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Machine-Learned Potentials: DFT-Level Accuracy for Real-World R&D

Cheng-Wei Lee, Materials Design, Inc.

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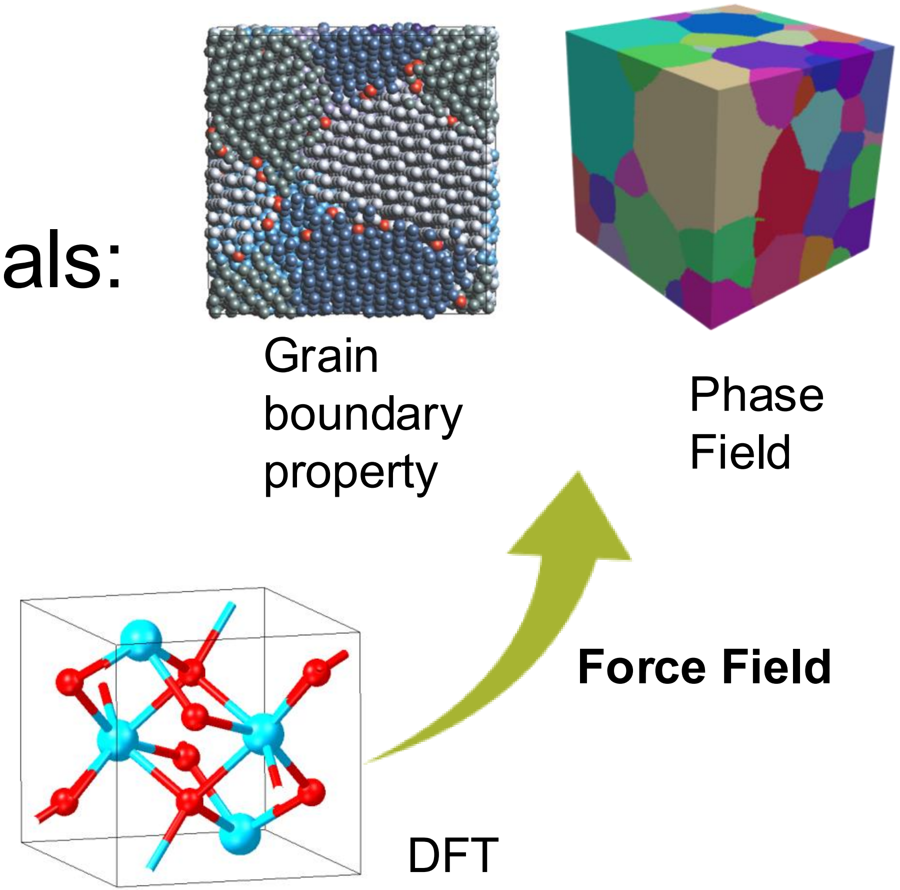

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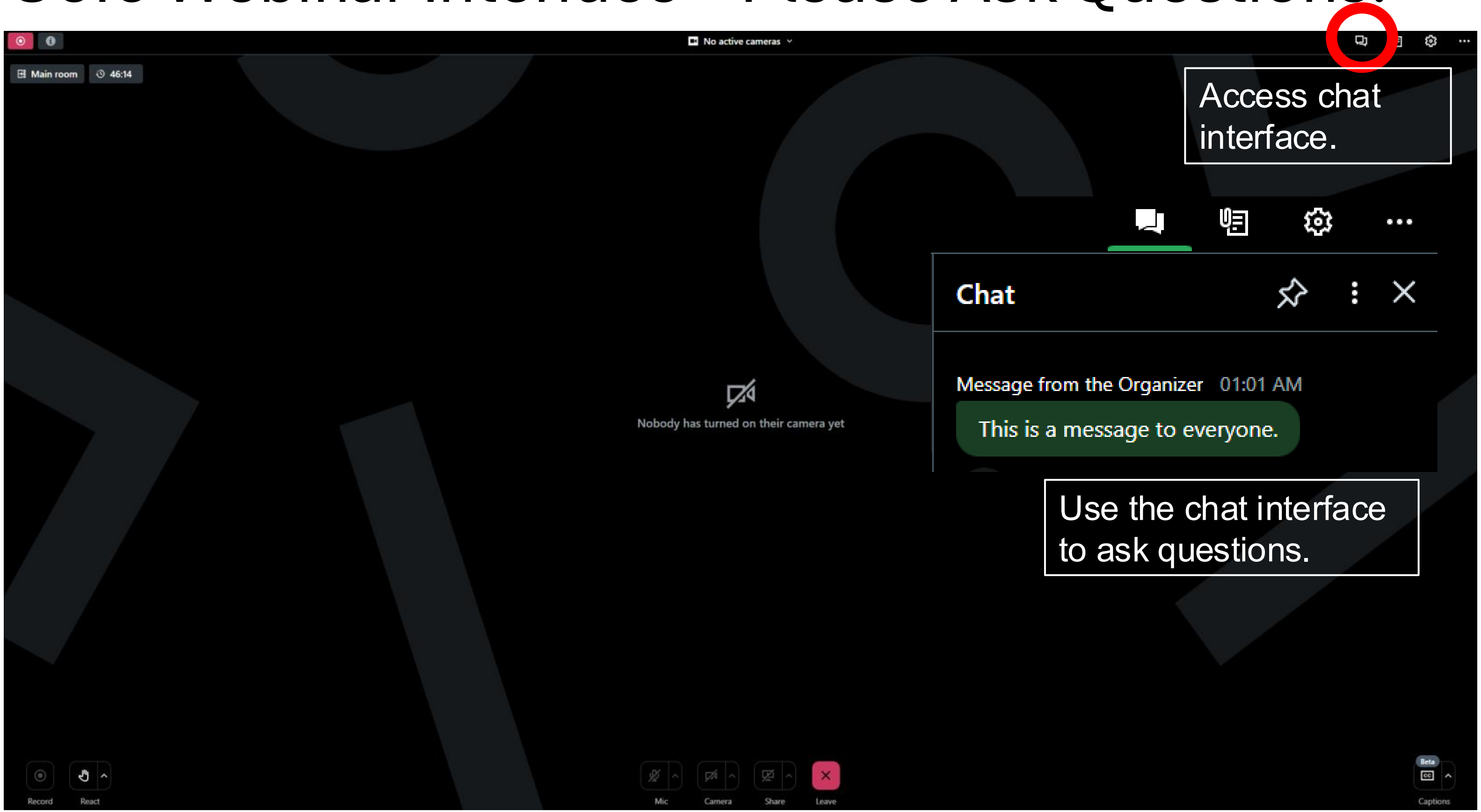

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Webinar Speakers

Katherine Hollingsworth *Dr. Cheng-Wei Lee* *Dr. Volker Eyert* *Dr. Michele Kotiuga*

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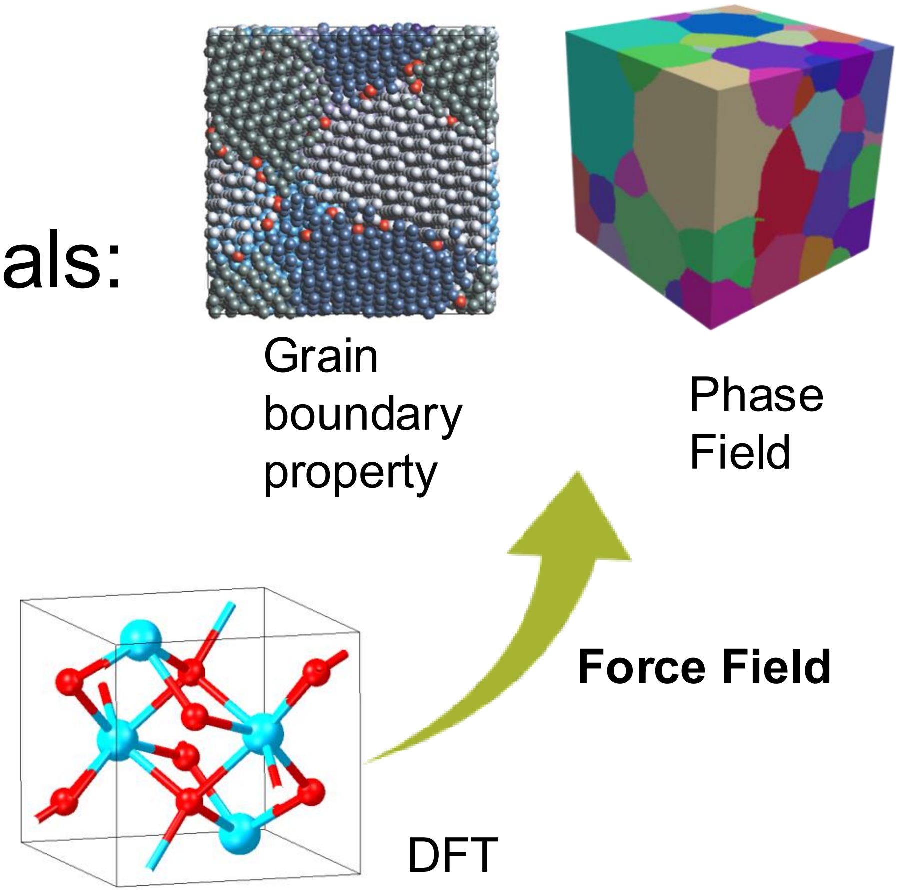
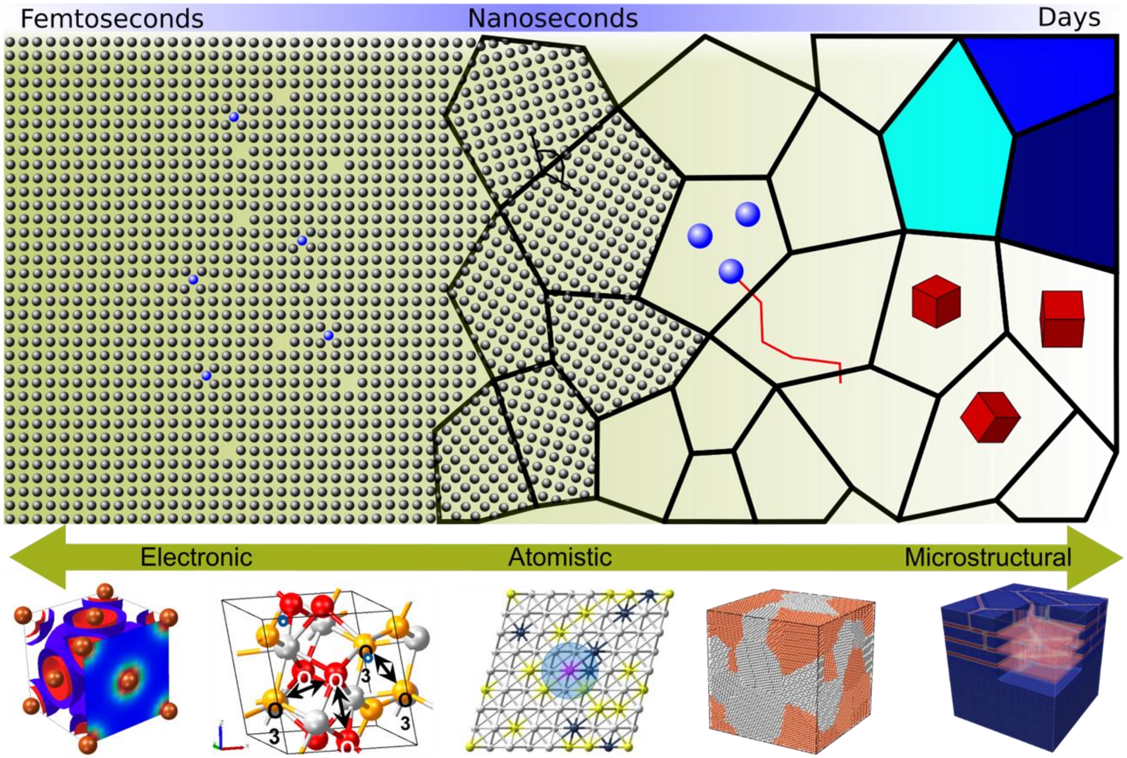


When Do We Need Multiscale Simulations?



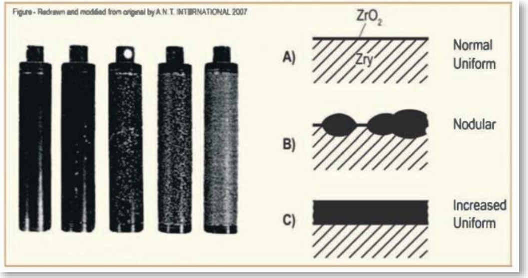
Corrosion

The global cost of corrosion is estimated to be US$2.5 trillion, which is equivalent to 3.4% of the global GDP. Numerous industries are affected including:

1) Energy:
   - Water-cooled reactors
     - Corrosion of fuel cells is one of the major life-limiting degradation mechanism in these reactors

2) Energy:
   - Oil & Gas
     - Corroding pipelines and various equipment in Oil and gas

3) Automotive:
   - Magnesium alloys have been used due to their mechanical properties and castability but they have poor corrosion resistance.



R. Adamson et al., *Corrosion mechanisms in zirconium alloys*, *ZIRAT12 Special Topic Report* (2007)

M. Askari, M. Aliofkhazraei, and S. Afroukhteh, J. Nat. Gas Sci. Eng. **71**, 102971 (2019) https://doi.org/10.1016/J.JNGSE.2019.102971

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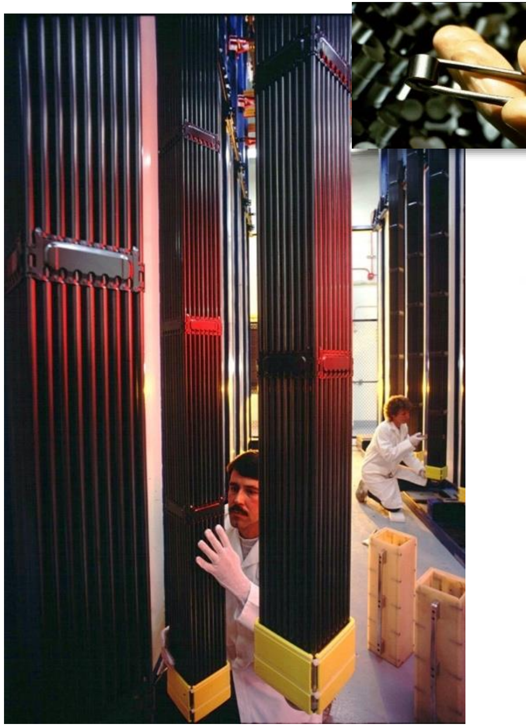
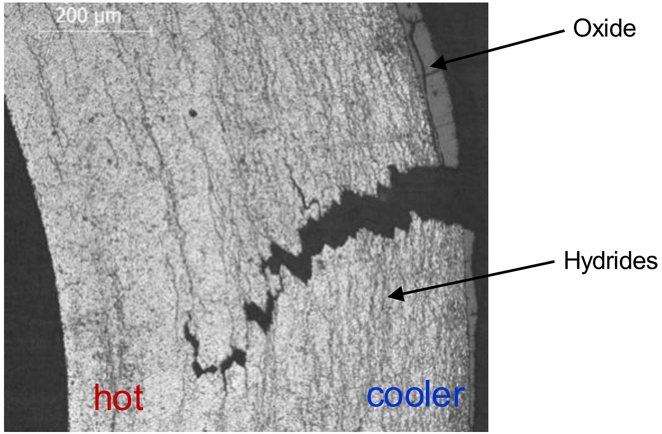
Hydrogen Embrittlement of Zirconium Alloys



95% Zr; Sn, Nb, Fe, O can be present



Cross section of fuel rod, Zr alloy

Corrosion of Zr alloys:

$$Zr + 2H_2O \rightarrow ZrO_2 + 4H$$

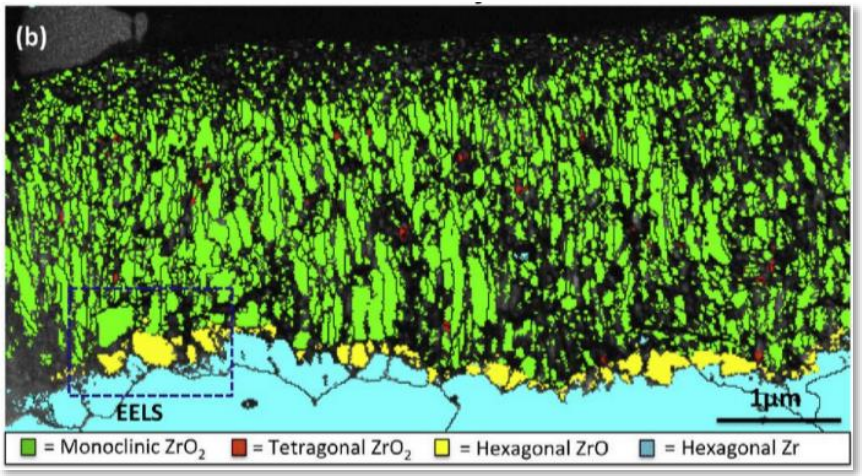
$$2H \rightarrow H_2$$

$$xH + Zr \rightarrow ZrH_x$$

embrittles

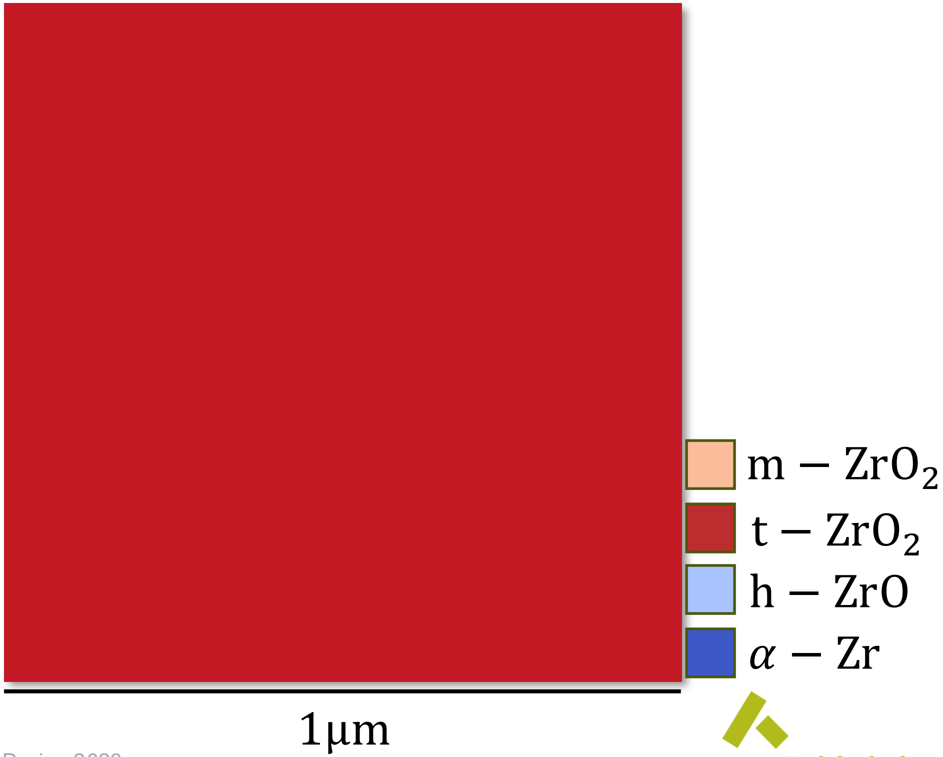
Corrosion in Zirconium Alloys

~1 year of experiment



Hu et al., Micron. **69**, 35 (2015)

