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Developments in Physics-Based Modeling and Machine Learning for Environmental Effects in Nuclear Materials

May 2024

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Changing the World's Energy Future

Idaho National Laboratory

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Developments in Physics-Based Modeling and Machine Learning for Environmental Effects in Nuclear Materials

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Modeling and simulation can predict environmental effects in nuclear materials

- Reactor environments are harsh (high temperatures, stresses, radiation, corrosive)
- As-fabricated materials must perform in these environments, and environmental effects can be lifetime-limiting (creep, creep-fatigue, IASCC, hardening…)
- Microstructures can significantly impact performance for a given material composition
- AM provides a huge range of microstructure space
- Physics-based modeling and appropriate application of machine learning can help design materials, reduce the need to test materials, and accelerate testing

A cohesive, modern approach to predict environmental effects in nuclear materials

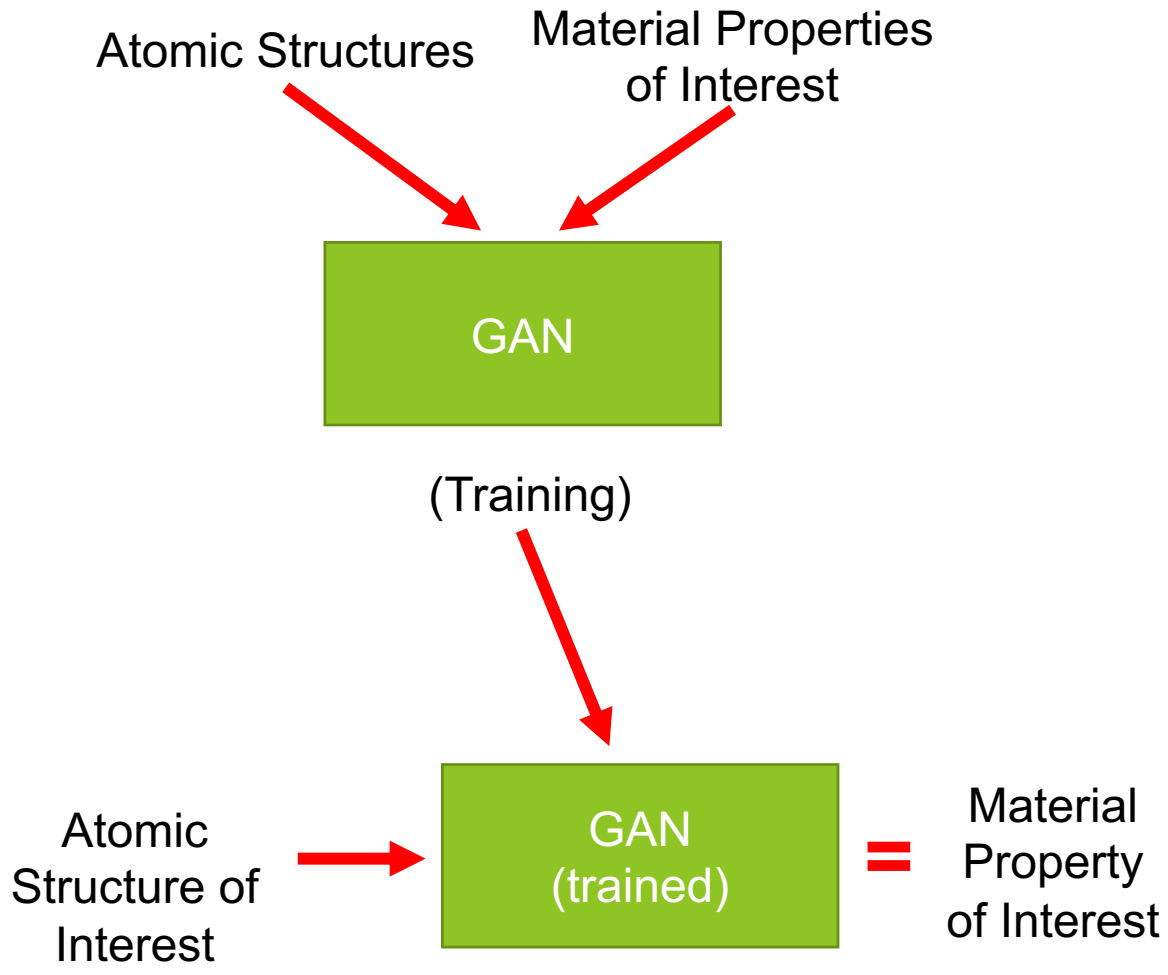
- Machine learning using density functional theory simulations to predict electronic structures of alloy systems
- Generalized workflow to predict thermodynamic and kinetic properties of multicomponent nuclear structural alloys using density functional theory, machine learning, and kinetic Monte Carlo
- Molecular dynamics-based quantification of irradiation damage metrics and comparisons of different defect recombination models
- MOOSE-based Stochastic Tools Module to support reduced order modeling, uncertainty quantification, etc.
- MOOSE-based crystal plasticity improvements and reduced order model development of bulk plastic behavior

- Designing materials from the ground up
- Basis of simulations for ion/neutron irradiation acceptance

