INL/MIS-21-63514-Revision-0

Physics based modeling and data analytics

May 2024

Changing the World's Energy Future

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Physics-based modeling and data analytics

Physics-based modeling and data analytics

- FY2021 goal: provide immediate computational capabilities to be leveraged and further developed within NMDQi and other programs
  - Improve physics-based modeling capabilities for structure-property relationships
    - High-fidelity mechanics
    - Point defect interactions with composition
  - New capabilities for statistical studies
  - New capabilities to interpret and work with experimental data
- Long-term goal: build the computational toolset and human expertise necessary to achieve NMDQi goals
  - Chemistry, mechanics, machine learning, statistical analysis, microstructure identification, irradiation effects

April 30, 2021

Dewen Yushu

Postdoctoral Research Associate, C650

Crystal Plasticity

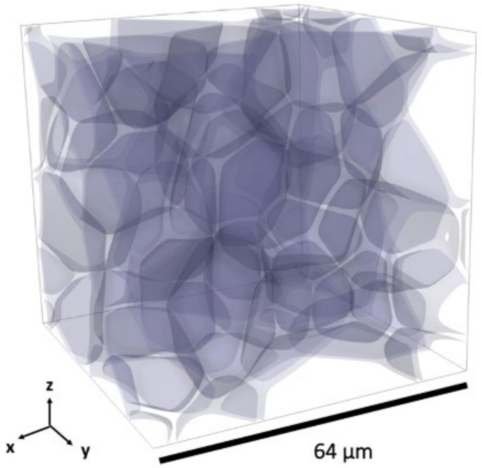
Why is Crystal Plasticity Important & What are the Challenges?

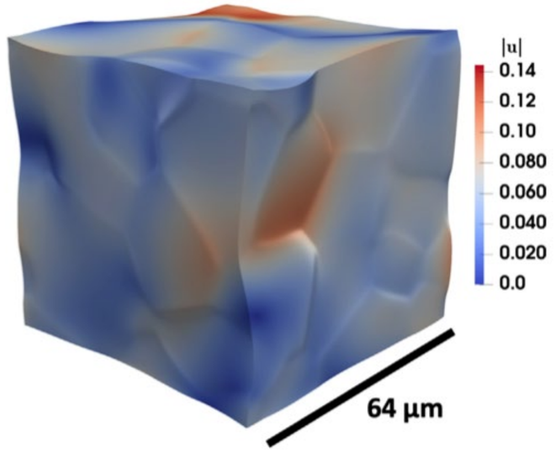
❑ Importance

- Fundamental in microstructure-based mechanical predictions
- Applicable to many kinds of deformation mechanism and various microstructures
- Accelerate new material discovery and qualification

❑ Challenges

- Various code branches & bases (Scattered in MOOSE, MARMOT, BISON)
- Most models are not very well documented
- Convoluted inputs (in .i file)
- Limited auxiliary input types (e.g., for microstructure, material parameters)
- Convergence is not great

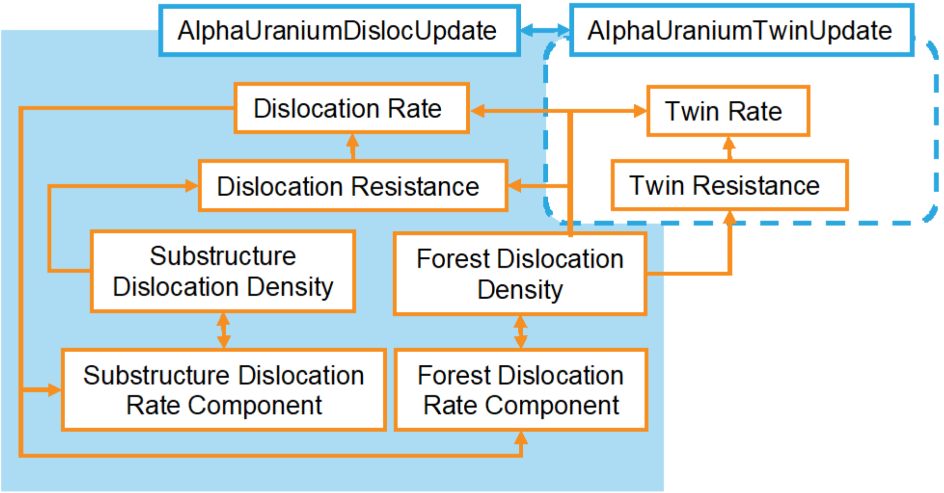




- Example grain structure and irradiation-induced microstructure distortion (A.M. Jokisaari, 2020)