~4 hr of Phase Field simulation



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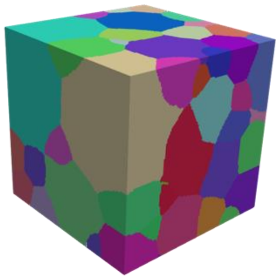
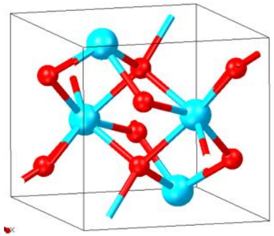
An Accurate Prediction Requires Accurate Inputs

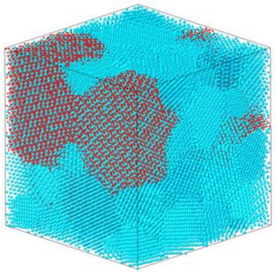
Continuum simulations
(phase field)





Electronic
structure

Atomic
microstructures



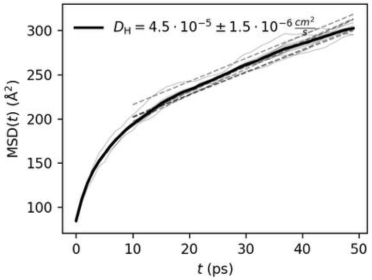
Required inputs:
Free energy
Interface energy
Diffusion (bulk& interface)
Elastic energy
… etc.

Length scale

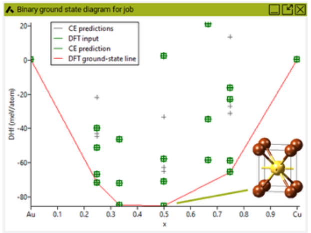
Time scale

DFT can Provide Most Key Inputs for Phase Field Models

Diffusion

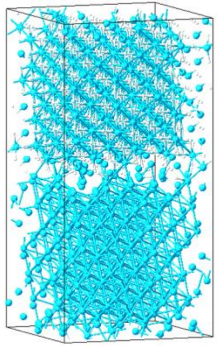


Free energy

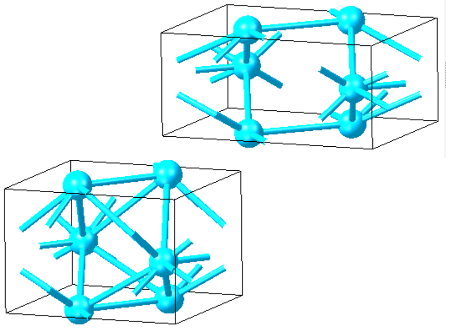


$$E = N \sum_F d_F \Pi_F(\mathbf{s})$$

Interfaces



Elastic energy



$$\frac{\partial c}{\partial t} = \nabla M(c, \eta, \sigma) \nabla \frac{\delta F}{\delta c}$$

$$\frac{\partial \eta}{\partial t} = -L \nabla \frac{\delta F}{\delta \eta}$$

$$F = \int dV \left[f_{chemical} + f_{interface} + f_{elastic}\right]$$

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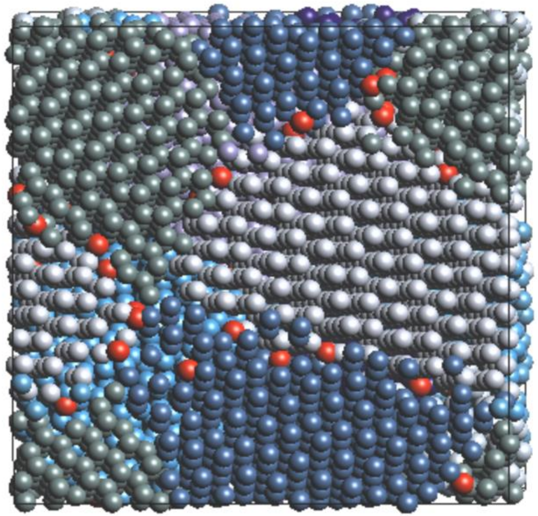
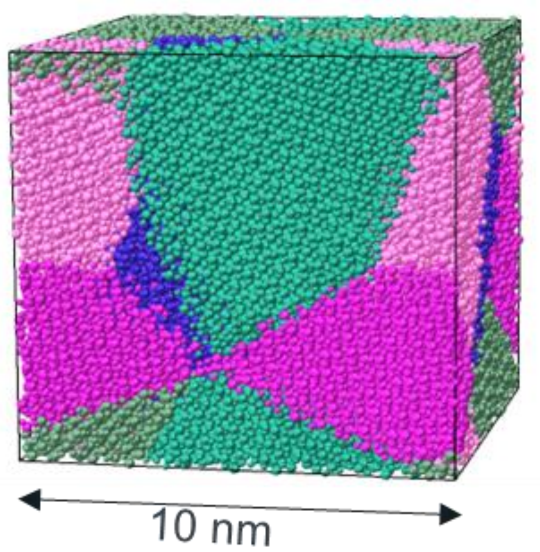
DFT with Grain Boundaries are Computationally Expensive

Diffusion in grain boundaries (GBs)



Grain boundary energy



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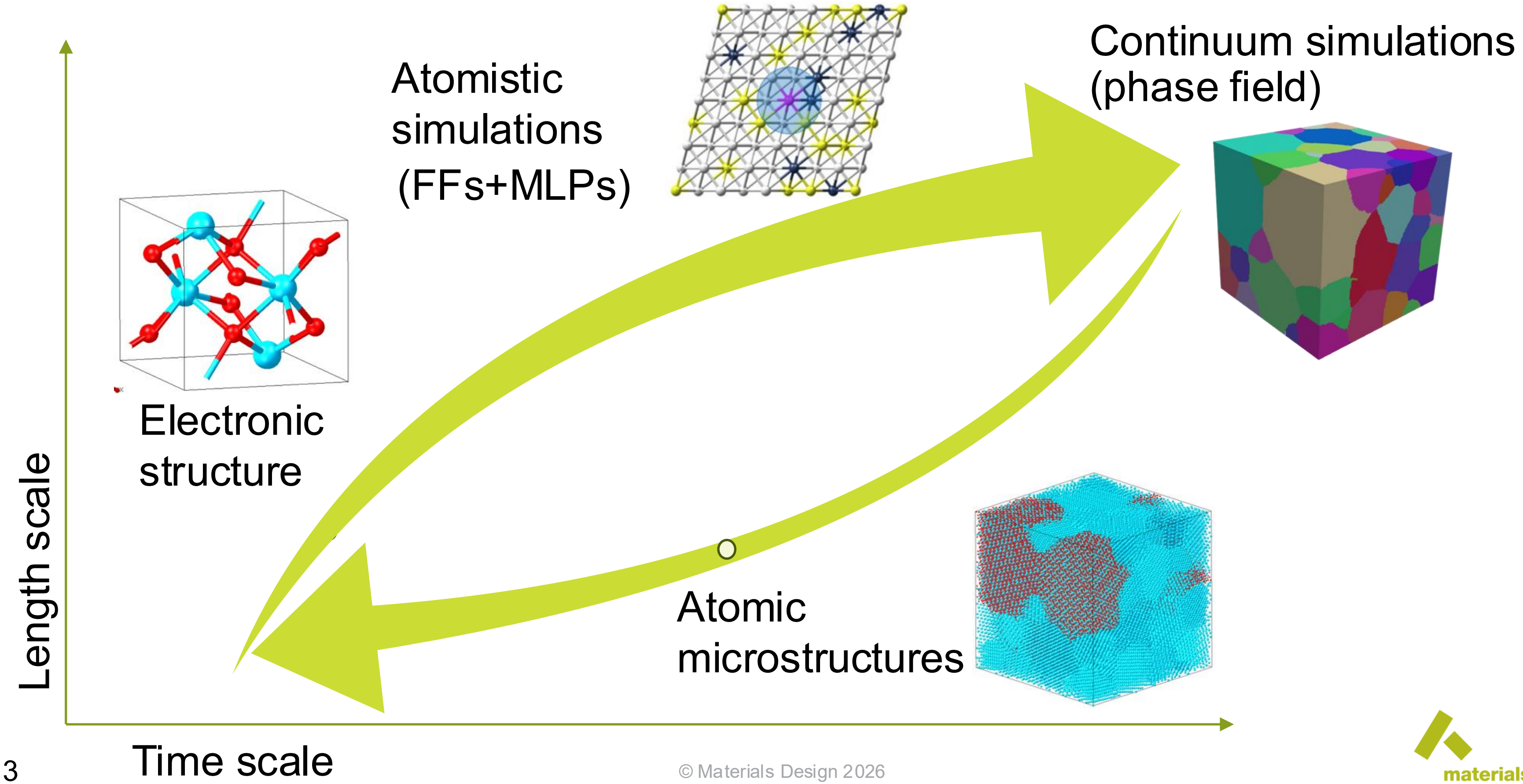
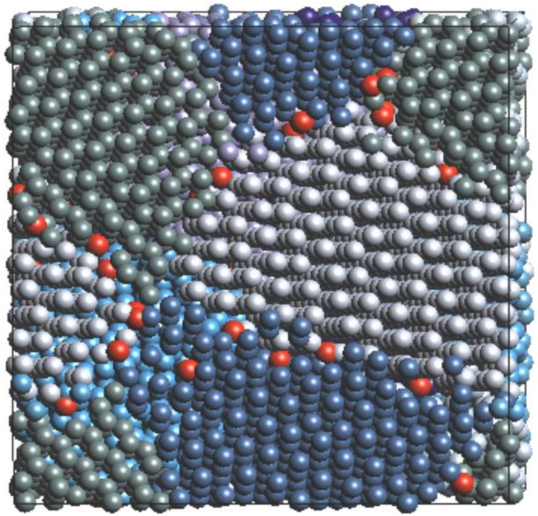
MLP Provides DFT Accuracy with Much Lower Cost



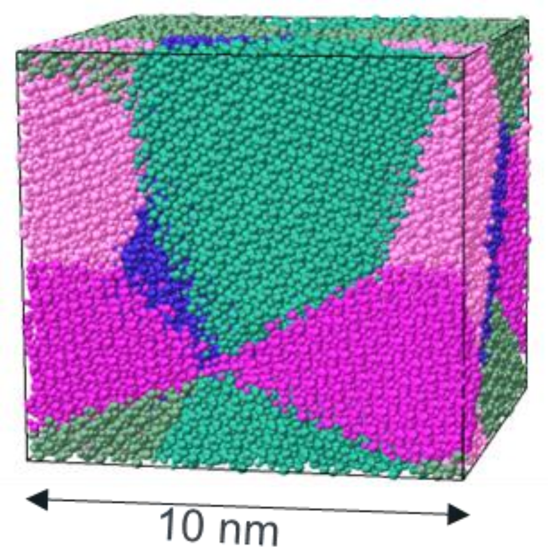
FFs/MLPs Bridge the Gap and Predicted GB Properties

Diffusion in grain boundaries (GBs)



Faster diffusion with grain boundaries

Grain boundary energy



m-ZrO_2 / m-ZrO_2: 2.6 J/m^2

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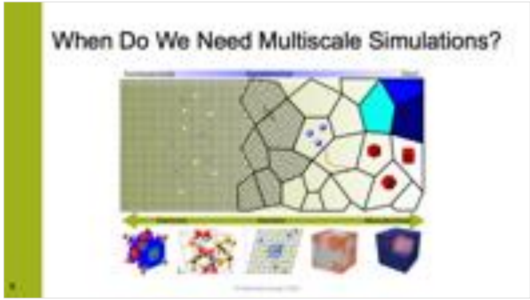
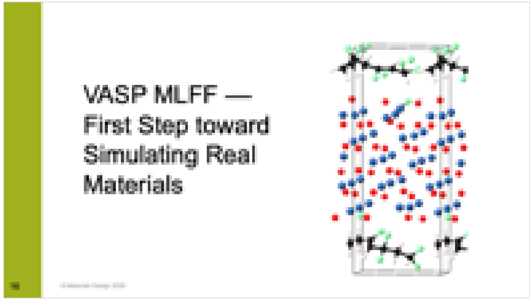
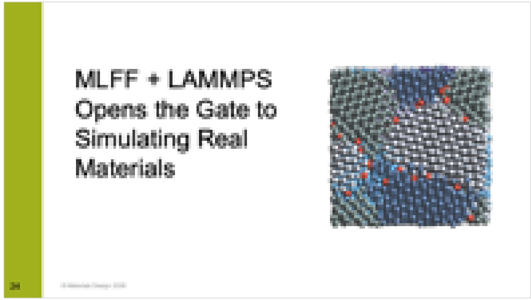
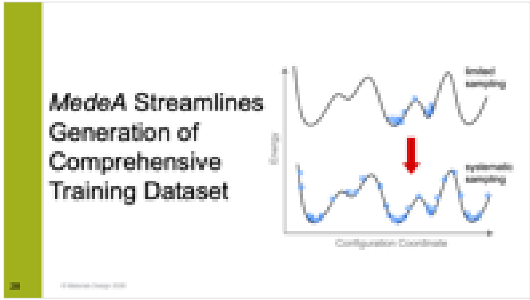
Outline









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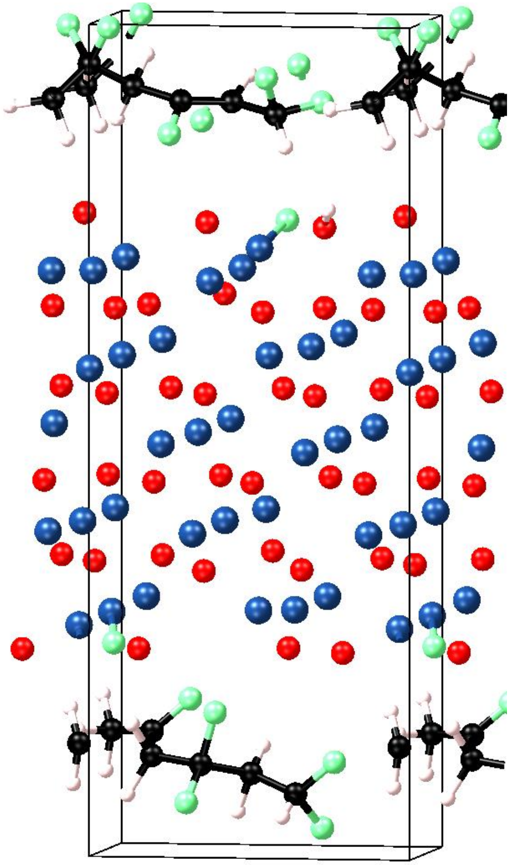
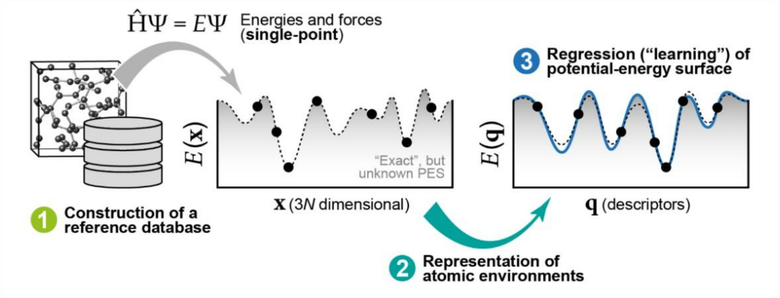
VASP MLFF — First Step toward Simulating Real Materials



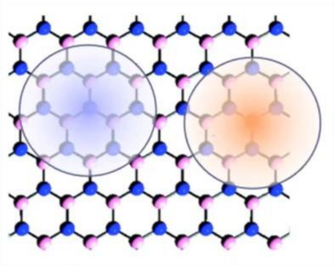
What is VASP MLFF?