- Creep, creep-fatigue

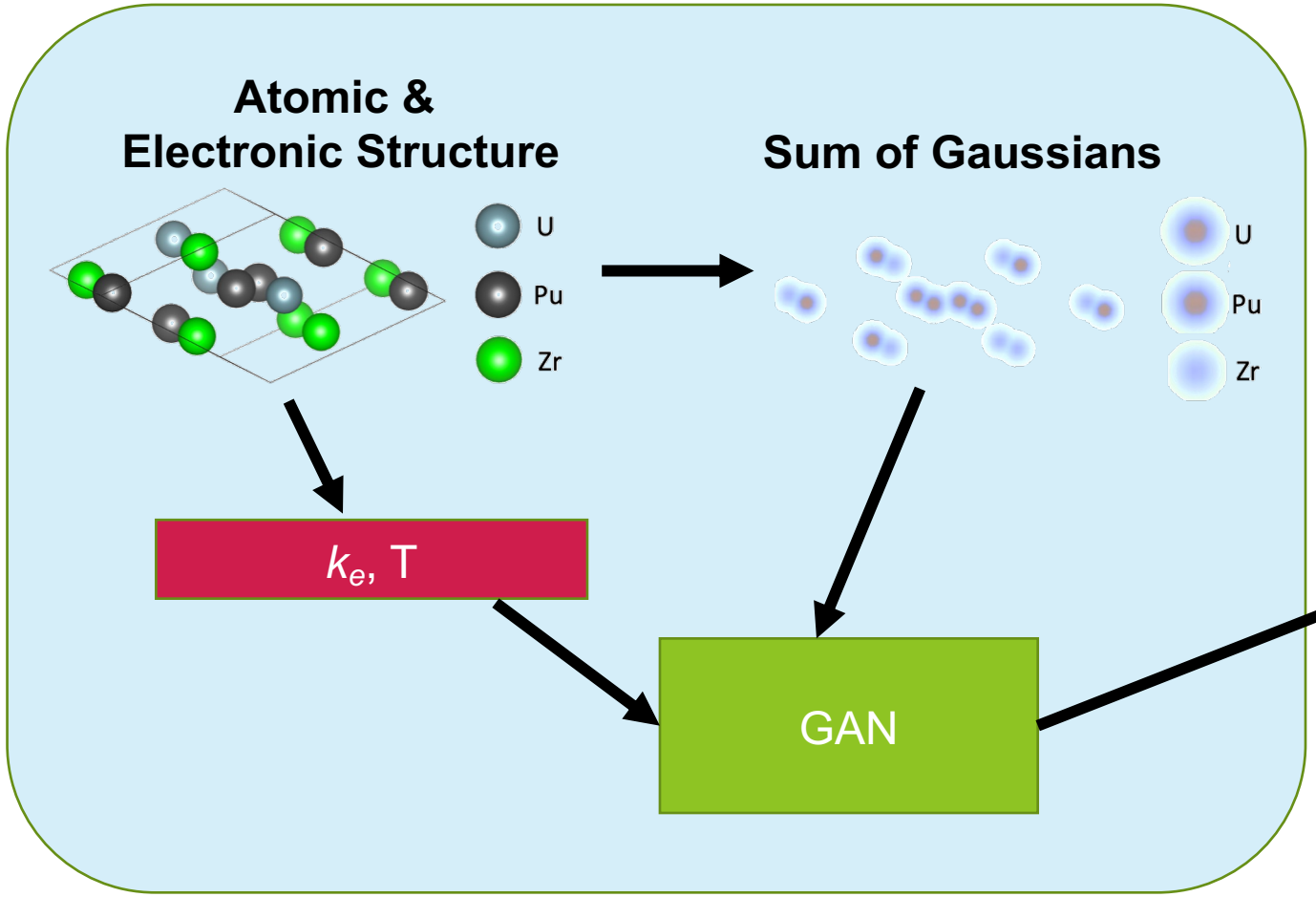
Machine learning using DFT to predict electronic structures of alloy systems

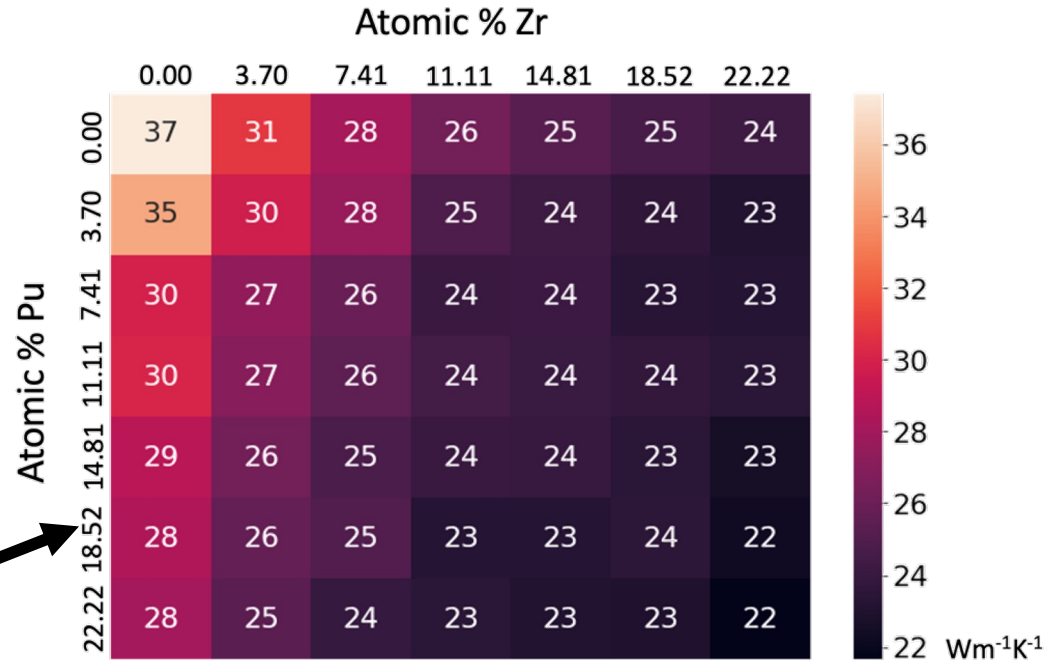
- DFT calculates electronic band structure and electron orbitals
- Orbitals are represented with sum of Gaussians
- Electronic structure is harvested for predicted material properties
- Generalized Adversarial Network (GAN) algorithm is trained and then makes property predictions for new structures
- This method is applicable to any property dependent upon spatial positions, mass, and electron density of each atom in the material
  - Tensile strength, modulus, yield strength, defect energies, corrosion behavior…



Practical example – calculating thermal conductivity of multicomponent alloy

- U-Pu-Zr alloys as a challenging system with some experimental data but little modeling