Crystal Plasticity Improvements

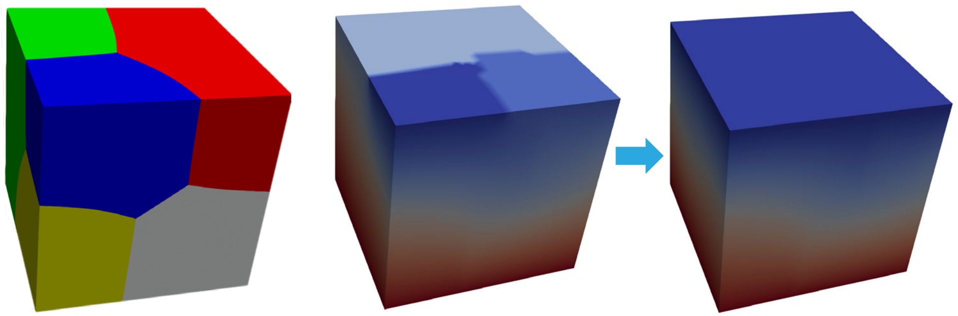
❑ Improved code structure



- **User & developer friendly**
  - Reduced number of classes & simplified input
- **Retained modularity**

❑ Improved robustness

- **Fixed BC issue related to sub-stepping**



❑ Added thermal eigenstrain

- Decomposition of ! :

$$F = F^e F^p F^{\checkmark}$$

- Evolution of thermal deformation gradient (! !):

$$\dot{F}^{\checkmark} F^{\checkmark -1} = \dot{\vartheta}\beta \quad \beta = \mathrm{diag}(\beta_1, \beta_2, \beta_3)$$

  where " is the thermal expansion coefficient.

- Shear stress for the # slip system:

$$\tau = \det(F^{\checkmark}) \; F^{\checkmark} S F^{\checkmark -1} : S_0$$

- Time integration for ! ! :

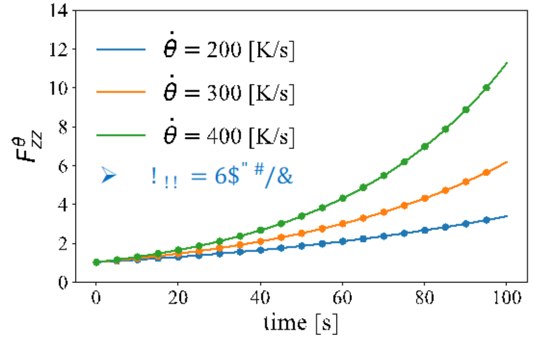
$$F_{n+1}^{\checkmark -1} = F_n^{\checkmark -1}(I - \Delta\vartheta\beta)$$

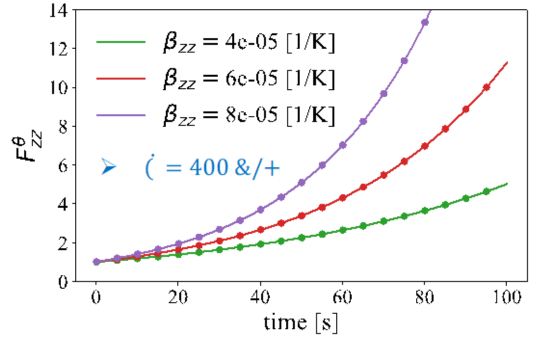
- Crystal plasticity Jacobian:

$$J = I - C : \left(\frac{\partial E^e}{\partial F^e} \frac{\partial F^e}{\partial F^{p-1}} \frac{\partial F^{p-1}}{\partial S} \right)$$