- Motivation: Map *ab-initio* potential energy surface (PES) with a set of local atomic descriptors

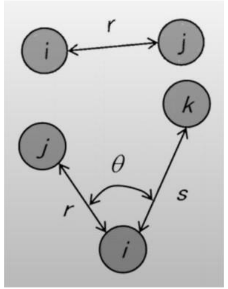


- Basic components
  - **Database**: Training set of reference structures with energies, forces, and stress calculated with a DFT method
  - **Descriptors:**
    - Describe the local environment of each atom in the database
    - Potential energy is a function of the sum of the energies of each atom depending on the local environment
  - **Regression:** determine the weight of each atomic contribution to the potential energy to obtain the best approximation of the DFT energy for each structure of the database

Atomic descriptors



Classical density distribution of atoms around a central atom



Pair-correlation and angular functions; translationally and rotationally invariant

Jinnouchi et al., *J. Chem. Phys*. 152, 234102 (2020)

Deringer et al., *Adv. Mater.* 31, 1902765 (2019)

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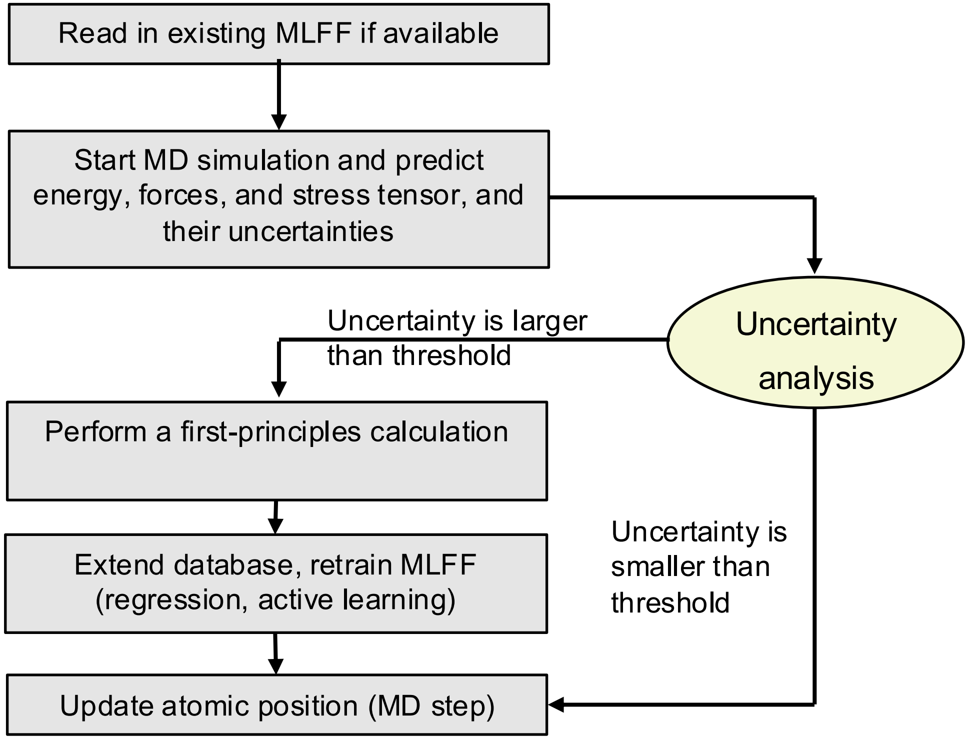
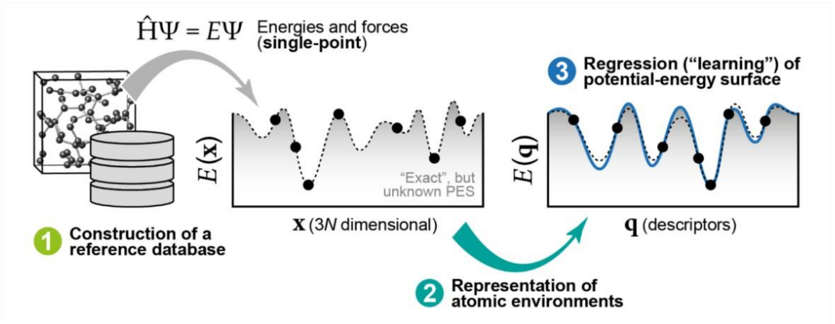
On-the-fly Training is the Major Strength of VASP MLFF



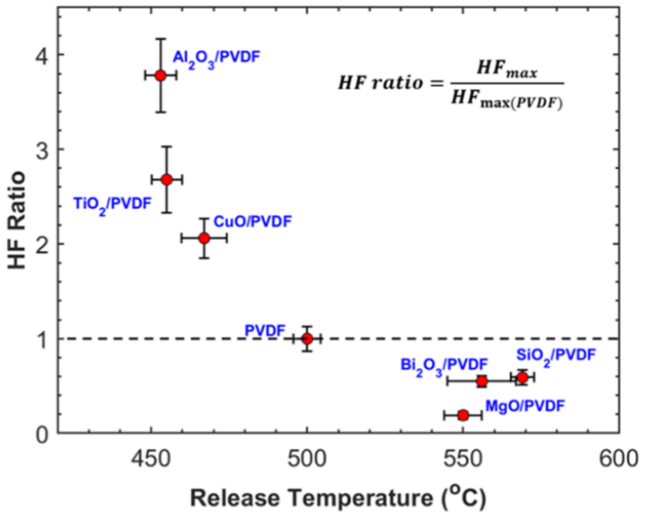
MLFF modes

- Create initial MLFF by on the-fly-learning
- Continue MLFF on-the-fly-learning
- Select mode: add special training data discard unwanted training data
- Refit MLFF with, e.g., modified descriptors

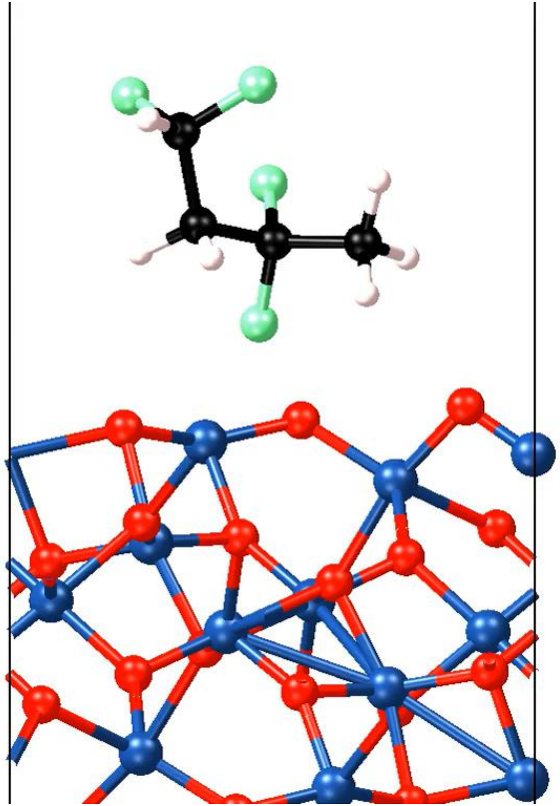


PVDF Decomposition Reactions Reported in Literature

- Measured HF release of PVDF/metal oxide composites [1]



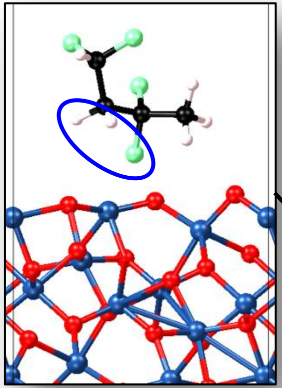
- Al_2O_3 enhance decomposition behaviour and the HF release of PVDF



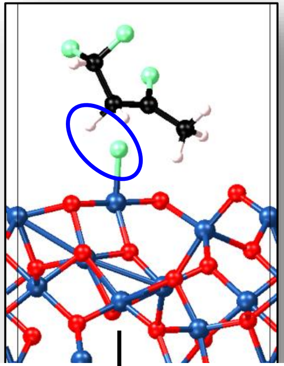
[1] Rehwoldt et al., High-Temperature Interactions of Metal Oxides and a PVDF Binder,Appl. Mater. Interfaces 14, 8938 (2022).

Verification of “HF” Abstraction with “Pure” DFT Calculations

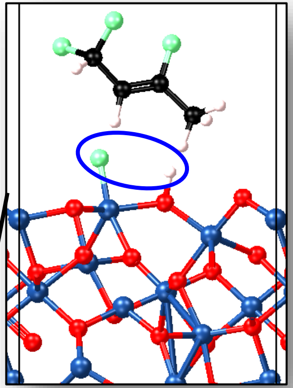
- The reaction mechanism is investigated with the nudged-elastic band (NEB) approach as implemented in *MedeA-TSS*; compute engine: *MedeA VASP* using the GGA method optB86b-vdW [1]



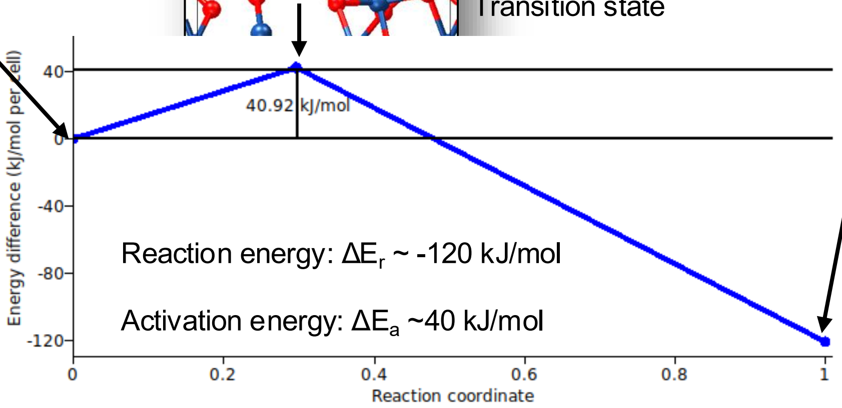
Educt



Transition state



Product



Estimated rate for 500 K:

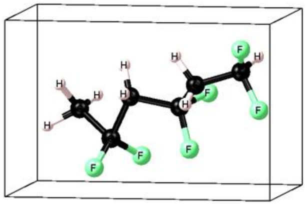
$$r = \frac{k_B T}{h} e^{-\Delta E_a/RT} \approx 0.5\ \mathrm{ns}^{-1}$$

[1] Klimeš et al., Chemical Accuracy for the van Der Waals Density Functional, J. Phys.: Condens. Matter 22, 022201 (2009).

VASP MLFF: On-The-Fly-Machine Learning Potential

On-the-fly learning procedure:

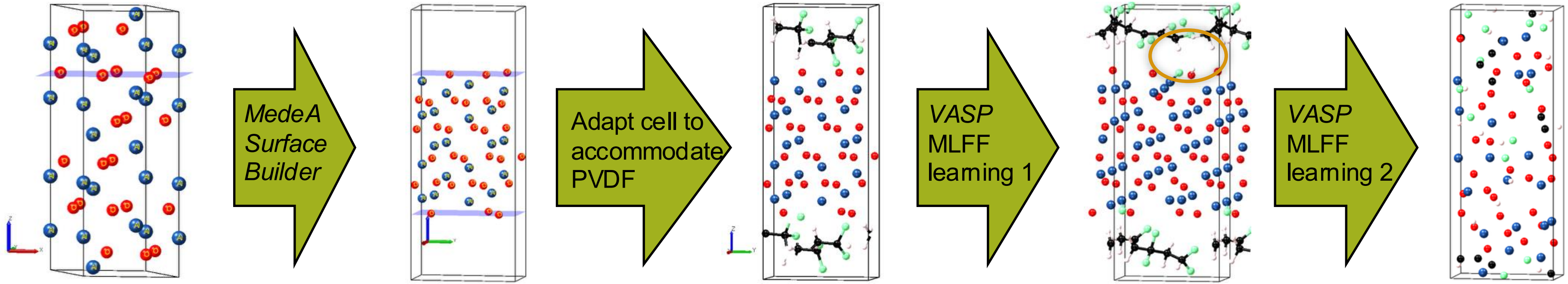
- **Step 1**: 1 ps NVT MD simulation,temperature ramp 500→1500 K
- **Step 2:** 0.5 ps NVT MD simulation, temperature ramp 500 →800 K
- Applied DFT method: optB86b-vdW [1]
- total compute wall time on 12 Intel CPU cores: ~14 h



PVDF 3mer: encompasses all key structural features of a polymer chain

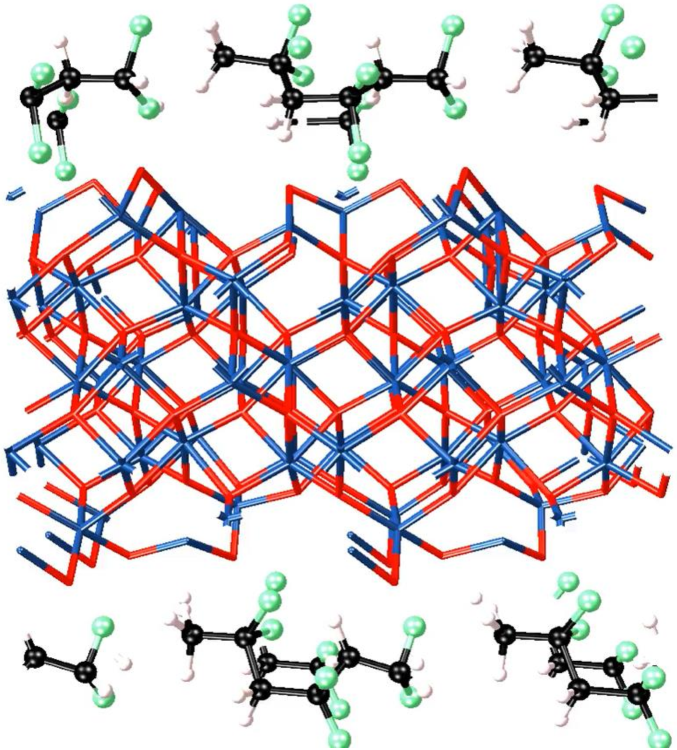
Al_2O_3 bulk: fully relaxed bulk structure (corundum)

Al_2O_3 (001) surface model: symmetric & stoichiometric



[1] Klimeš et al., Chemical Accuracy for the van Der Waals Density Functional, J. Phys.: Condens. Matter 22, 022201 (2009).

VASP MLFF Application



Simultation details:

- PVDF 3mer on Al_2O_3 (001) slab
- 100 ps NVT MD simulation @ 500 K,
- Wall time on 16 Intel CPU cores: ~95 h

What we gain with MLFF?

- More realistic model
- Temperature effect

optimization knobs

- Long MD trajectory with reasonable resource

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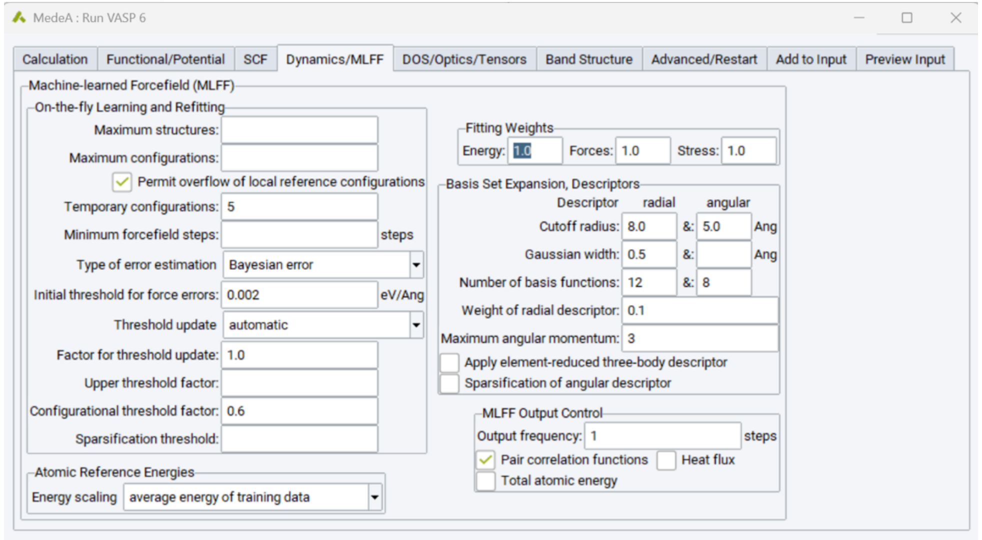
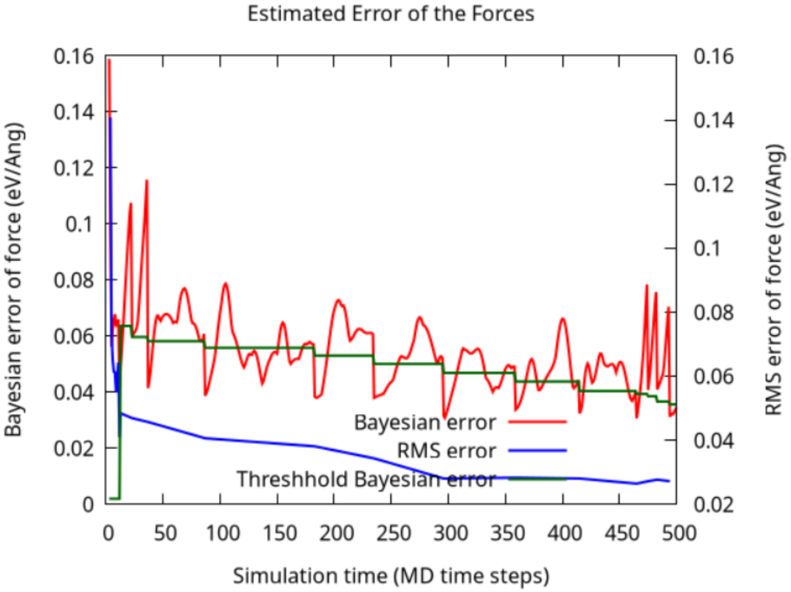
MedeA VASP Allows Easy Adoption of MLFF