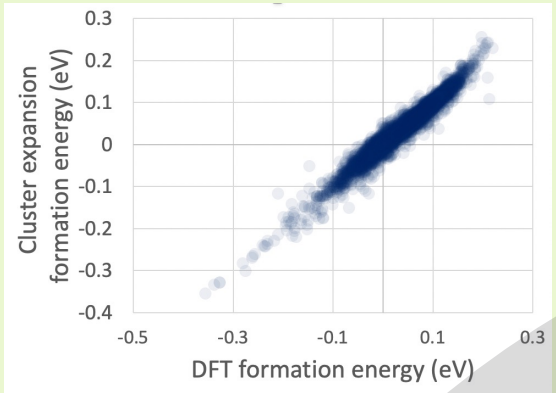


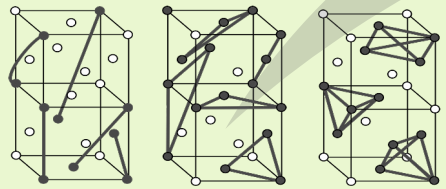
General workflow to predict thermodynamic and kinetic properties of multicomponent alloys

- Uses density functional theory, machine learning, cluster expansion and kinetic Monte Carlo

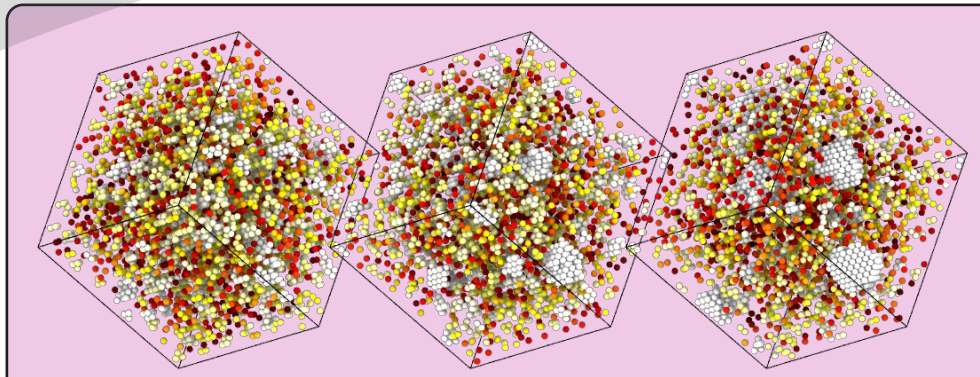
Ion vs neutrons, accelerated testing

From ab initio DFT data to properties

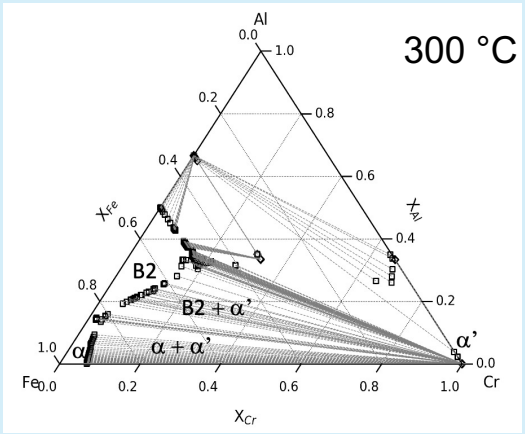




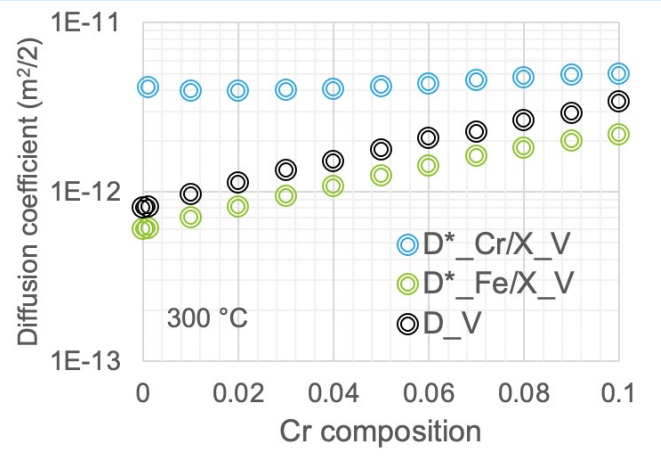
DFT and cluster expansion



kinetic Monte Carlo simulation of precipitation



Low temperature phase diagram

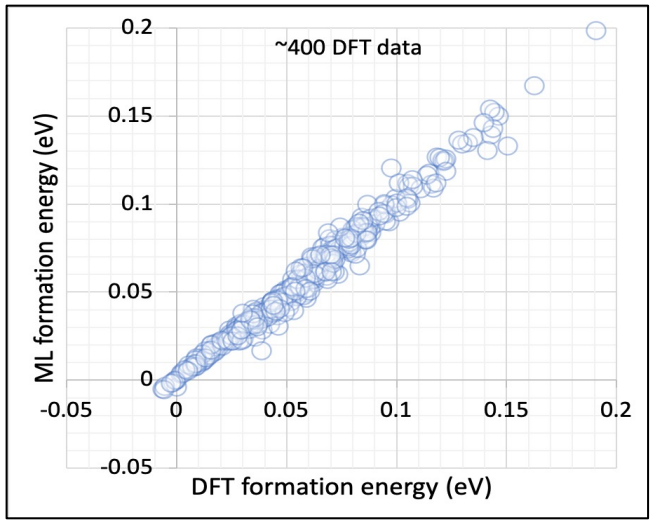


Non-dilute solute effect on diffusion

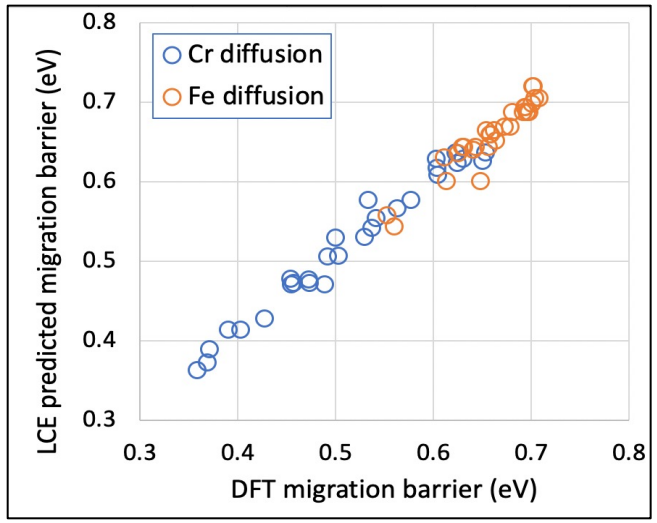
Predicting energetics, diffusivities, and phases

