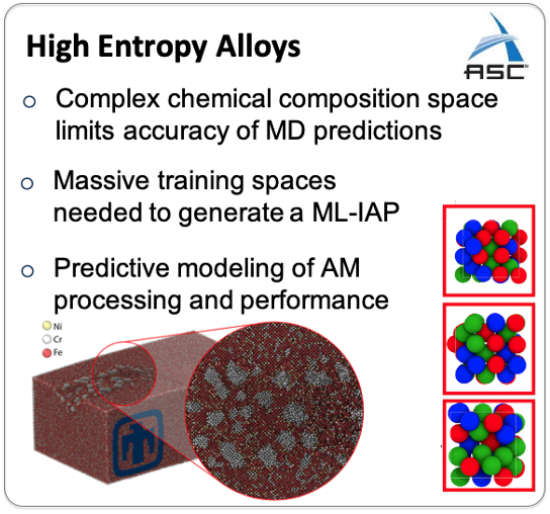

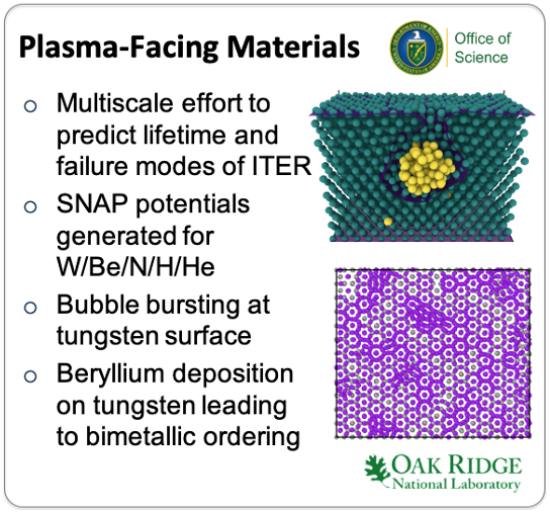

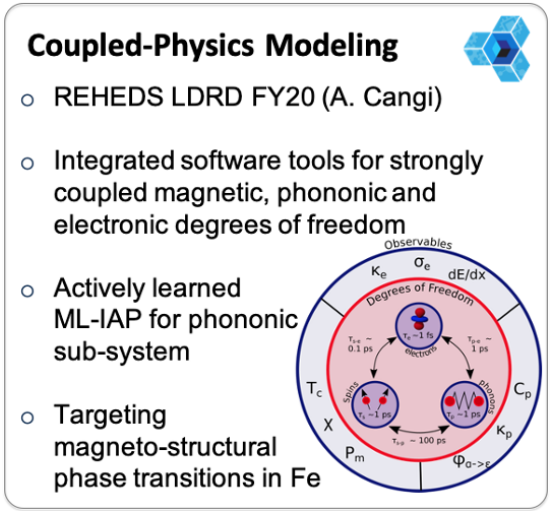

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Can train a SNAP potential for a **specific material or application**

New ML potential framework in LAMMPS

Work with Nick Lubbers (LANL)

- All MLIAPs perform 3 steps in MD context:
  1. compute descriptors from atoms
  2. compute model gradients with respect to descriptor gradients
  3. compute forces from model gradients
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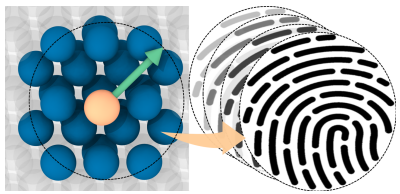
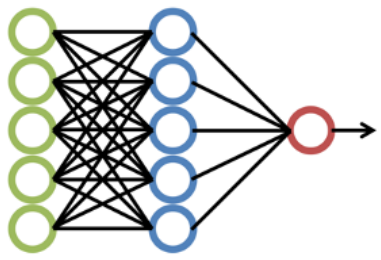
moment tensors, SOAP, bispectrum, ACE

Energy Models:

linear & kernel-ridge regression, Gaussian process

non-linear opt, NNs & hierarchical NNs





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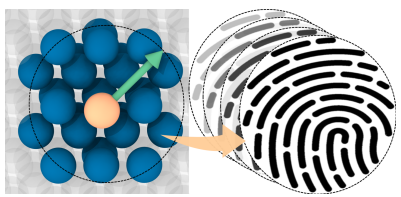

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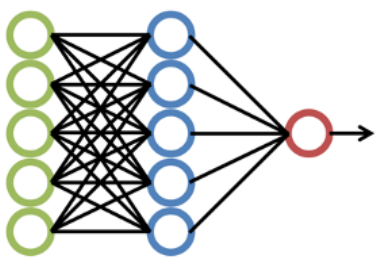

New pair style MLIAP allows:

- **mix-and-match** any Descriptor with any Model
- call back to Python, link with **PyTorch** for GPUs

Thanks for your attention

Thanks to Tom Swinburne (CINaM) & Noam Bernstein (NRL)
for lib examples, and to Ryan Elliott (U Minn) for OpenKIM work

LAMMPS: https://lammps.sandia.gov

MolSSI MDI: https://molssi-mdi.github.io/MDI_Library

OpenKIM: https://openkim.org

Email questions to:

athomp at sandia.gov (machine learning)
mitwood at sandia.gov (fitSNAP or SNAP applications)
sjplimp at sandia.gov (anything else)