GUI streamlines input files



Integrated tracking of the process



We are here to support your R&D activities

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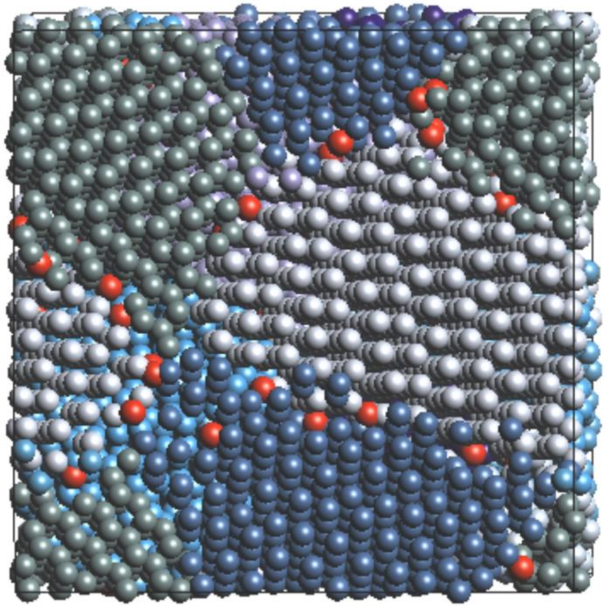
MLFF + LAMMPS Opens the Gate to Simulating Real Materials



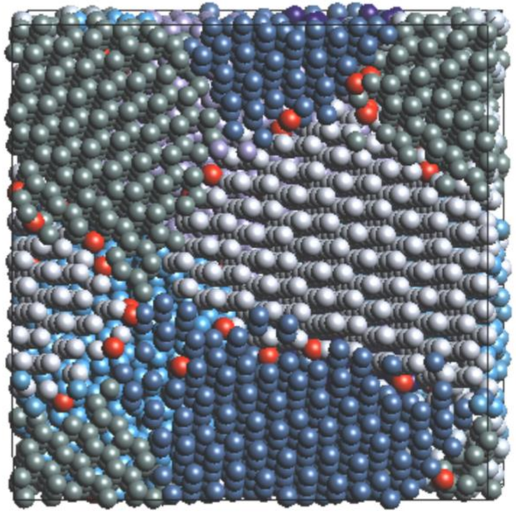
LAMMPS Can Better Account for Real-World Scenarios

Capability	VASP	LAMMPS
System Size	Typically < 10^4 atoms	Millions to Billions
Ensemble Variety	NVE, NVT, NPT, NPH	Also includes µVT
Mechanical Testing	Restricted to small cell	Realistic microstructure
Combined Potentials	No	Yes
Spatial handling	Only global cell	Group and region
On-the-fly Analysis	Basic	Customized

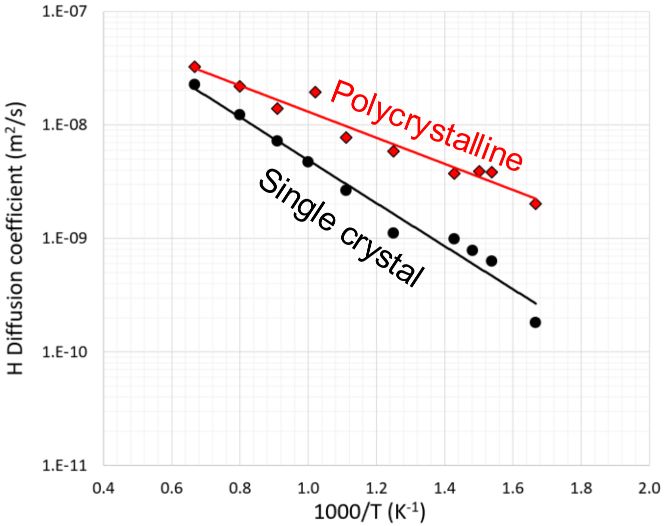
MedeA has a suite of properties modules utilizing LAMMPS unique features

H grain boundary diffusion in Zr

Polycrystalline model of Zr with atoms in GBs can be built directly in the Microstructure Builder



H diffusion as function of T in polycrystalline or single crystal model



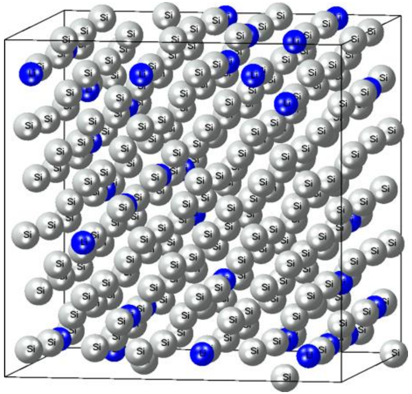
Faster diffusion in polycrystal than in single crystal

1) Build 2 models:
   1) Polycrystalline
   2) Single crystal – no GBs
2) Populate with H and compute diffusion coefficient
3) Diffusion of H is enhanced when GBs are present

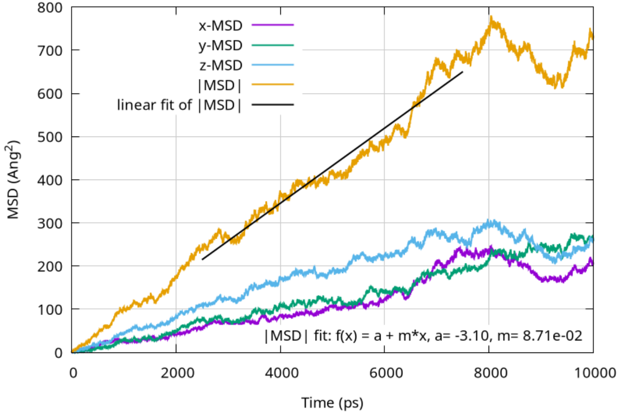
MedeA Has a Suite of Property Modules & Flowcharts

- *MedeA LAMMPS*
- *MedeA MD Phonon*
- *MedeA Diffusion*
- *MedeA Thermal Conductivity*
- *MedeA Viscosity*
- *MedeA CED*
- *MedeA Surface Tension*
- *MedeA Deposition*

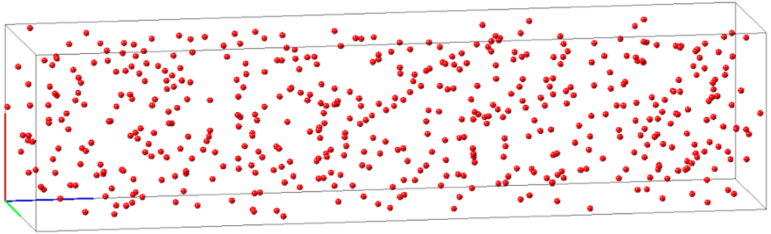
Li insertion in Si



Li diffusion in $LiPF_6$



Thermal conductivity of structurally complex system



https://www.materialsdesign.com/property-modules

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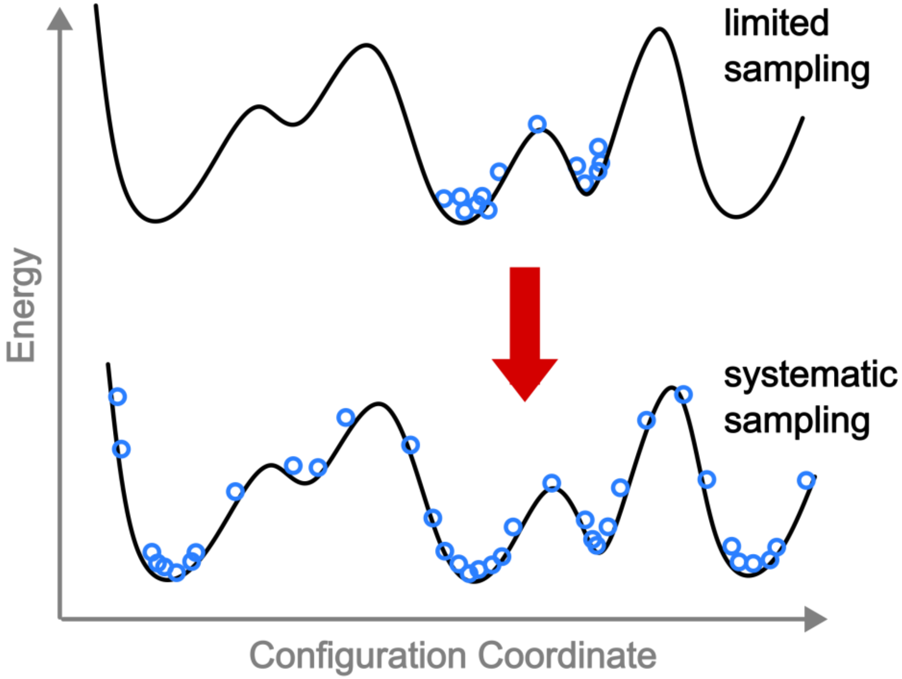
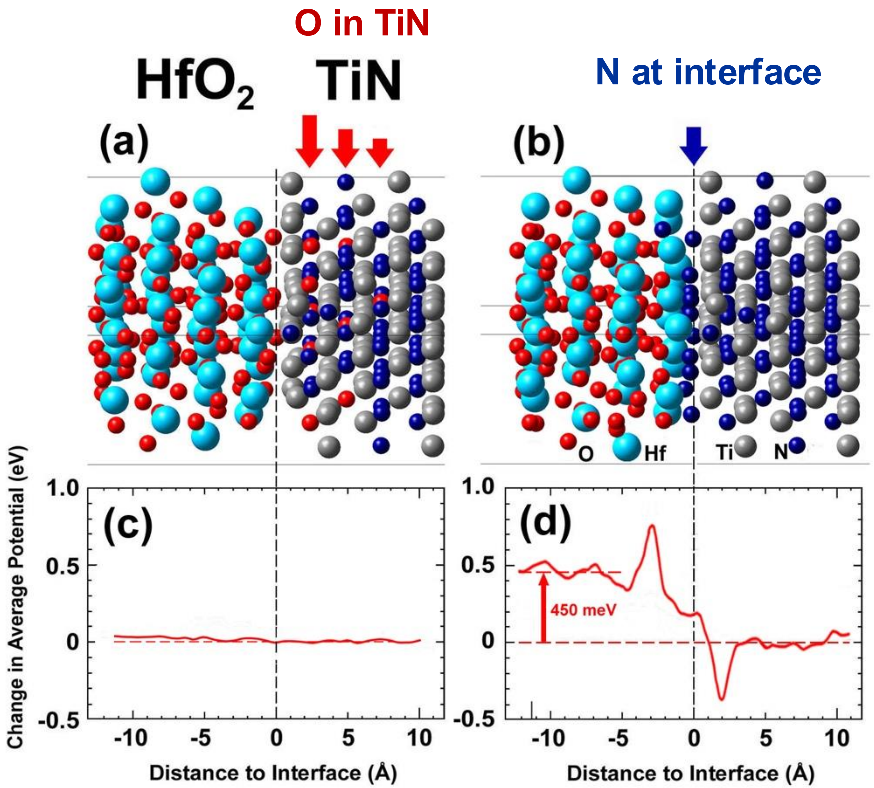
MedeA Streamlines Generation of Comprehensive Training Dataset



Atomic Details at the Interface Determines the Property



HfO_2: gate dielectrics
TiN : Metal gates

- Experiments show that effective work function (EWF) changes when high [O] near interface
- DFT shows that :
  1. O atoms filling N vacancies has minimal effect on EWF
  2. The N segregation at the interface cause significant changes

MLP can enable detailed investigation of interface structure

Hinkle et al., *Appl. Phys. Lett.* 96, 103502 (2010)

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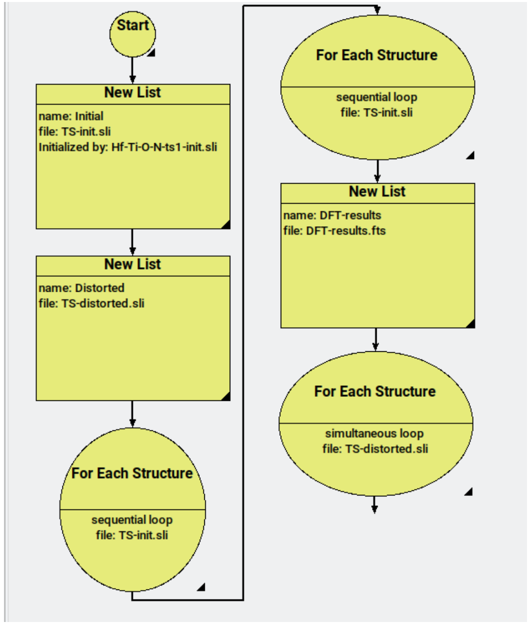
Training Set Creation at a Glance

All calculations use *MedeA* High-Throughput

Retrieve initial structures from *MedeA* InfoMaticA, the internal structure database

Systematic perturbation for diverse structures

High-throughput DFT calculations for final training set



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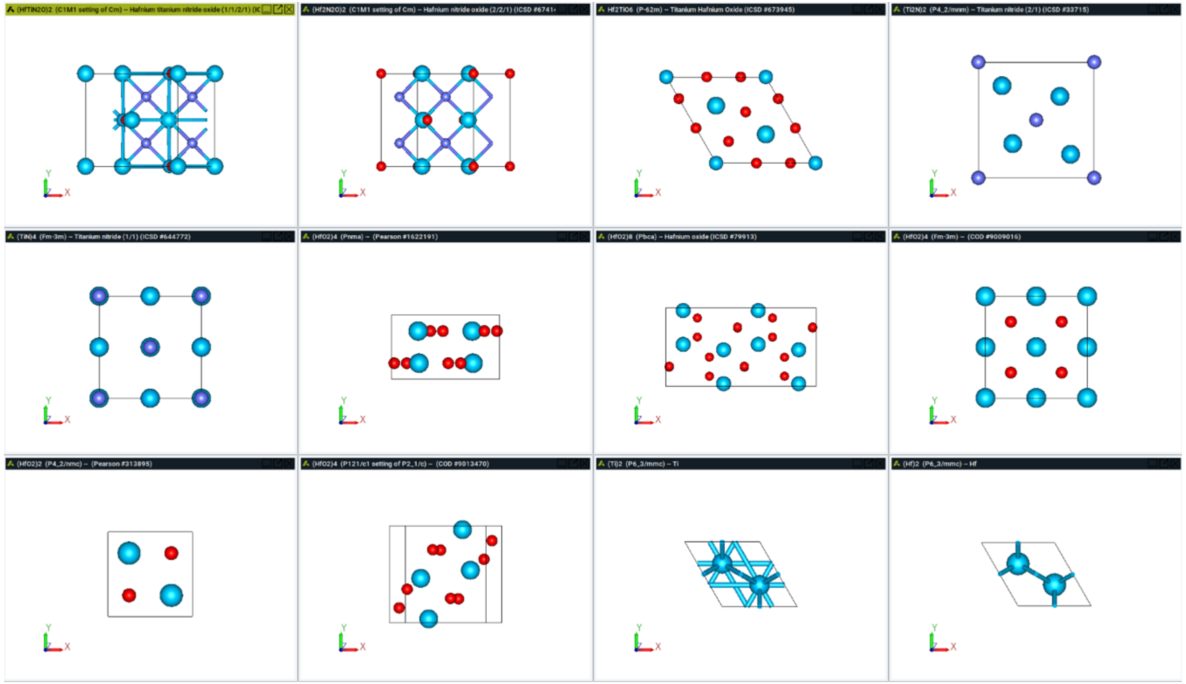
Initial Structures from *MedeA* InfoMaticA



Structures containing Hf, Ti, O, and N

- Search InfoMaticA for all unary, binary, and ternary compounds containing Hf, Ti, O, and N
- Select relevant structures
  - Relevant composition range
  - High-score structures
  - Experimentally verified structures
  - Small structures (≤ 50 atoms)

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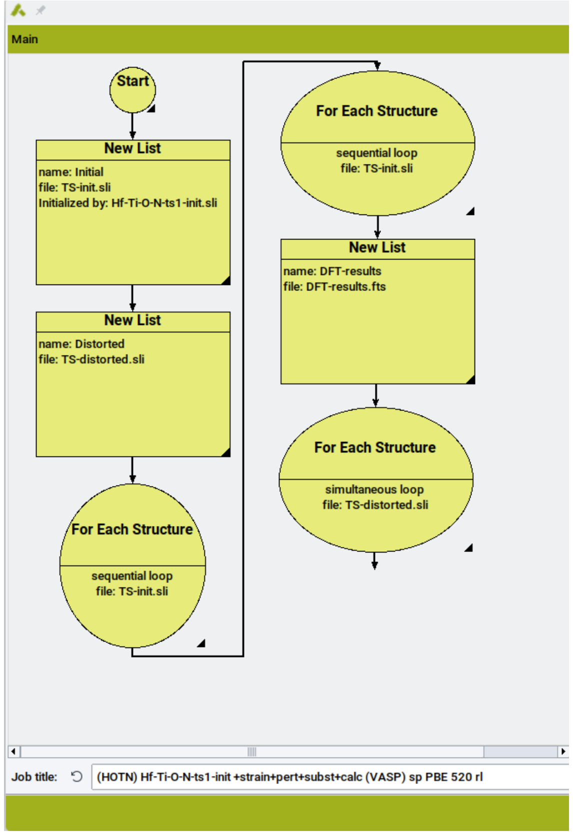
Main Flowchart Has Three Major Stages