DFT vs ML prediction for Fe-Cr binary system

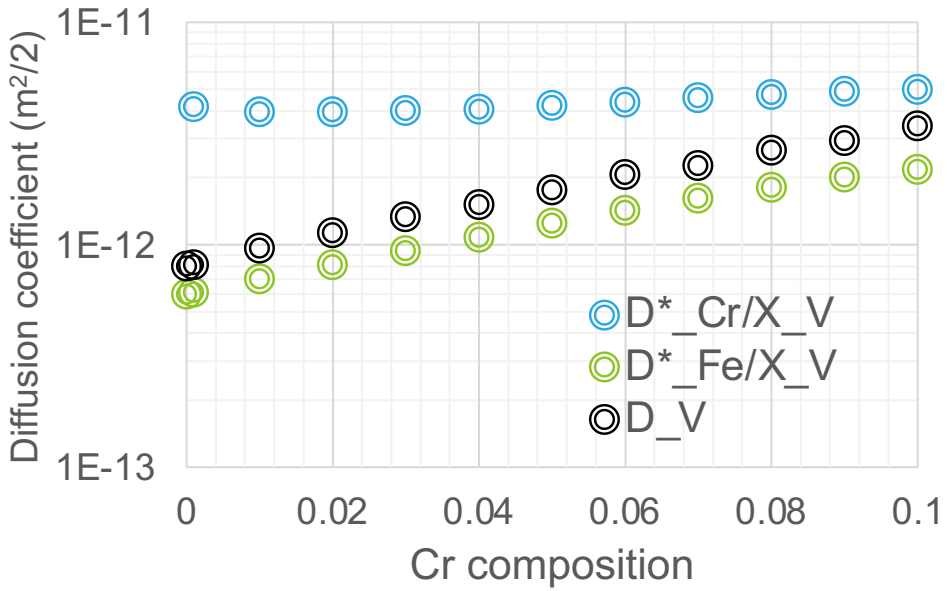
Formation energy (thermodynamics)



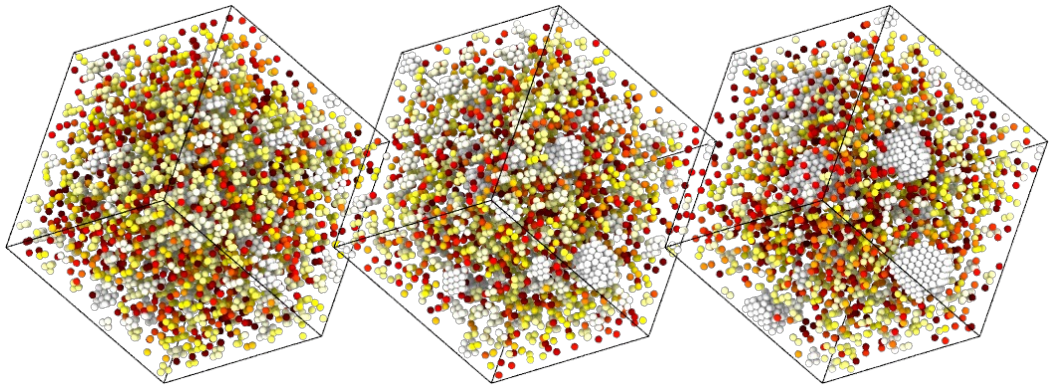
Migration barrier (kinetics)



Cr effect on atom and vacancy transport (300 °C)

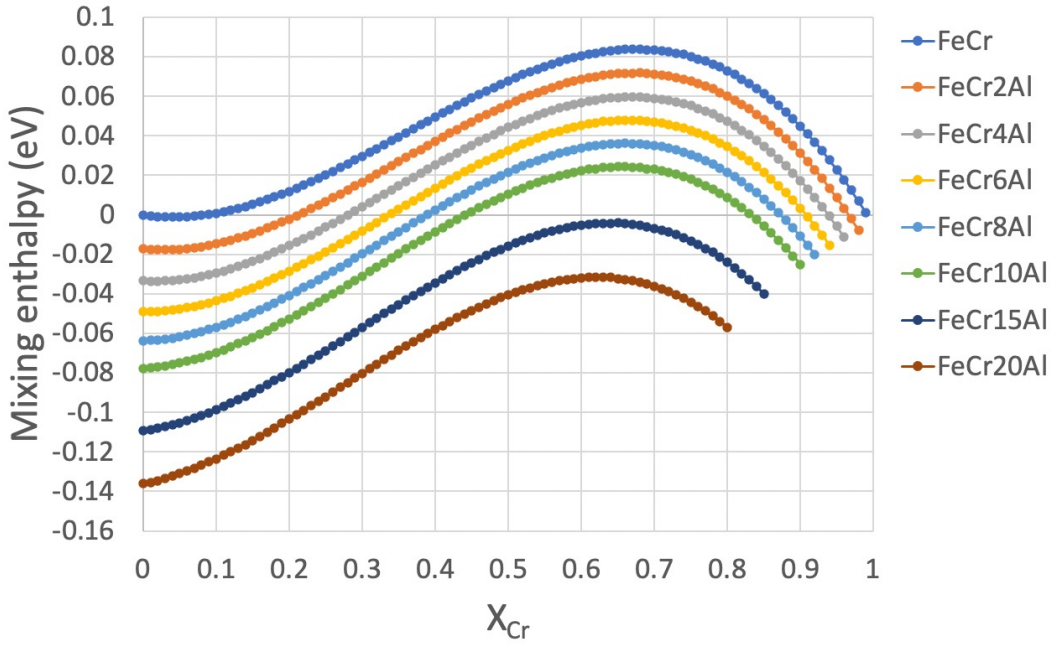


Cr-rich cluster nucleation and growth (15Cr, 300°C)