- Elasto-plastic tangent moduli:

$$\frac{\partial \sigma}{\partial F} = \left(\frac{\partial \sigma}{\partial S} \frac{\partial S}{\partial F^e} + \frac{\partial \sigma}{\partial F^e} \right) \frac{\partial F^e}{\partial F}$$





❑ Plans

- **Publication**
- **Extend eigenstrain types**
- **Improve performance & robustness**
- **Expand microstructural input types**

April 30, 2021

Md Riaz Kayser

Postdoctoral Research Associate, C610

Recombination of cascade damage in metals and alloys

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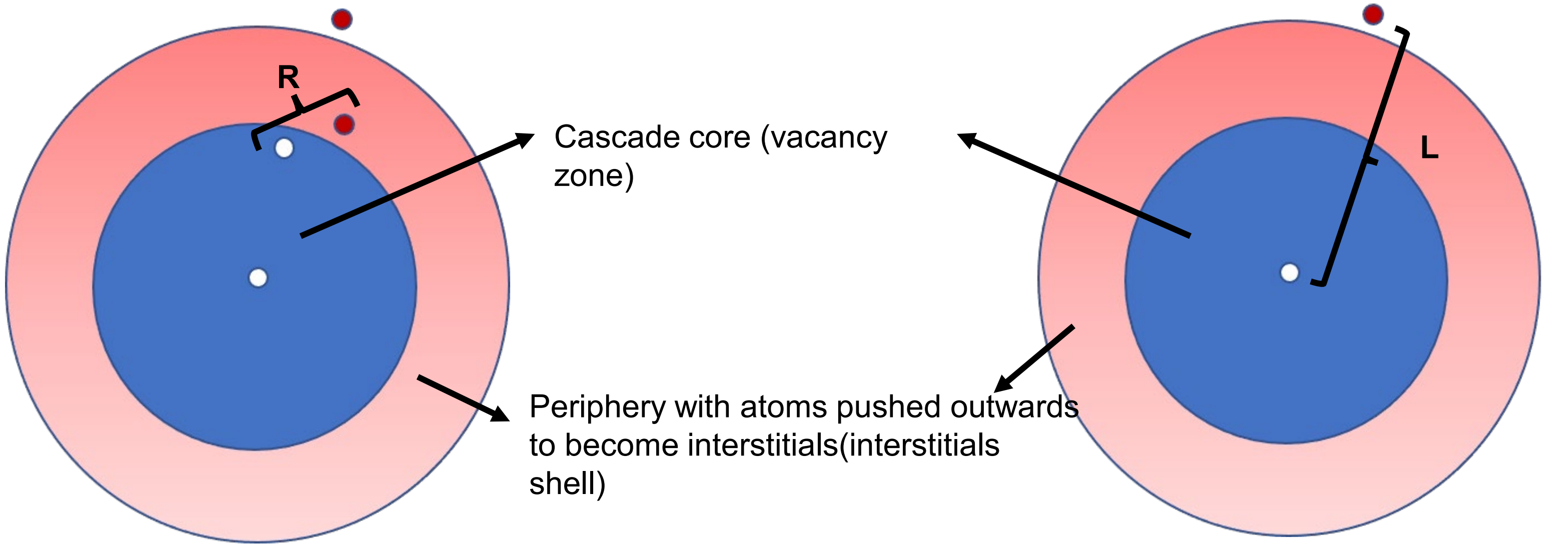
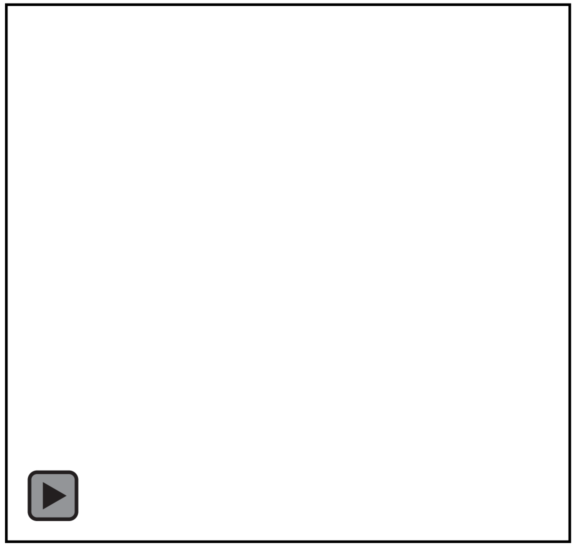
Local, evolving damage distribution