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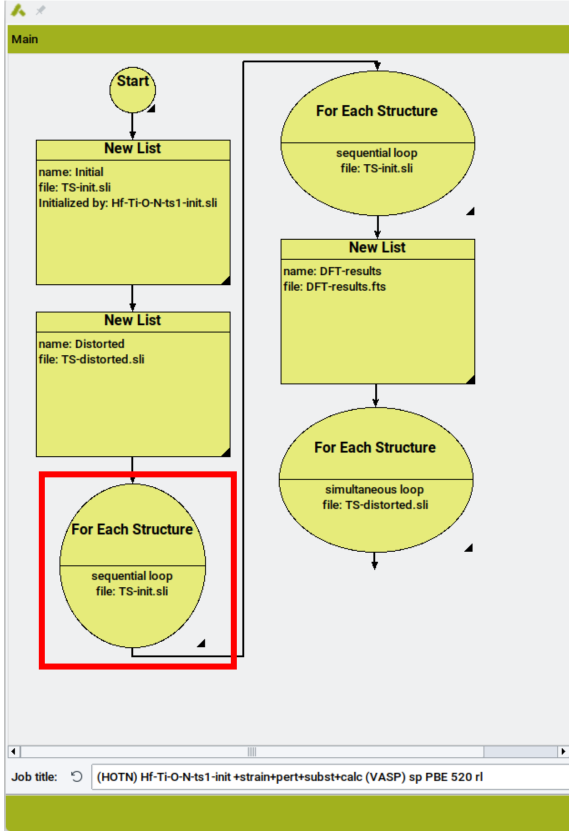
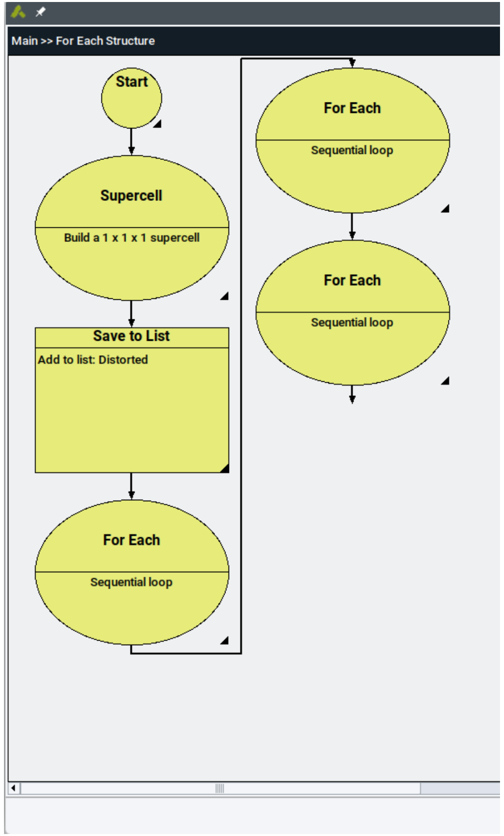
First **For Each Structure** Stage Perturbs Unit Cell Shape





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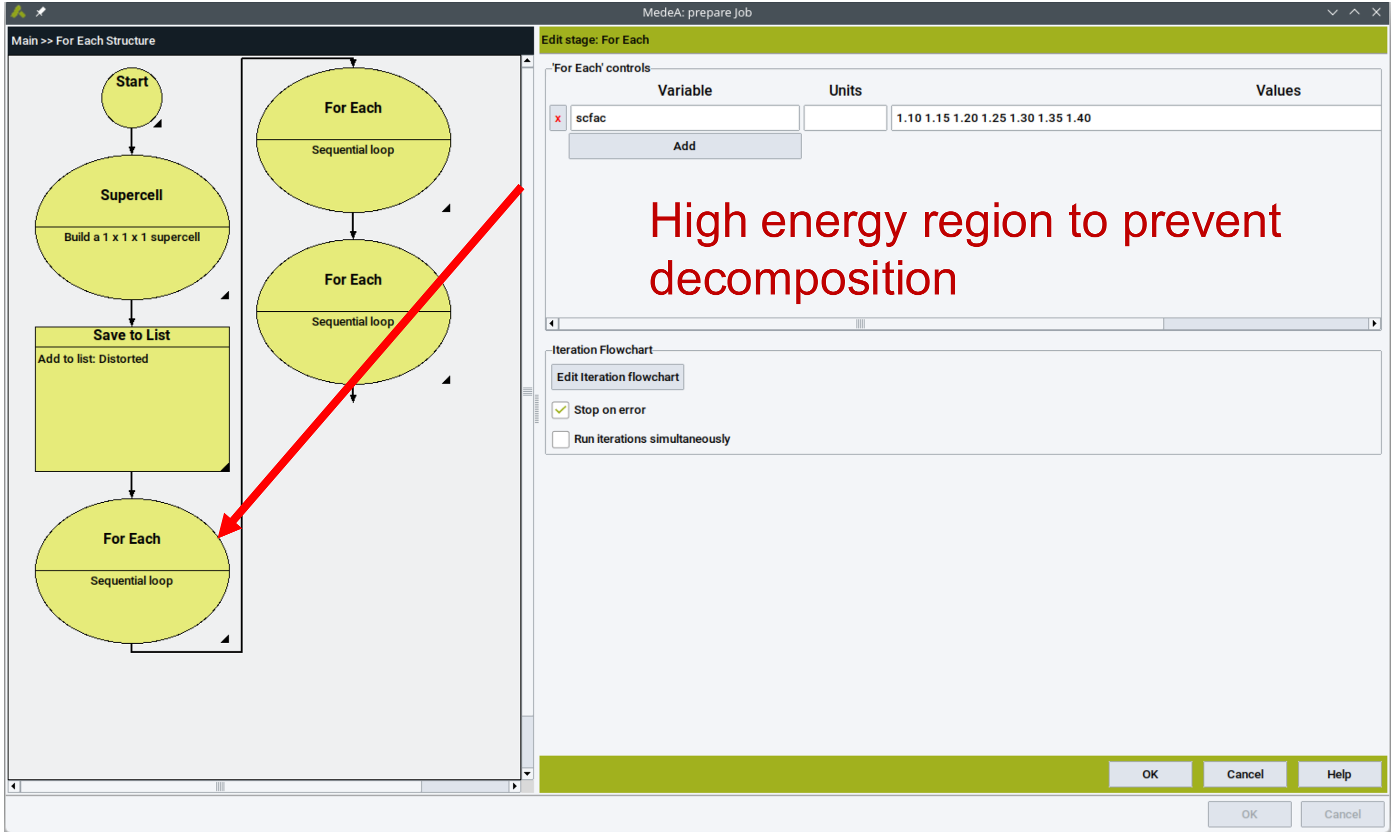
First **For Each Structure** >> First **For Each**



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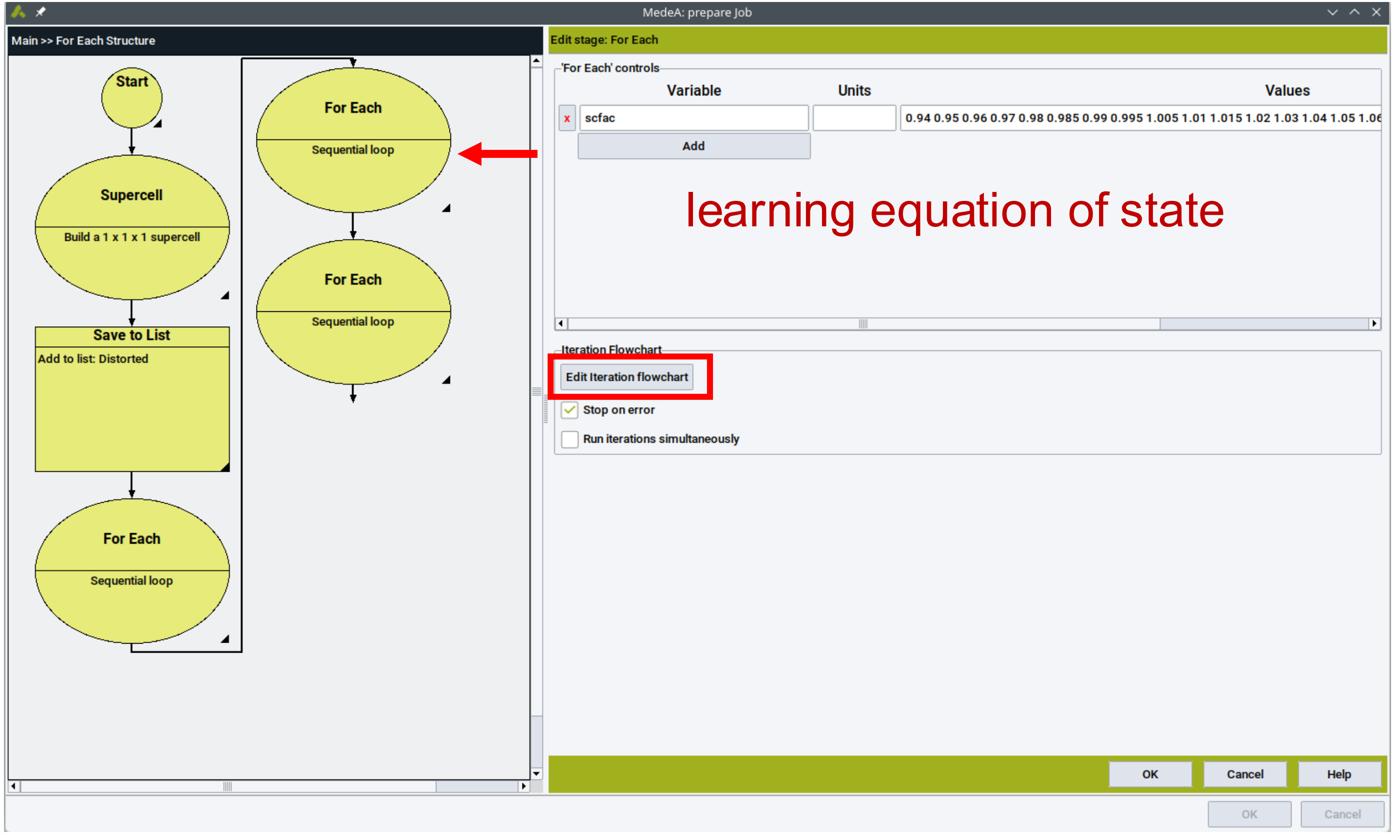
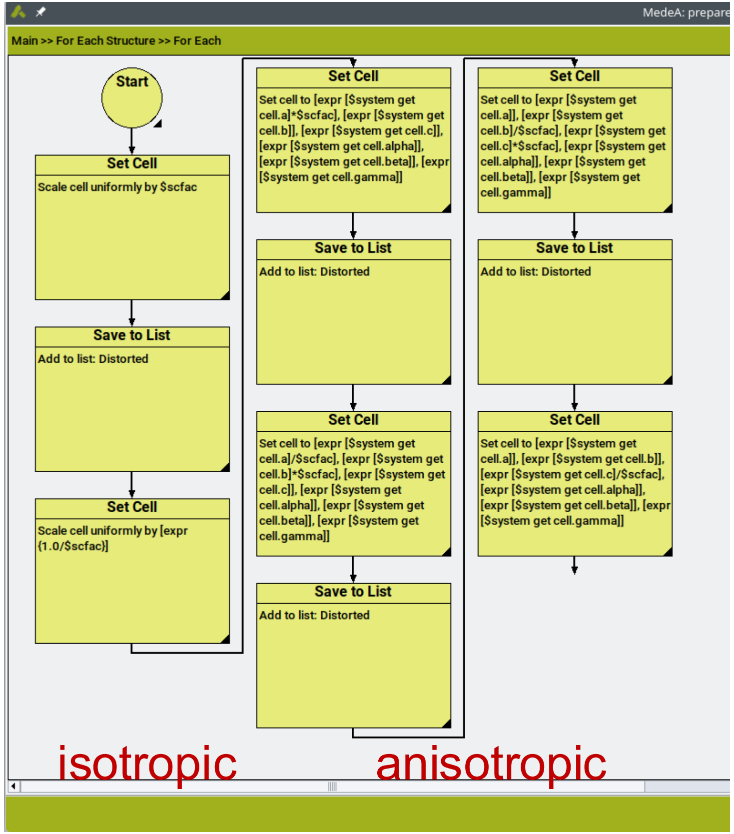
First **For Each Structure >> Second For Each**



First **For Each Structure** >> Second **For Each** >> …



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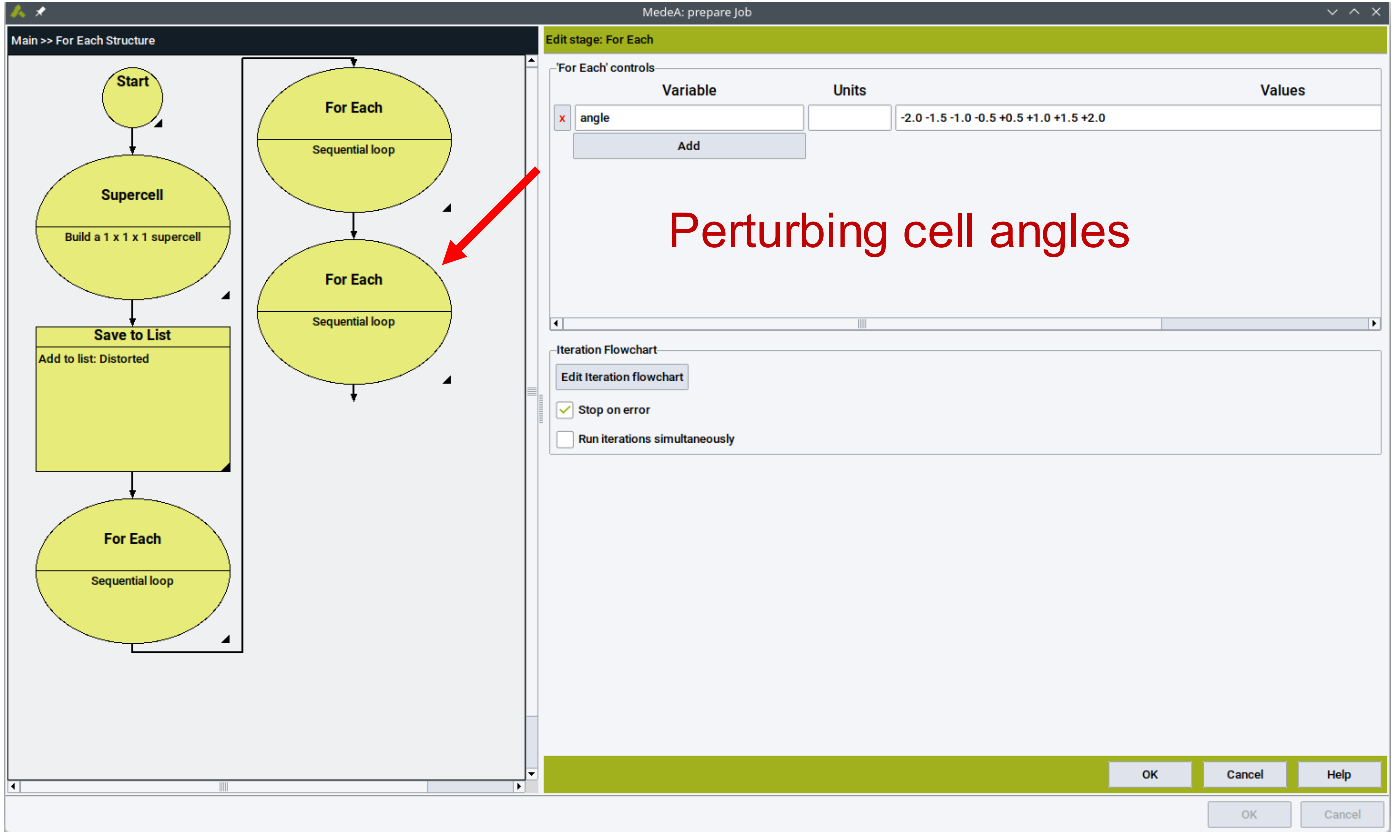
First **For Each Structure** >> Third **For Each**



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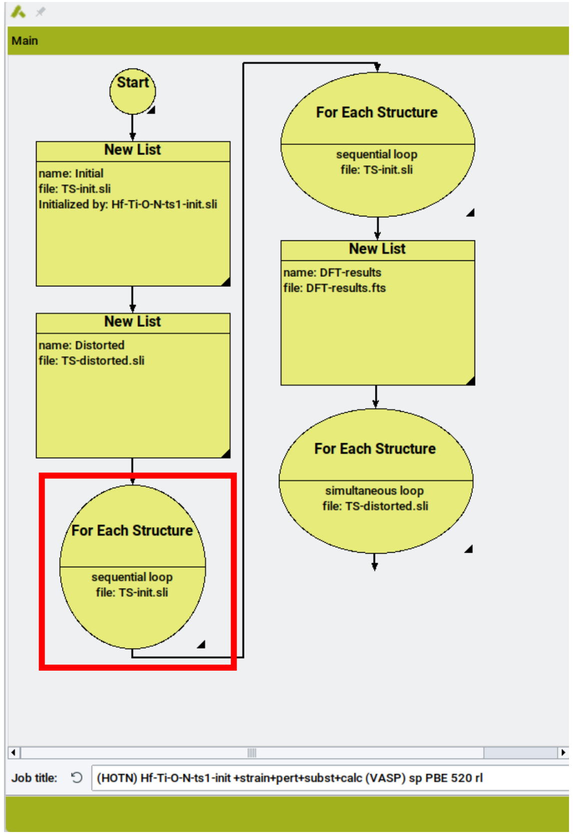
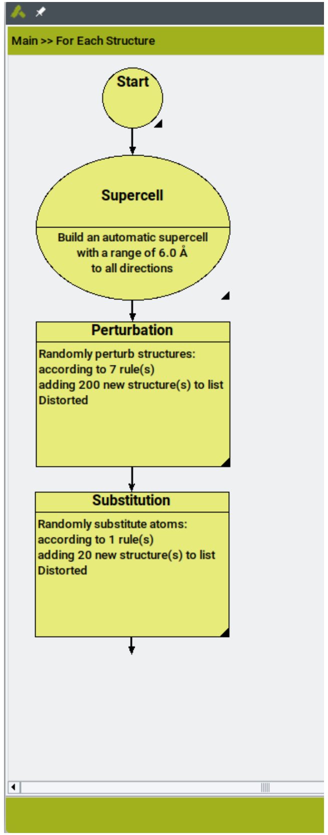
Second **For Each Structure** Stage Perturbs Supercell