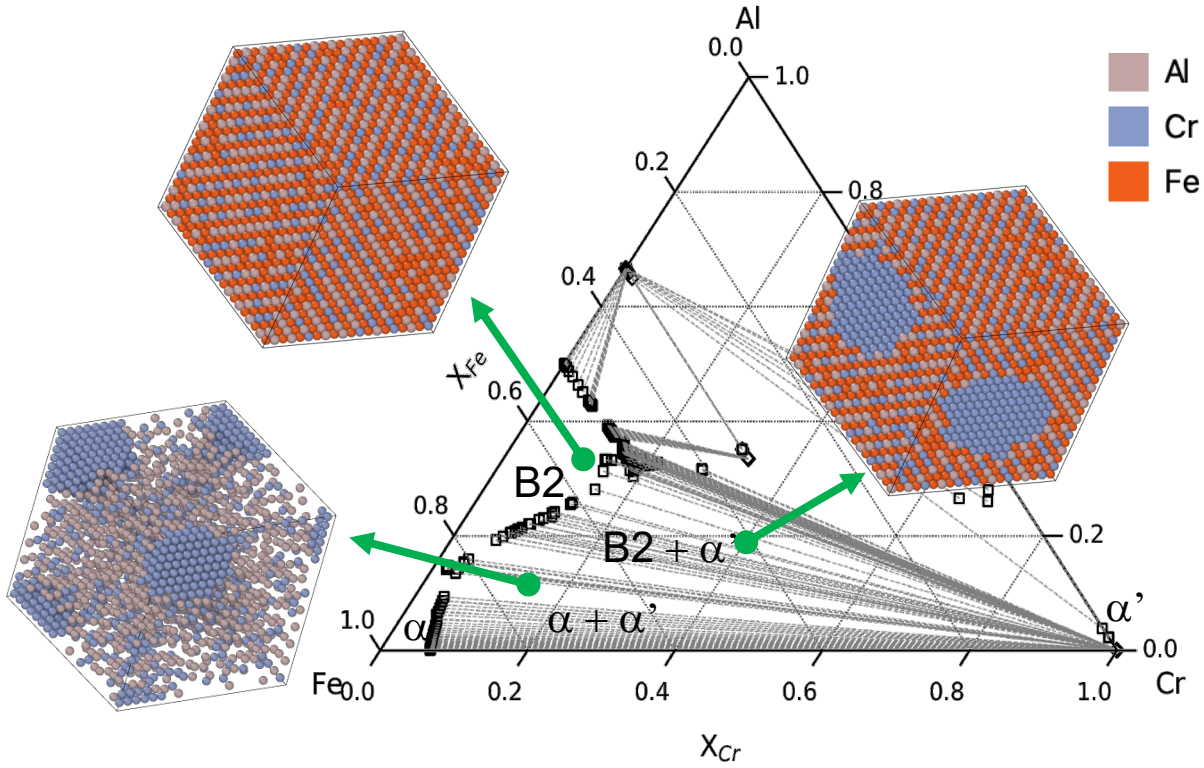


Practical applications to multicomponent Fe-Cr-Al alloys

FeCr-*x*Al mixing enthalpy



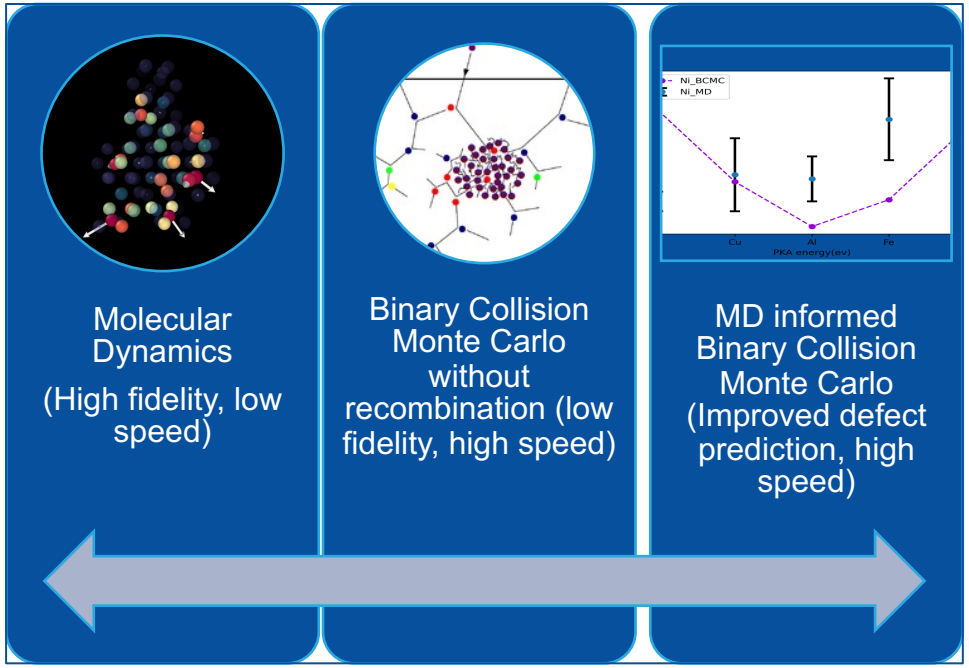
Predicted Fe-Cr-Al phase diagram (300 °C)



- Fe-Cr-Al phase diagram constructed by thermodynamics integration and Monte Carlo simulations

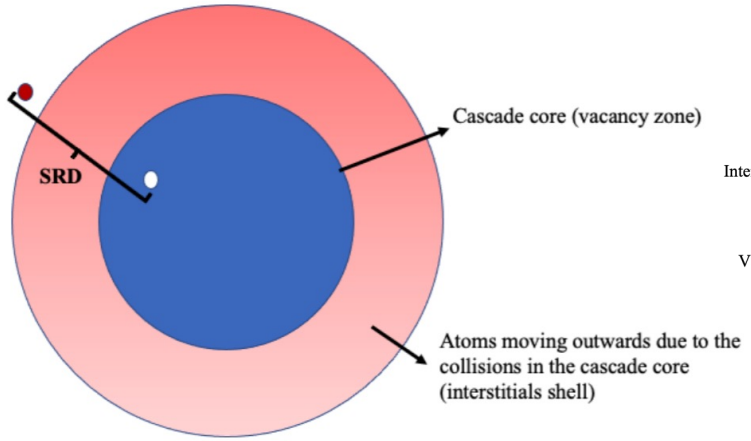
Providing realistic irradiation-induced defect quantities to model microstructure evolution