- Recombination of defects controls the microstructure evolution of materials
- To design new materials, it is vital to understand defect recombination in metals, alloys and its interfaces
- The recombination radius (R): maximum distance between the monovacancy and SIA center allowing immediate recombination
- Spontaneous recombination distance (L): minimum physical separation of the interstitial and vacancy survival of initially created Frenkel defects



Vacancy Interstitial

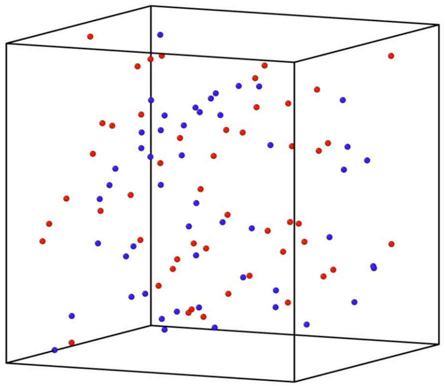


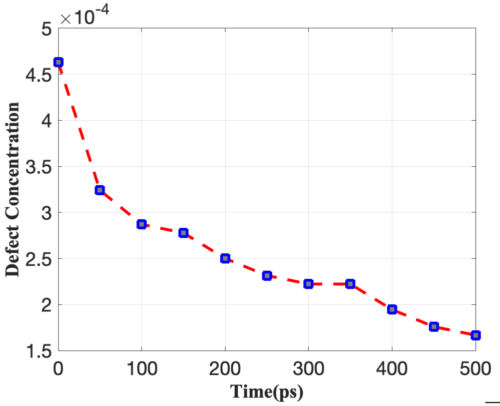
Difference between interstitial and vacancy zone for PKA 5 KeV of Ni

Quantifying cascade damage and recombination

Material system	Temp (K)	Maximum number of defects	Stable number of defects	Recombination time (ps)	Recombination rate (number of Frenkel defects/ps)	Radius of interstitial zone (Å)	Radius of vacancy zone (Å)	Spontaneous recombination distance (L)
Ni	300	306	6	3.7	83.90	16.12	11.35	8.93
Cu	300	764	9	10.6	143.43	23.41	18.65	14.72
Al	300	466	8	6.7	69.38	26.76	22.43	13.94

Diffusion model for recombination radius





Material	Diffusion coefficients of single interstitial atom (nm^2/ns)	Diffusion coefficients of monovacancy (nm^2/ns)	Recombination constant of vacancies and SIAs (ns^{-1})	Recombination radius (nm)	Spontaneous recombination distance (nm)
Ni	**18.35**	**2.18**	**18616.91**	**$2.21\times a_o$**	**$2.55\times a_o$**
Mo	**17.77**	**2.05**	**9643**	**$1.9\times a_o$**	**-**
Al	**17.61**	**0.99**	**7807.33**	**-**	**$3.45\times a_o$**