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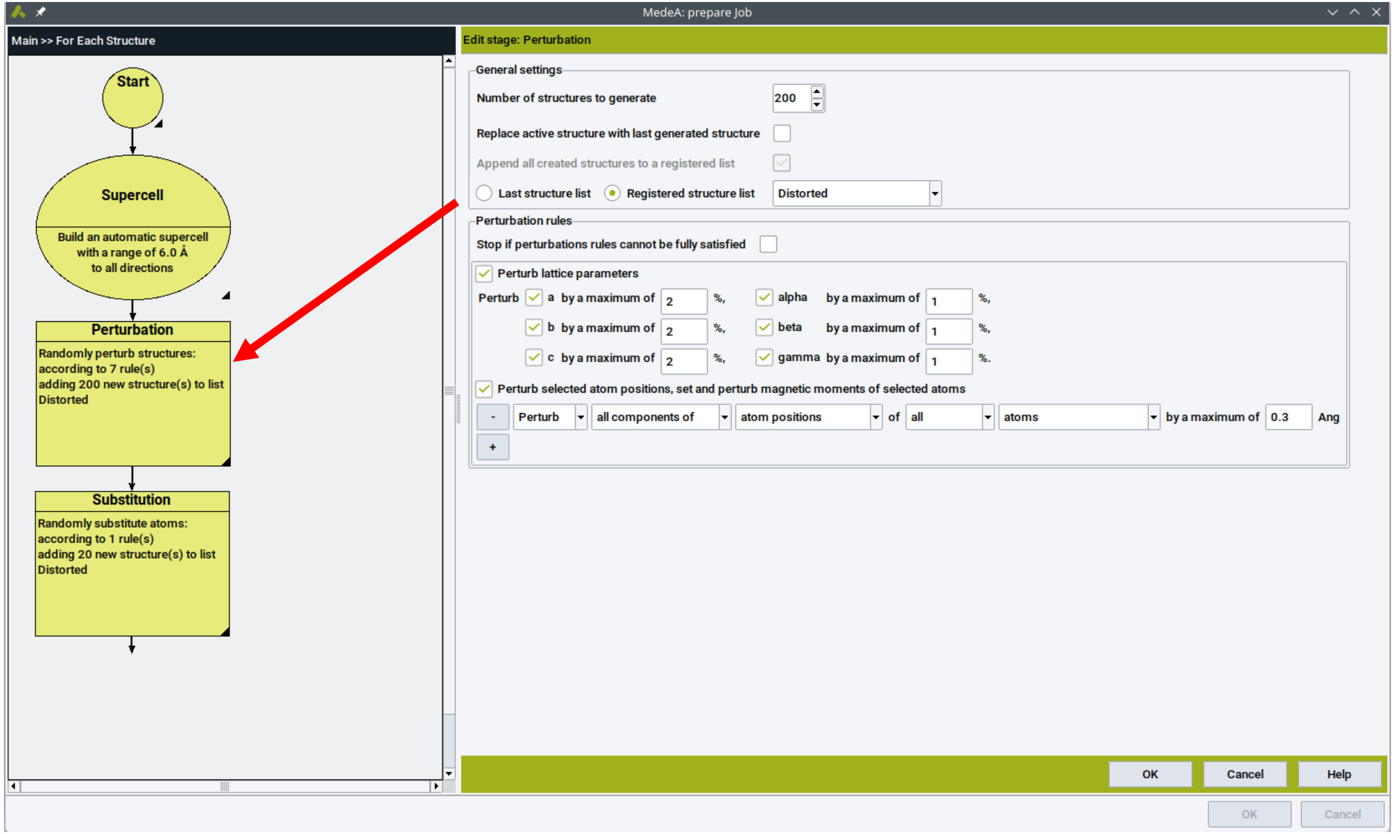
Perturbation Applies to All Degree of Freedom



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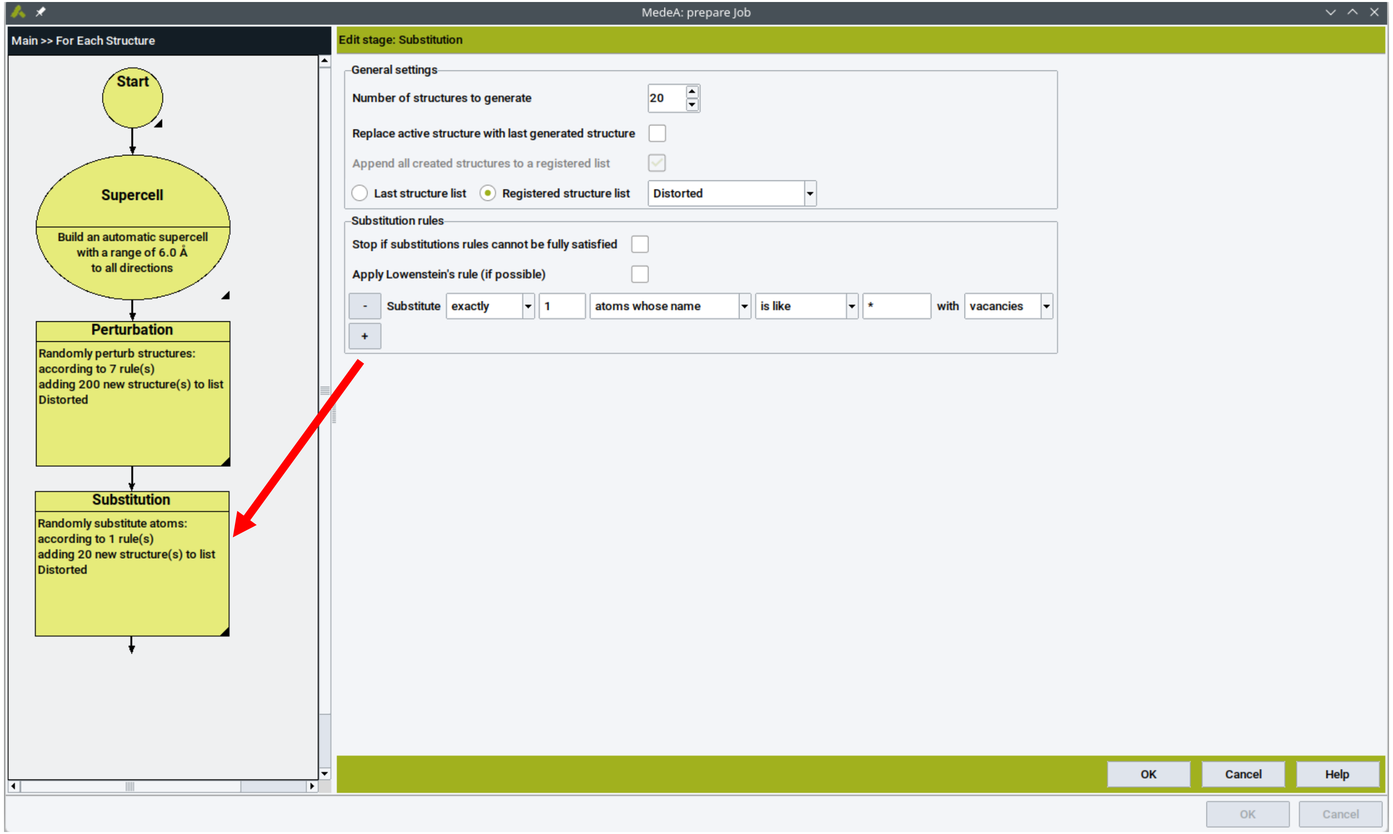
Chemical Substitution and Vacancies Can be Included



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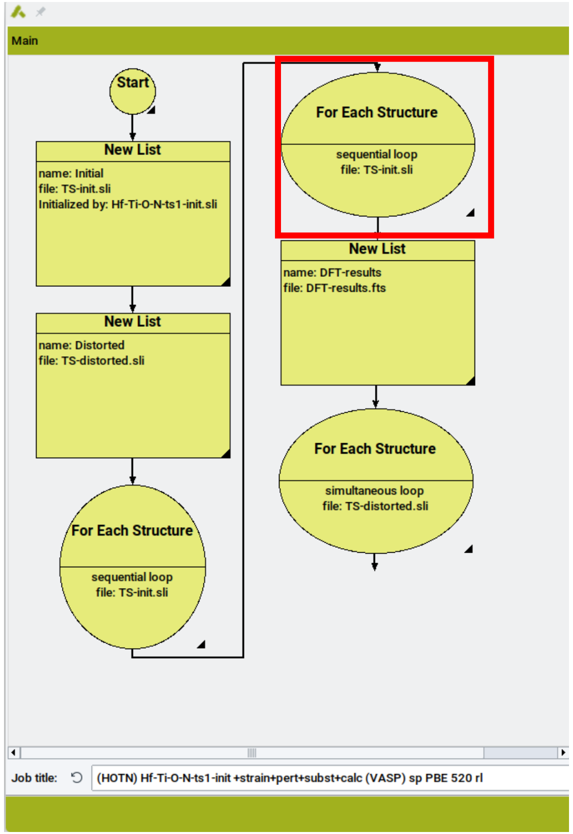
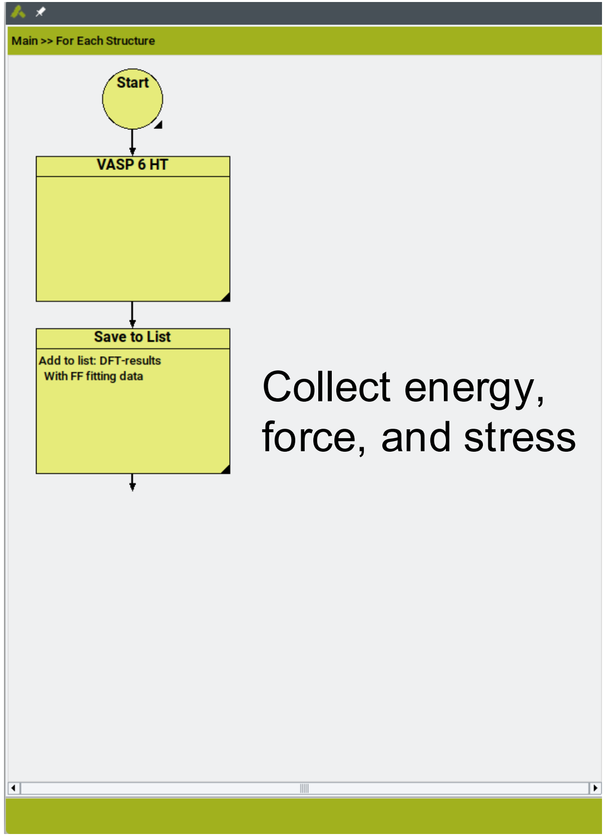
Third **For Each Structure** Stage is DFT calculations





Collect energy, force, and stress

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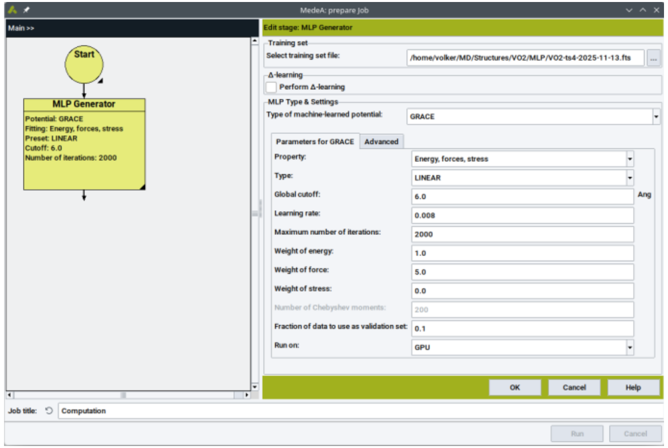
MedeA MLP Generator

Collection of tools to generate MLPs from user-created training sets for subsequent use with *MedeA* LAMMPS



Spectral Neighbor Analysis Potential (**SNAP/qSNAP**)

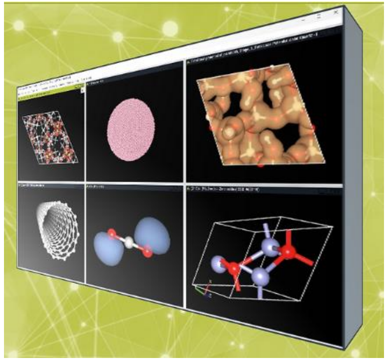
- A. Thompson and M. Wood
- FitSNAP code by Sandia group

Neural Network Potential (**NNP**)

- J. Behler and M. Parrinello
- n2p2 code by A. Singraber, Vienna

Atomic Cluster Expansion (**ACE**) and Graph ACE (**GRACE**)

- R. Drautz, Y. Lysogorskiy, A. Bochkarev, and M. Mrovec
- PACEMAKER/GRACEMAKER code by ICAMS group



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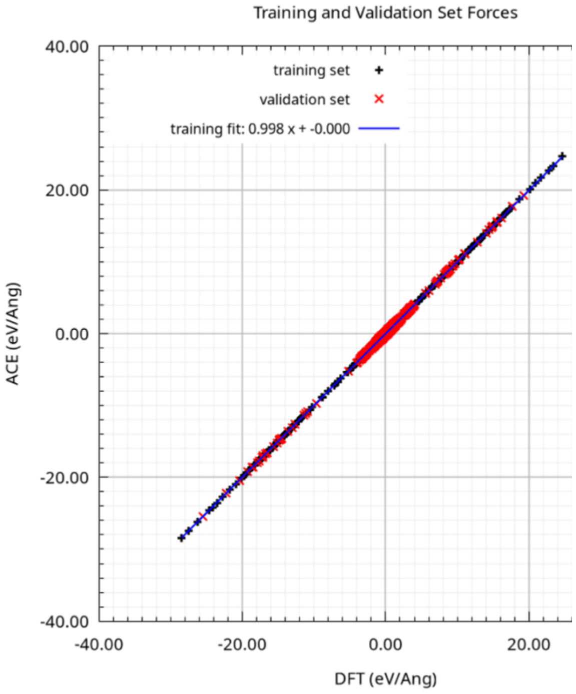
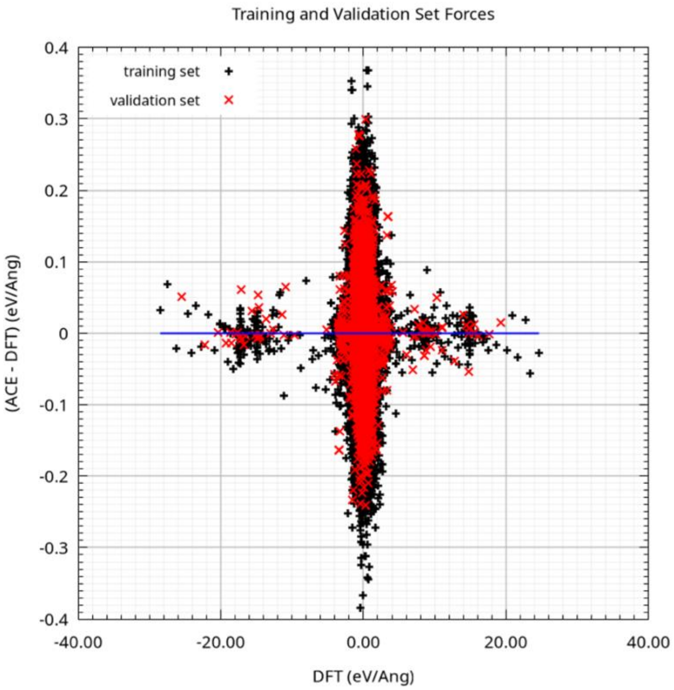
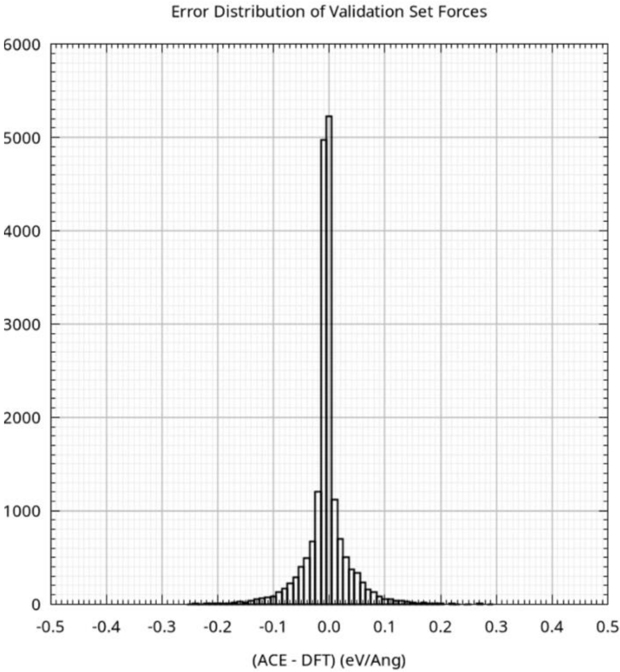
MedeA MLPG Makes Models Assessment Simple







We are here to support your R&D activities

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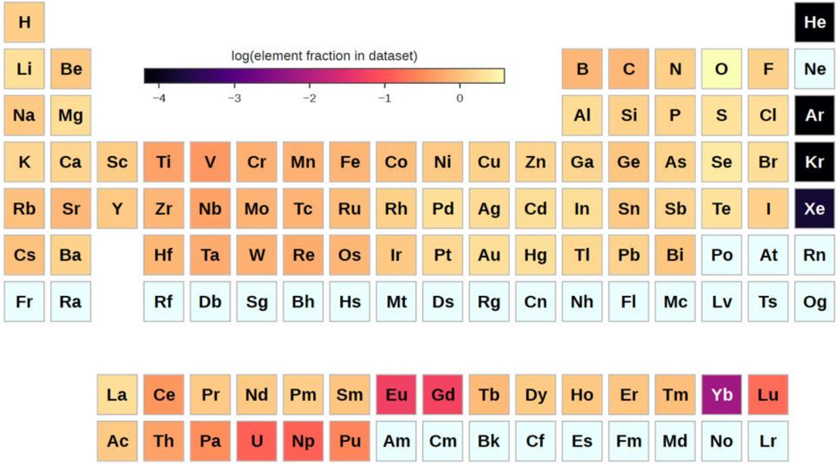
GRACE Foundation Model + *MedeA* is a Virtual Lab for Materials Discovery

MedeA MLPs

Collection of pre-trained MLPs ready to use with *MedeA* LAMMPS



Foundational GRACE

- **True Universality**: The elemental composition of the underlying training set spans most of the periodic table, covering 89 chemical elements, with a focus on inorganic bulk materials.
- **Foundation**: OMAT24 dataset includes more than 110 million structures; OAM models are composed of the OMAT24 dataset, fine-tuned with the subsampled Alexandria (sAlex) and MPTraj (Materials Project) datasets.