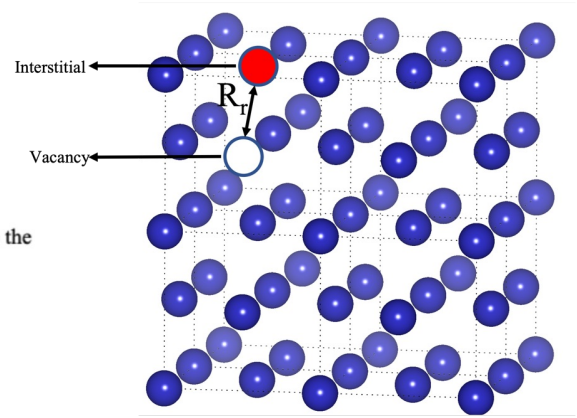
- Equating different irradiation conditions requires fast and accurate calculations of irradiation-induced defects
- **MAGPIE code:** INL researchers developed a MOOSE-based binary collision Monte Carlo (BCMC) code called MAGPIE
- MAGPIE contains a novel defect recombination model designed to address the overestimation of defect populations by BCMC
- We focus on molecular dynamics-based quantification of irradiation damage metrics and comparisons of different defect recombination models to test the MAGPIE recombination model
- Fast and accurate calculations of defect populations means microstructure evolution under different irradiation conditions can be quantitatively studied

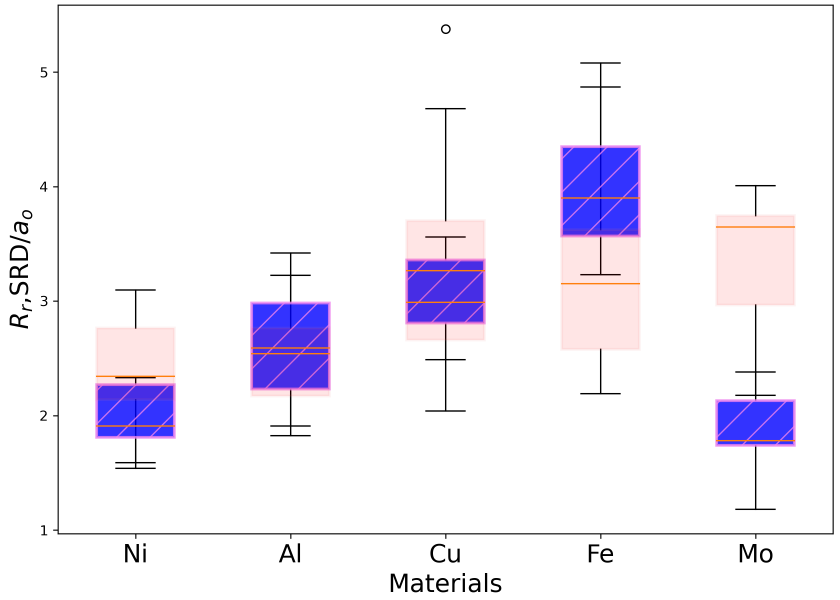


Ion vs neutrons, accelerated testing

Are two recombination metrics actually equivalent?





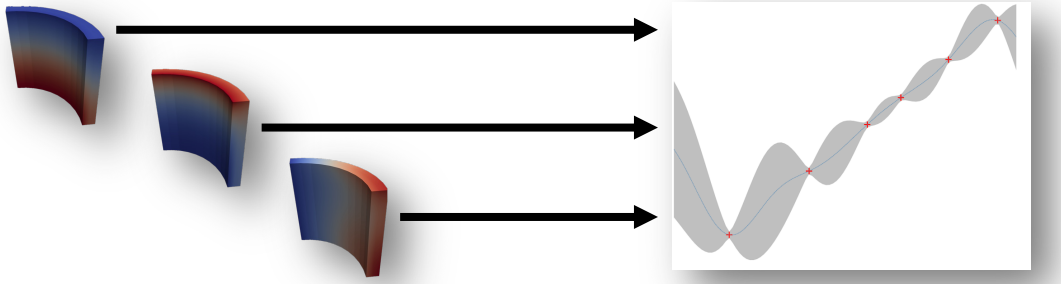


- Spontaneous recombination distance: calculated from collision cascade simulations
- Recombination radius: calculated from diffusional simulations
- Typically, these two metrics are equivalent within statistical significance, but may vary for heavier elements

Introduction to Stochastic Tools Module

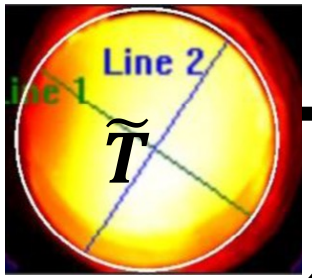
- Provide a MOOSE-like interface for performing stochastic analysis on MOOSE-based models
- Sample parameters, run applications, and gather data that is both efficient (memory and runtime) and scalable
- Perform UQ and sensitivity analysis with distributed data

- Train meta-models to develop fast-evaluating surrogates of the high-fidelity multiphysics model
- Provide a pluggable interface for these surrogates



Material inversion determines material properties that reproduce experimental results

Experimental, $\tilde{T}$

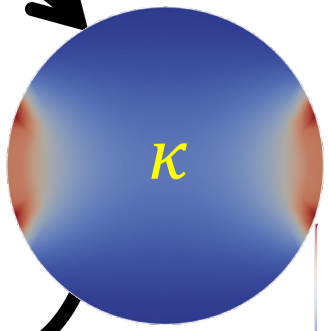


Objective Function:

$$\min_{\boldsymbol{p}} J(T,\boldsymbol{p}) = \frac{1}{2}\sum_{i=1}^{N}\left(T_i - \tilde{T}_i\right)^2$$

Modify $\boldsymbol{p}$ until J is minimized

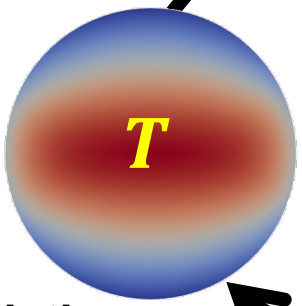
Unknown material property, κ



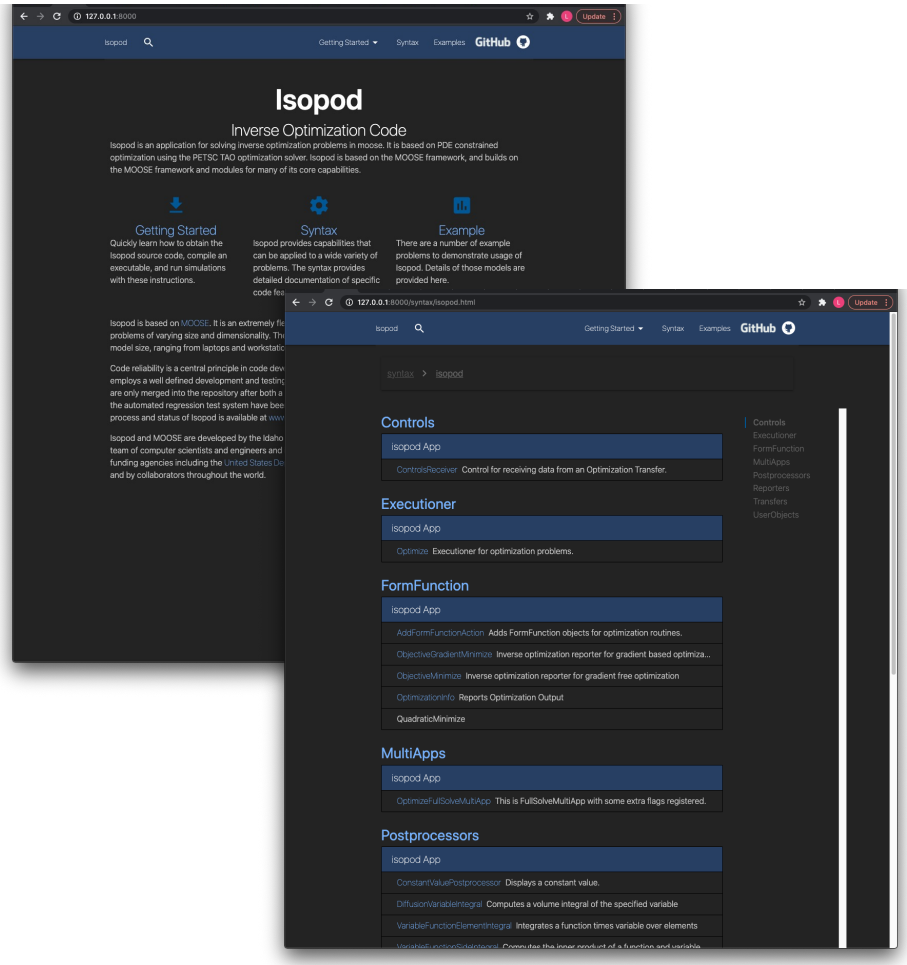
Physics Model:

$$\boldsymbol{g}(T,\boldsymbol{p}) = \nabla^T \kappa \nabla T + q_v = 0$$

Solve the forward problem

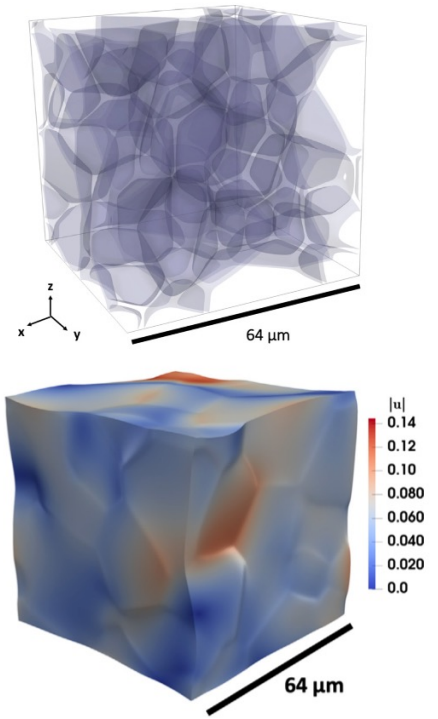


Simulation, T



Why is Crystal Plasticity Important & What are the Challenges?

- Importance
  - Fundamental in microstructure-based mechanical predictions
  - Applicable to many kinds of deformation mechanisms and various microstructures
  - Accelerate new material discovery and qualification
- Challenges for MOOSE implementation
  - Scattered in various code branches & bases
  - Not user-friendly
  - Limited auxiliary input types (e.g., for microstructure, material parameters)
  - Robustness and speed can be improved



- Example grain structure and irradiation-induced microstructure distortion (A.M. Jokisaari, 2020)

Capability & Usability Improvements

- Expanded inputs by creating pipeline from Dream3D to MOOSE to generate microstructures from statistical information