High Accuracy & High Efficiency

- **Validated Accuracy**: Extensively benchmarked against quantum calculations. Unlike simpler models, GRACE accurately predicts difficult properties, such as thermal conductivity and elastic moduli, right out of the box.
- **Unmatched Efficiency**: GRACE models establish a new ***'Pareto front'***, offering the best available balance between **high accuracy** and **computational speed**.

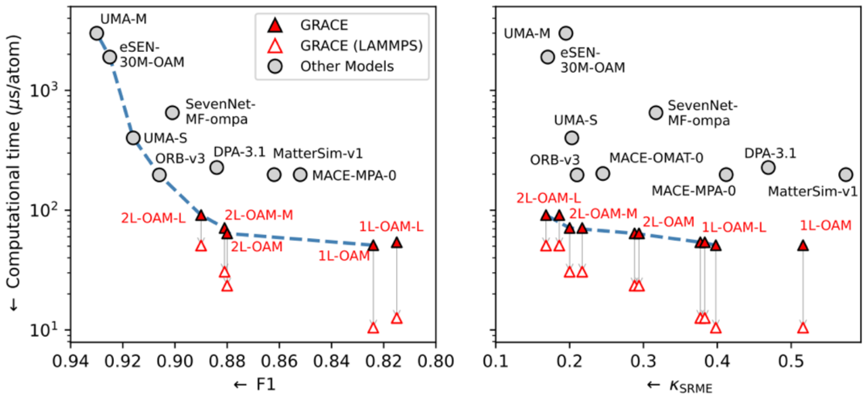


FIG. 1. Model performance for stable structure identification (F1 score in MatBench Discovery benchmark) and thermal conductivity prediction (κ_{SRME}) versus computational time per atom. A higher F1 score and lower κ_{SRME} indicate better performance. The blue dashed line links Pareto optimal models. Computational performance is estimated via ASE (filled symbols) and LAMMPS (open symbols), with GRACE models indicated in red.

Lusogorskiy, Bochkarev and Drautz "***Graph atomic cluster expansion for foundational machine learning interatomic potentials***" https://doi.org/10.48550/arXiv.2508.17936

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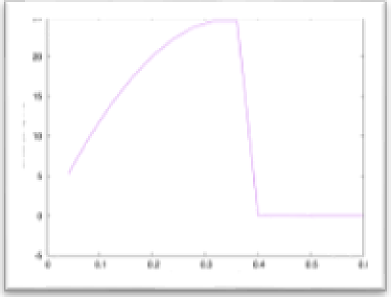
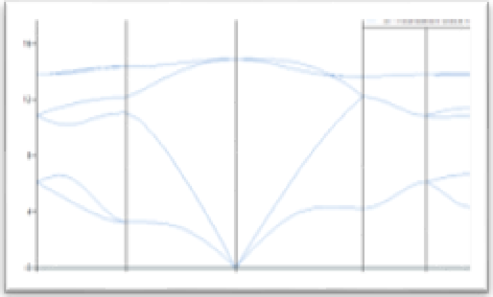
Seamless Integration

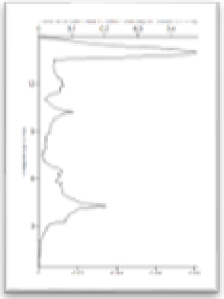
Use with *MedeA LAMMPS* and the *MedeA LAMMPS* modules

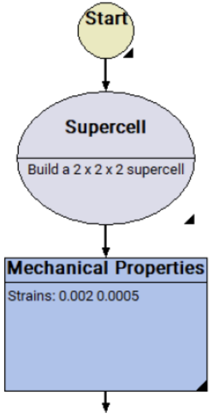
- *MedeA Diffusion*
- *MedeA Thermal Conductivity*
- *MedeA Deformation*
- *MedeA MT*
- *MedeA Phonon*
- *MedeA MD Phonon*

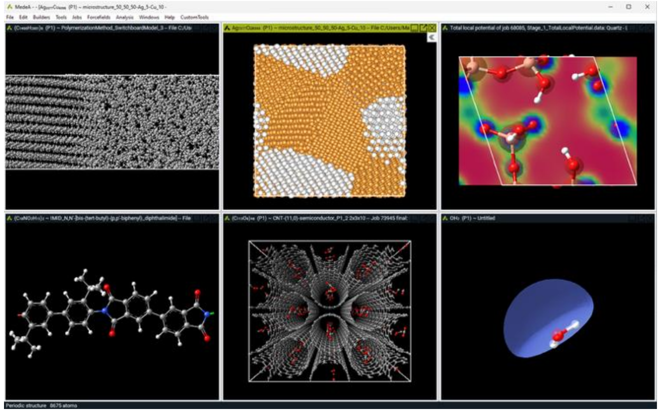
Transport · Mechanical · Vibrational











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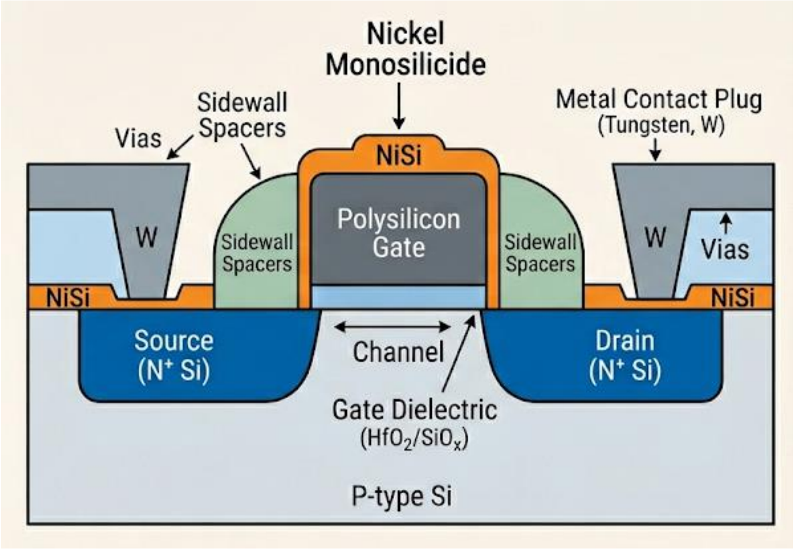
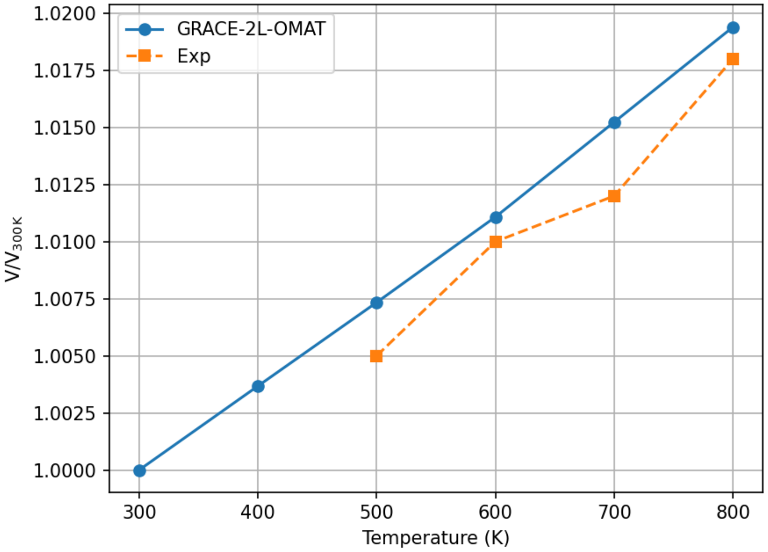
Thermal Expansion is Critical for Heterogenous Integration





- NiSi is a common contact material for semiconductor devices
- Complexity in thermal treatment increases with advance in heterogenous integration

- GRACE-2L prediction for bulk materials are consistent with experimental results

Goel et. al, Front. Chem. 6:331 (2018)

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Summary

- Multiscale simulation beyond DFT is the key to engineer real materials
- VASP MLFF speeds up MD simulation by roughly 10 times
- Trained MLFF/MLP can simulate properties of real materials easily with *MedeA*
- *MedeA* streamlines dataset generation and MLP selection
- GRACE Foundation Model can accelerate materials research

Question and Answer Session

Dr. Volker Eyert

Materials Design

Dr. Michele Kotiuga

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Datasheets, Tutorials, Documentation

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MedeA MLP
Efficient and Flexible Machine Learning Potential Support

At-a-Glance

MedeA®[1] *MLP (Machine Learning Potential)* provides full *MedeA* support for LAMMPS based machine learning potential simulations, including the simulation of mechanical, vibrational, and transport properties combined with comprehensive *MedeA* based analysis of simulation results.

MedeA MLP includes a library of published machine learning potentials derived from the Spectral Neighbor Analysis Potential (SNAP)[2] formalism supported by LAMMPS.

MedeA LAMMPS based simulations using *MedeA MLP* typically show excellent agreement with first-principles methods for systems that are well represented by the training set employed in creating the machine learning potential.

Key Benefits

Productivity
- Extends *ab initio* simulation results to larger length and time scales through substantially reduced energy and force calculation times
- Efficient use of published machine learning potentials
- Automates the handling of files and data for efficient simulation

Access
- Supports the SNAP machine learning potential form
- Allows access to all *MedeA LAMMPS* simulation properties with machine learning potential accuracy
- Can be employed with the *Machine Learning Potential Generator (MedeA MLPG)* to access newly derived machine learning potentials
- Handles diverse atomic geometries including making and breaking of bonds

Machine learning methods allow rich first-principles datasets to be mined and employed in interpolation and inference. Such techniques are having a dramatic effect in many areas of science. In materials science, they allow researchers to obtain the accuracy and freedom from bias of *ab initio* methods at reasonable computational cost for substantial simulation times and system sizes.

'All science depends on past work. Machine Learning depends more than other science on previous work: it needs examples.'

Michael Levitt, Nobel Laureate.

Machine learning based methods for energy and force calculation have been used for a number of years. For example, Blank et al. in 1995 employed a neural net based methodology to probe the energetics of CO on the Ni(111) surface[3]. In recent years it has become increasingly clear that such approaches, employing novel descriptors and advanced machine learning techniques, can yield exceptionally accurate reproduction of quantum mechanical training data at substantially reduced computational cost[4].

MedeA MLP provides easy to use and efficient access to such methods. By making such machine learning potentials accessible for use with *MedeA LAMMPS*, *MedeA MLP* extends the range of *ab initio* methods to much larger length and time scales, while relying on first-principles results for

[1] MedeA and Materials Design are registered trademarks of Materials Design, Inc.
[2] A. P. Thompson, L. P. Swiler, C. R. Trott, S. M. Foiles, and G. J. Tucker, *Spectral neighbor analysis method for automated generation of quantum-accurate interatomic potentials*, J. Comp. Phys. 285, 316 (2015)
[3] T. B. Blank, S. D. Brown, A. W. Calhoun, D. J. Doren, *Neural network models of potential energy surfaces*, J. Chem. Phys., 103, 4129 (1995)
[4] J. Behler, and M. Parrinello, *Generalized neural-network representation of high-dimensional potential energy surfaces*, Phys. Rev. Lett. 98, 146401 (2007)

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MedeA MLPG
Efficient Flexible Machine Learning Potential Generator

At-a-Glance

The *MedeA*®[1] *MLPG* (Machine Learning Potential Generator) enables users to create their own machine learning potentials (or force-fields) from training-set data previously generated by quantum mechanical calculations. The resulting potentials allow users to perform simulations of systems substantially larger in size and for much larger simulation times than can be typically accessed using quantum mechanical methods while at the same time reflecting the high accuracy and validity of the latter.

In addition to managing selection of training and validation data, the *MedeA MLPG* allows you to generate machine learning potentials using the Spectral Neighbor Analysis Potential (SNAP)[2] formalisms. The potentials created are ready for subsequent use with *MedeA MLP*. Combined with the *MedeA* Flowchart interface as well as VASP and LAMMPS, the *MedeA MLPG* thus provides efficient access to machine learning based simulation techniques.

Key Benefits

Productivity
- Automates the creation of machine learning potentials using the SNAP formalism
- Extends *ab initio* precision to larger length and time scales
- Manages training set data
- Full Ziegler-Biersack-Littmark (ZBL) potential support

Accuracy
- Yields machine learning descriptions based on the SNAP methods
- Provides access to all calculation details and information
- Provides machine learning potentials for use with all *MedeA LAMMPS* property calculation types

Machine learning potentials employ efficient descriptors of atomic environments combined with machine learning based correlative methods to describe the energetic behavior of atomic and molecular systems. The *MedeA MLPG* allows users to generate machine learning potentials by accurately reproducing supplied target first-principles data for a training set of structures.

Figure 1: The MedeA Machine Learning Potential Generator (MLPG) is integrated within the MedeA environment allowing straightforward use of first-principles information from VASP in the creation of MLPs.

The *MedeA MLPG* manages training-set data derived from first-principles calculations as the target to be reproduced by the MLP (machine learning potential). Configuration dependent energies, forces, and stresses can be considered in the fitting process. Using the SNAP approach the *MedeA MLPG* creates a machine learning potential by minimizing the deviations from the target energies, forces, and stresses calculated by quantum mechanical methods. While this process is guided by meaningful default parameters, the full flexibility of the underlying methods can be accessed by advanced settings. The *MedeA MLPG* has been developed as part of active research and development projects and is thoroughly validated.

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[2] A. P. Thompson, L. P. Swiler, C. R. Trott, S. M. Foiles, and G. J. Tucker, *Spectral neighbor analysis method for automated generation of quantum-accurate interatomic potentials*, J. Comp. Phys. 285, 316 (2015)

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FMNT

INTERNATIONAL CONFERENCE

FUNCTIONAL MATERIALS & NANOTECHNOLOGIES

15–18 JUNE 2026 — RIGA, LATVIA

Dr. Volker Eyert

WELCOME to the International Conference Functional Materials and Nanotechnologies

FM&NT 2026 brings together scientists, students, companies, industry representatives, and experts from research institutes and universities across the Baltic Sea Region and beyond.

Explore the latest achievements in research, innovative solutions, and applications that foster international cooperation and advance the field of functional materials and nanotechnologies.

https://fmnt.lv/en/fmnt/

Dr. Eyert’s Presentation and Training

- Volker’s talk **‘*Machine-Learned Potentials for Transition-Metal* Oxides’** is scheduled for early afternoon on **June 17**.
- Volker will give a [MedeA Software Environment]() Training on the afternoon of **June 18**.

Dr. Volker Eyert

Conference Topics

The following topics will be included in conference:

- **Materials for Energy |** batteries, supercapacitors, hydrogen, nuclear power
- **Materials for Photonics |** emission, detection, transformation of light, quantum photonics
- **Ferroelectrics and Functional Materials |** functional (inorganic, organic and hybrid), low dimensional materials, Van der Waals, hybrid, topological and other ferroelectrics
- **Microfluidics and Biomedical technologies |** organ-on-chip, lab-on-a-chip, microfluidics devices, biosensors, micro and nano sensing, micro-nano robotics, biomaterials for biomedical technologies
- **Theoretical Modeling of Functional Materials and Devices |** prediction of Next-Generation Materials and their properties, application of Artificial Intelligence
- **Technologies and Devices |** nanotechnologies, sensors, thin film and coating technologies, fibre optics, lasers
- **Large-Scale Research Infrastructures, Science Policy and Collaboration |** synchrotrons, neutron sources, FP10, collaboration in materials research, nano technologies and innovation

Highlighted *MedeA* Modules

***MedeA* Environment**: The *MedeA* software package is the leading environment for the atomistic simulation of materials. *MedeA* enables professional, day-to-day deployment of atomic-scale and nano-scale computations for materials engineering, materials optimization and materials discovery. In *MedeA*, world-class simulation engines are integrated with elaborate property prediction modules, experimental databases, structure builders and analysis tools, all in one user-friendly environment.