Statistical data

EBSD data

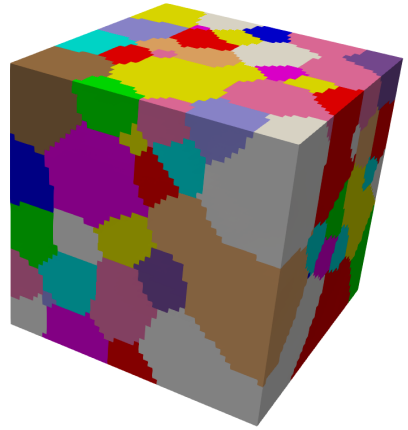
…

DREAM.3D BlueQuartz Edition

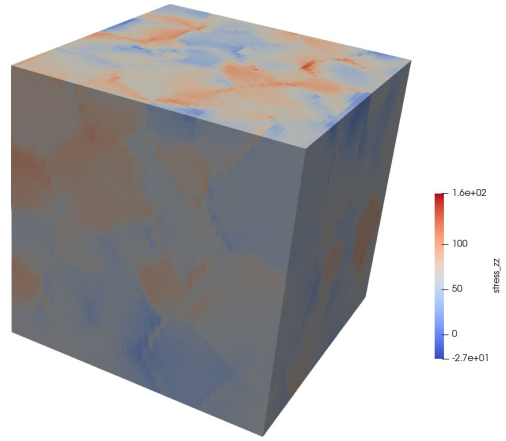
.inp files

coreform Cubit™

Exodus file

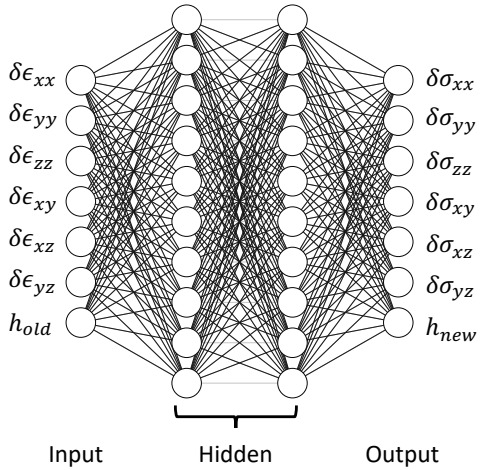


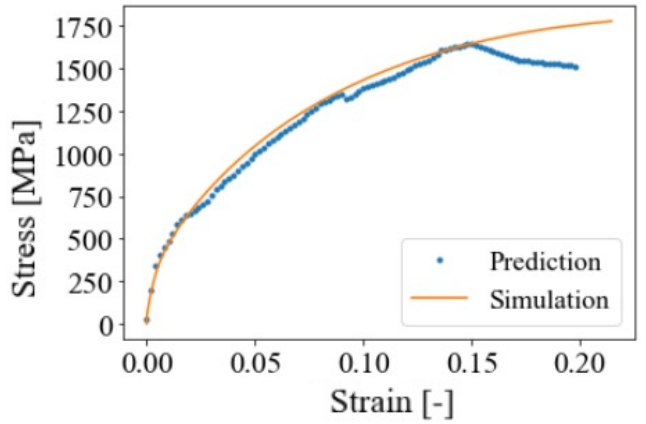
MOOSE-based simulation tools



- Added thermal expansion eigenstrain
- Improved robustness and efficiency
  - Crystal orientation update
  - Boundary condition bug during substepping
  - Improved code structure for usability and modularity
  - Reduced order model development to speed crystal plasticity solves

Prediction by NN can accelerate FEM prediction

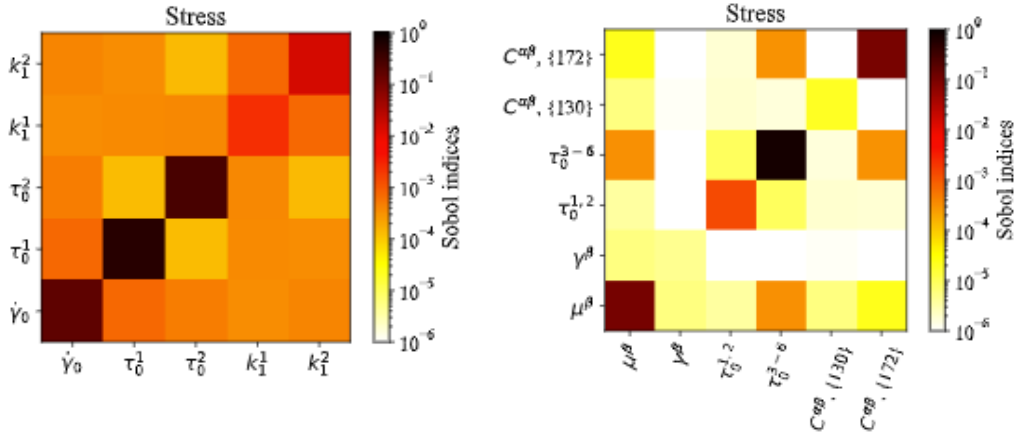




Stochastic Tools Module leverages power of crystal plasticity

❑ Sensitivity analysis

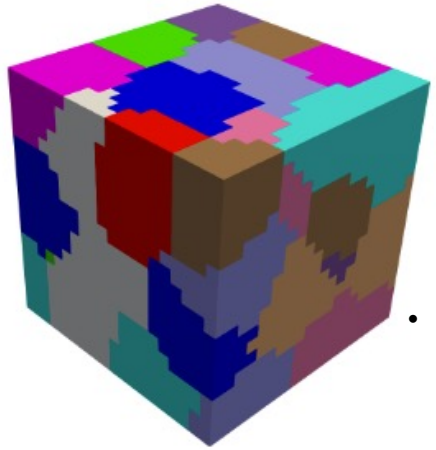
- **Leverage stochastic tools module (STM) in MOOSE**
  - Crystal plasticity model is highly complex and includes a lot of parameters from different slip systems
  - Use STM enables the possibility to examine the most important properties that has the most impact on the material response/behavior



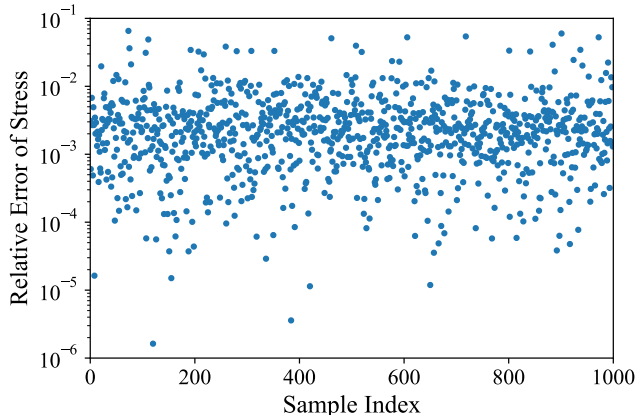
- Sobol indices (first and second order) for the stress. Material parameters are chosen from the slip (left) and twin (right) based deformation modes, respectively.

❑ Surrogate model training

- **STM also enables surrogate model training**
  - Polynomial chaos, Polynomial regression, Proper orthogonal decomposition, Gaussian process
  - Successfully applied for heat conduction problems
  - Produces accurate prediction of the final stress state for a CP model
  - However, does not do well in capturing transient states



- Polycrystal sample with 45 grains



- Example polynomial chaos surrogate model. Relative error of stress (@ t_end) for 1K samples. Similar error magnitude is observed for slip and twin rates.

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