***MedeA* Machine-Learned Potential Generator (MLPG)**

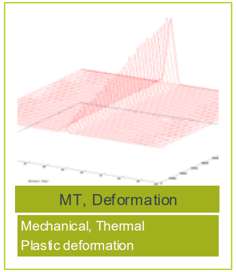
The *MedeA* Microstructure Builder

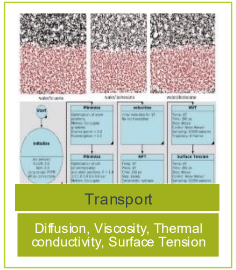
***MedeA* PhaseField**

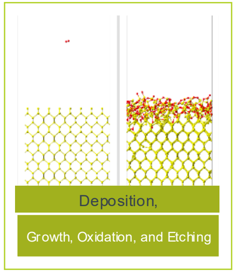
***MedeA* Machine-Learned Potentials (MLP)**

***MedeA* Diffusion**

***MedeA* Thermal Conductivity**







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Related *MedeA* Webinars

Modeling Interfaces and Microstructures with MedeA:

https://www.materialsdesign.com/webinars/recorded/modeling-interfaces-and-microstructures-with-medea

Accessing the Mesoscale with Phasefield Modeling

https://www.materialsdesign.com/webinars/recorded/accessing-the-mesoscale-with-phase-field-modeling

Precision at Scale MLP:

https://www.materialsdesign.com/webinars/recorded/precision-at-scale-with-machine-learned-potentials

Related *MedeA* Tutorials

VASP MLFF Thermal Expansion NiSi

Thermal Conductivity Ar Mueller Plathe NEMD

Generating an ACE MLP for Ti

Tutorial Phasefield WO Oxidation

Question and Answer Session

Dr. Volker Eyert

Materials Design

Dr. Michele Kotiuga

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Questions about Materials Design Webinars

Katherine Hollingsworth

khollingsworth@materialsdesign.com

materials design

info@materialsdesign.com

www.materialsdesign.com

MedeA

Innovation by Simulation

Question and Answer Session

Dr. Volker Eyert

Materials Design

Dr. Cheng-Wei Lee

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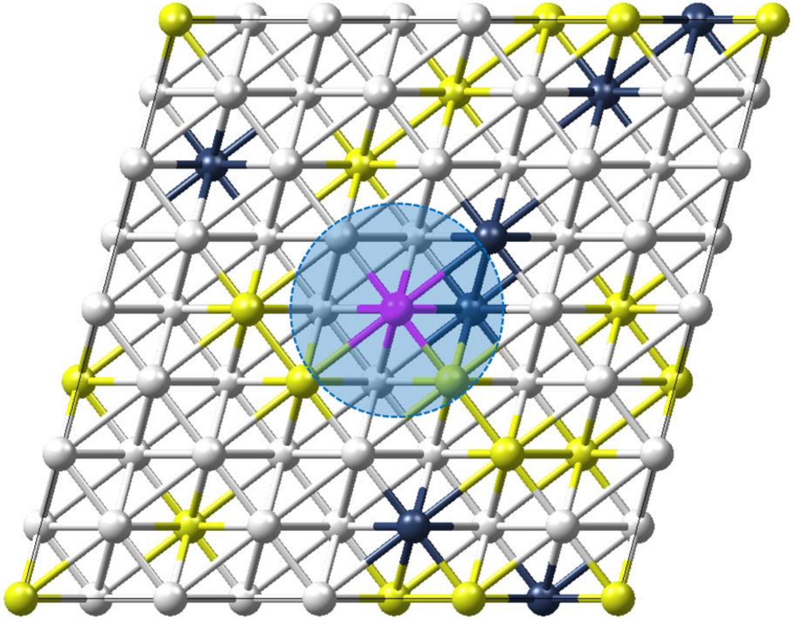
Descriptors and Regressors

Descriptor: describes atomic structures



- Divide structure into local atomic environments/clusters
- Describe local atomic structures in terms of atom positions and types

$$B_i = B_i\,(\{\boldsymbol{r}_{ji}, A_j, j = 1, N_i\}),\ i = 1, N$$

  - $\boldsymbol{r}_{ji}$ in local coordinates (r, ϑ, φ), or
  - all pairwise distances r_{jl} in cluster
  - A_j: atomic weighting factor
  - N: all atoms, N_i: all atoms in cluster i

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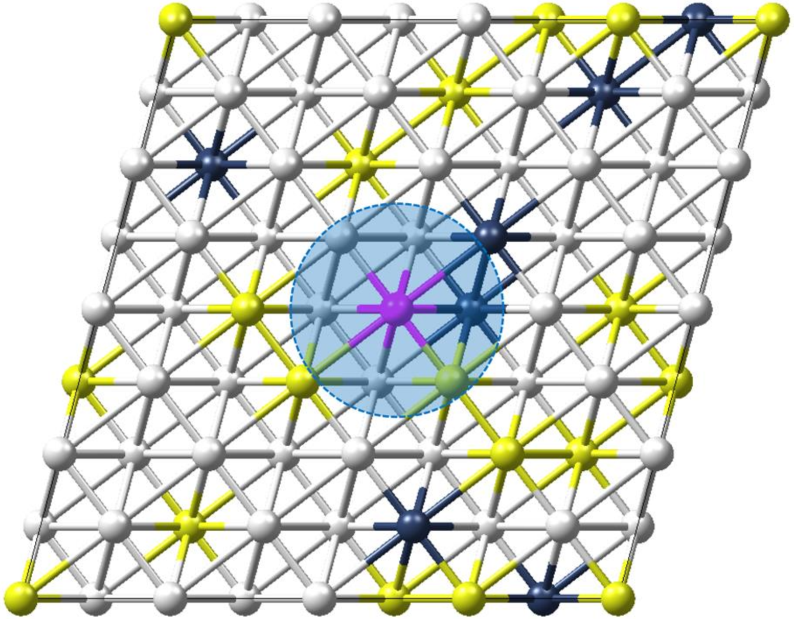
Descriptors and Regressors

Regressor: maps structures to energies/forces/stresses



- Divide energies/forces/stresses into contributions from all clusters

$$E = \Sigma_i E_i$$

- Express energies/forces/stresses in terms of descriptors B_i

$$E_i = \beta_0 + \Sigma_k \beta_k B_{i,k}$$

$$\boldsymbol{F}_{i,j} = -\nabla_j E_i = -\sum_k \beta_k \frac{\partial B_{i,k}}{\boldsymbol{r}_j}$$

- Determine (train) coefficients β_k using *ab initio* calculations

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Initial Structures for Ti-Hf-O-N from InfoMaticA

Structures | Properties

Order	Name	Structural formula	# atoms	# configurations	Symmetry	Cell parameters
1	Hf	Hf_2	2	1	P63/mmc	3.1964 3.1964 5.0511 90 90 120
2	Ti	Ti_2	2	1	P63/mmc	2.9504 2.9504 4.6833 90 90 120
3	(COD #9013470)	Hf_4O_8	12	1	P121/c1	5.1156 5.1722 5.2948 90 99.18 90
4	(Pearson #313895)	Hf_2O_4	6	1	P4_2/nmc	3.6437 3.6437 5.296 90 90 90
5	(COD #9009016)	Hf_4O_8	12	1	Fm-3m	5.115 5.115 5.115 90 90 90
6	Hafnium oxide (ICSD #79913)	Hf_8O_{16}	24	1	Pbca	10.0177 5.2276 5.0599 90 90 90
7	(Pearson #1622191)	Hf_4O_8	12	1	Pnma	5.5544 3.307 6.4572 90 90 90
8	Titanium nitride (1/1) (ICSD #644772)	Ti_4N_4	8	1	Fm-3m	4.241 4.241 4.241 90 90 90
9	Titanium nitride (2/1) (ICSD #33715)	Ti_4N_2	6	1	P42/MNM	4.9452 4.9452 3.0342 90 90 90
10	Titanium Hafnium Oxide (ICSD #673945)	Hf_2TiO_6	9	1	P-62m	5.547 5.547 3.1519 90 90 120
11	Hafnium nitride oxide (2/2/1) (ICSD #674145)	$Hf_4N_4O_2$	10	1	C1M1	5.5425 5.5723 5.7592 90 112.33 90
12	Hafnium titanium nitride oxide (1/1/2/1) (ICSD #674155)	$Hf_2Ti_2N_4O_2$	10	1	C1M1	5.4105 5.4387 5.5491 90 112.961 9(

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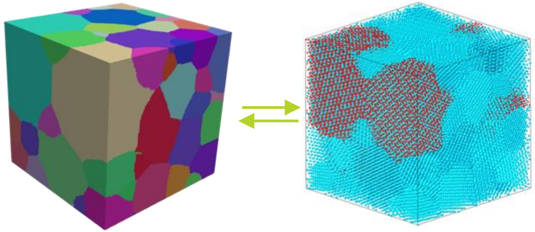
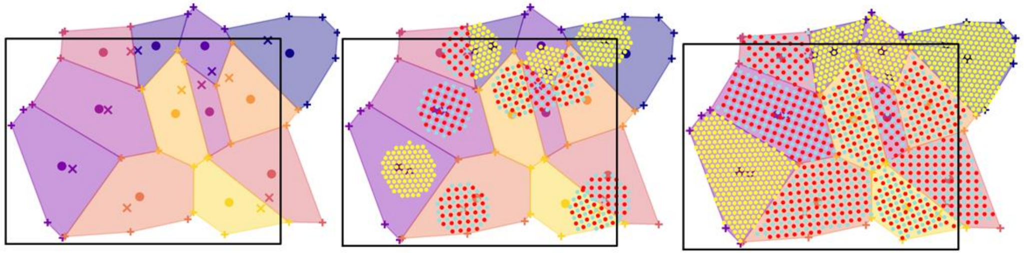
Building atomic microstructures



1) Generate atomic microstructures *via* "Seed & Growth" algorithm:

- Define seed points where "crystal growth" initiates.
- Grow crystals from seed point until other grains are met.
- Constrain interatomic distance or phase stoichiometry.

2) Populate existing microstructure definition with atoms



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The *MedeA* Microstructure Builder

Select components:

- Phases and number of grains
- Growth speed (*via* weight)
- Voids (empty space)
- GB interstitial atoms

Set growth parameters:

- Stoichiometric growth
- Interatomic distances at GB

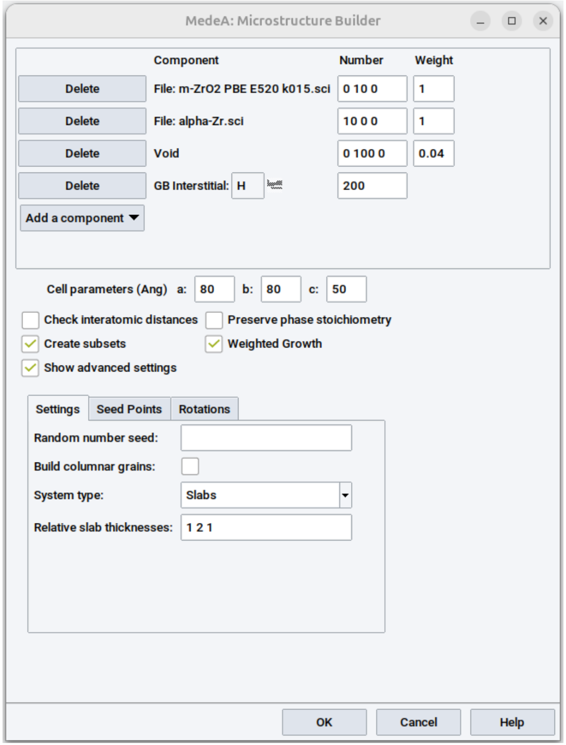
Advanced settings:

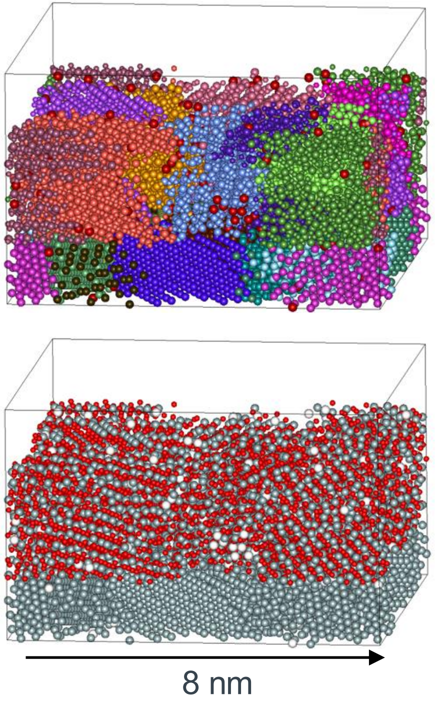
- Seed point coordinates
- Grain rotations (Euler or *hkl*)
- Interatomic distance thresholds
- Columnar & slab geometries

Output options:

- Analysis of grains & interfaces

Green: New feature in MedeA 3.12





A slab microstructure of ZrO2 grains on top of α-Zr grains

materials design

Solving the phase field equations

The energy becomes a functional of the order parameters η, concentration c, stress σ, etc.

Driving forces

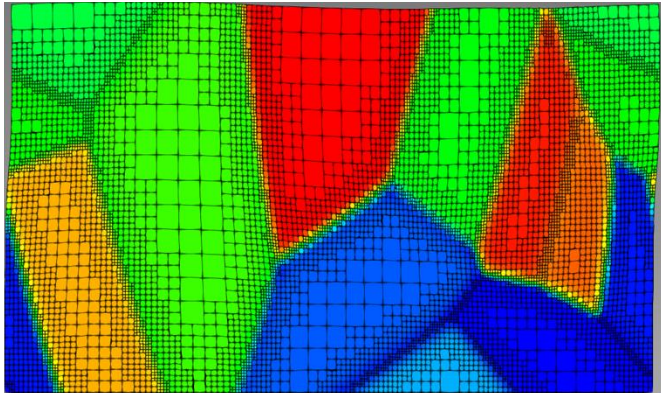
$$F = \int dV\, [f_{chemical} + f_{interface} + \cdots]$$

$$\frac{\partial c}{\partial t} = \nabla\, M(c, \eta, \sigma) \nabla \frac{\delta F}{\delta c}$$
$$\frac{\partial \eta}{\partial t} = -L \nabla \frac{\delta F}{\delta \eta}$$

Update

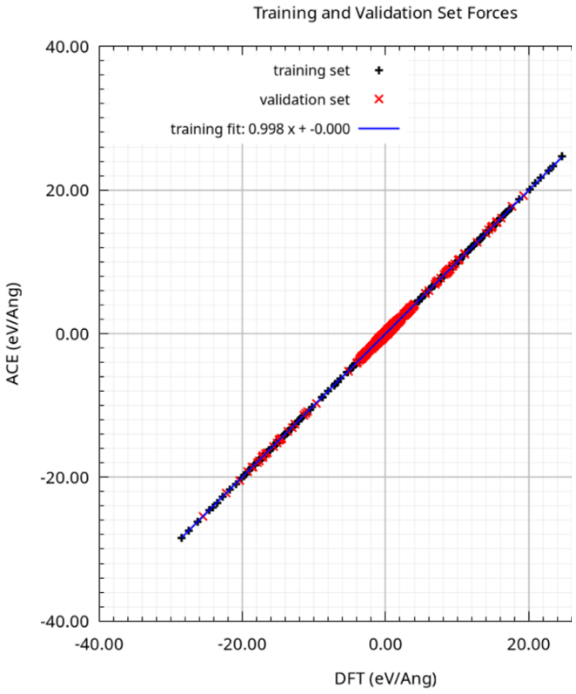
A set of PDEs are solved iteratively and propagated in time via response functions (e.g., Fick's diffusion equation, Allen-Cahn equation, etc).

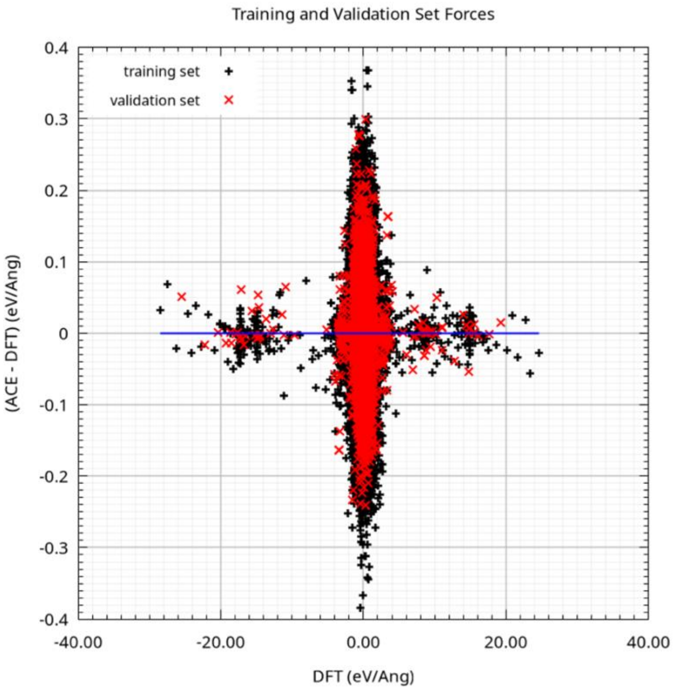
We solve the phase-field equations on an adaptive mesh using Finite Elements:

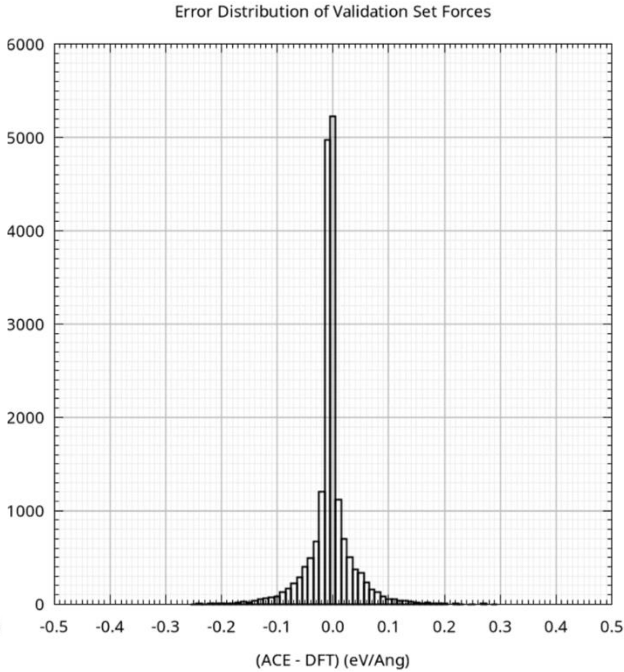


MedeA PhaseField

MedeA MLPG Makes Models Assessment Simple







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MLPs Enable DFT Accuracy for Multiscale Simulations