Change of defect concentration of nickel at 1500 K

April 30, 2021

Zachary Prince

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Lynn Munday

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Andrew Slaughter

Computational Scientist, C510

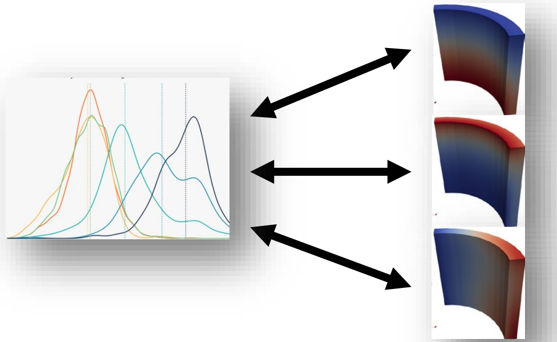
Stochastic Tools Module

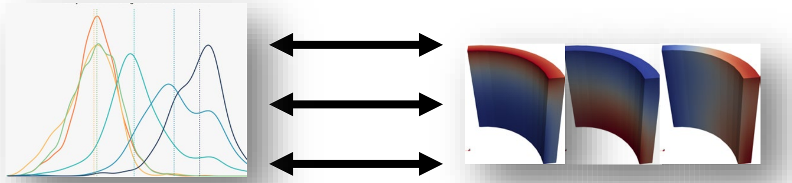
Idaho National Laboratory

Introduction to Stochastic Tools Module

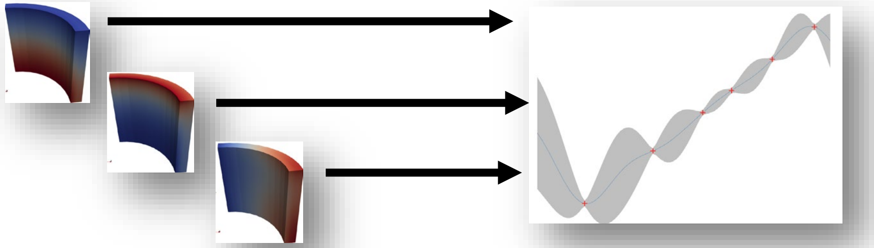
The Stochastic Tools Module (STM) is an open-source MOOSE module available to all MOOSE-based applications.

- 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.

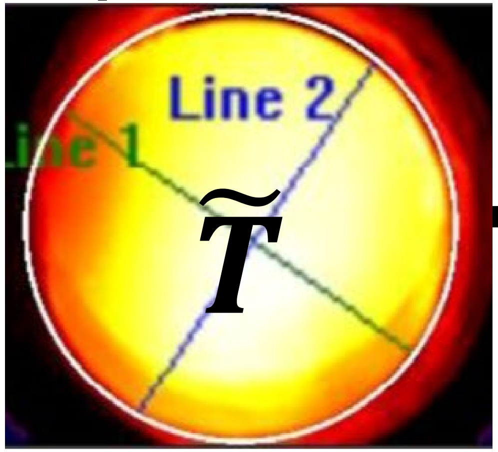


Stochastic Tools Module Update

- Ability to specify number of processors to use per sample run
  - Better memory management for stochastically running large models
  - Syntax:
    - `Sampler/*/min_procs_per_row=<num>`
    - `MultiApps/*/min_procs_per_app=<num>`
  - Example: 1,000 samples with 100 processors
    - Previously: 100 apps with 1 processor running 10 samples
    - With `min_procs_per_app = 10`: 10 apps with 10 processors running 100 samples
- Generalizing surrogate model training data
  - Reporter system allows output of any “type” of quantity of interest in MOOSE simulations
  - STM can now transfer arbitrary data types from sub apps to accumulate theses quantities
  - Surrogate trainer system can access the accumulated data for building surrogate models
- Looking for applications for showcasing capabilities
  - Building surrogate models to quickly perform statistical analysis
  - Multiscale modeling with surrogate models

PDE Constrained Optimization

Experimental, $\tilde{T}$

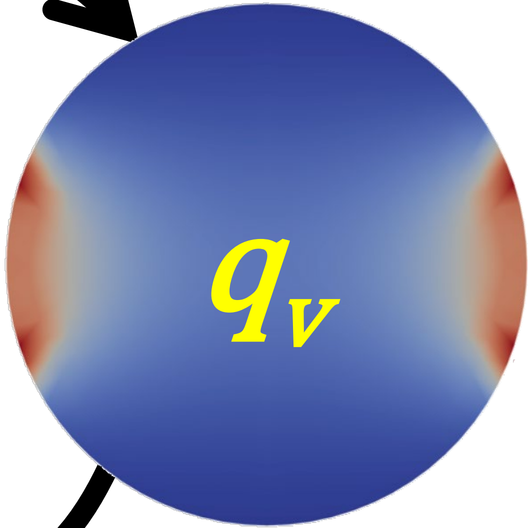


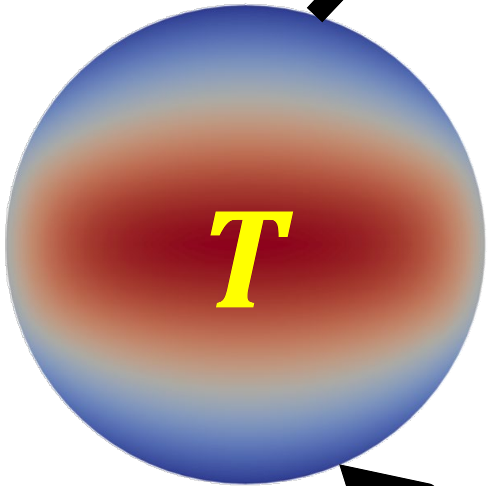
Objective Function:

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

Modify $\boldsymbol{p}$ until J is minimized using Stochastic Tools (Monte Carlo), RAVEN (gradient-free) or **TAO (gradient)**

Unknown parameter:
Heat Source, q_v





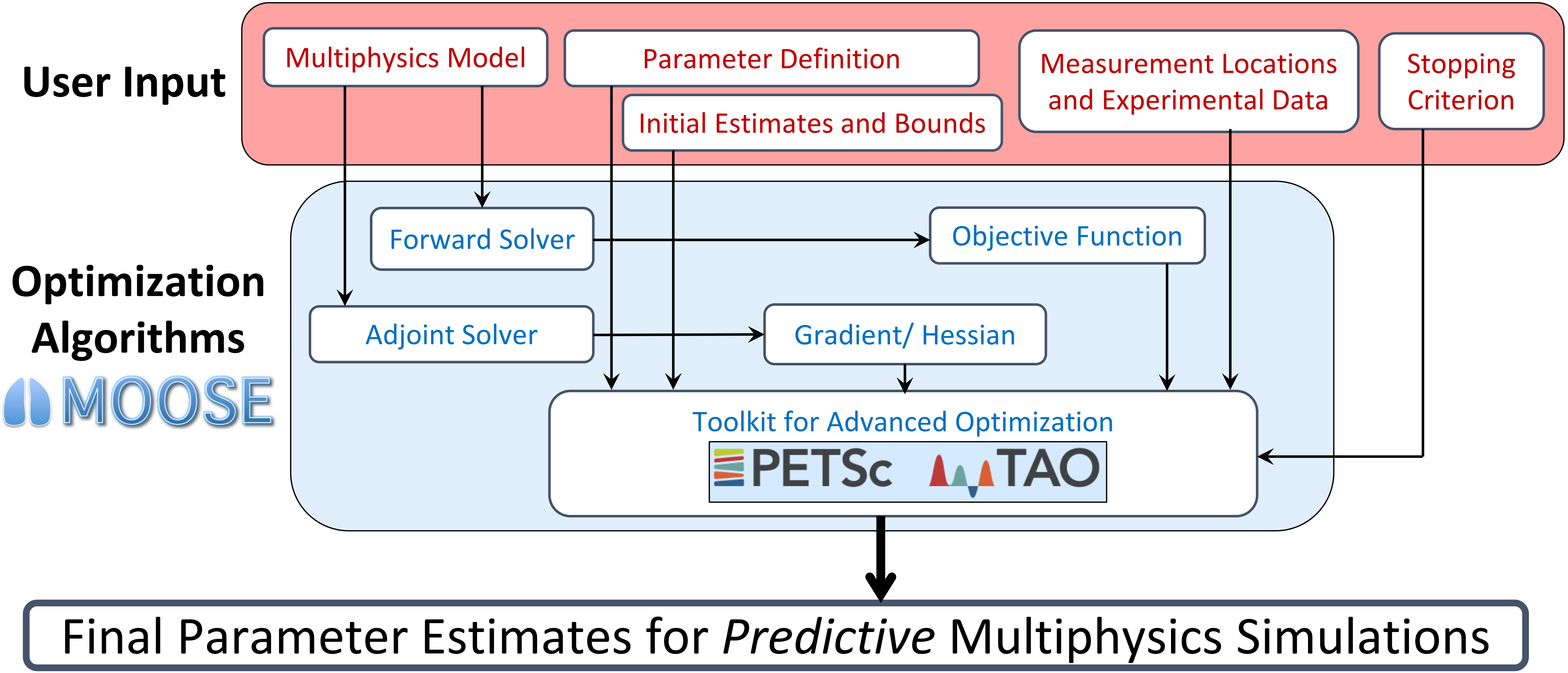
Simulation, T

Physics Model:

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

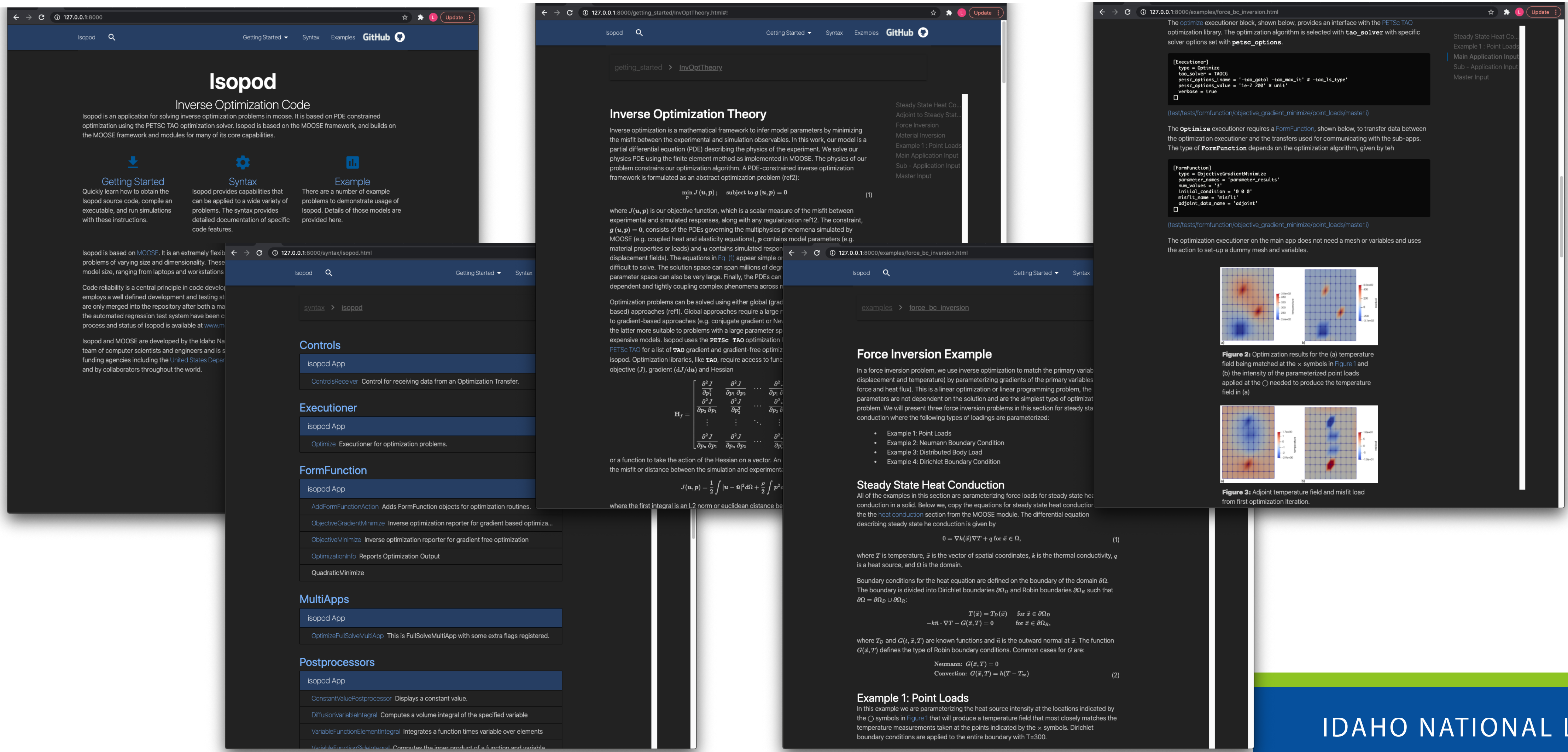
Forward Problem

Computational framework for isopod



Documentation

The current plan is to merge the isopod app into the MOOSE stochastic tools modules which requires documentation along with examples, and maybe a little code clean-up.



April 30th, 2021

Jia-Hong Ke

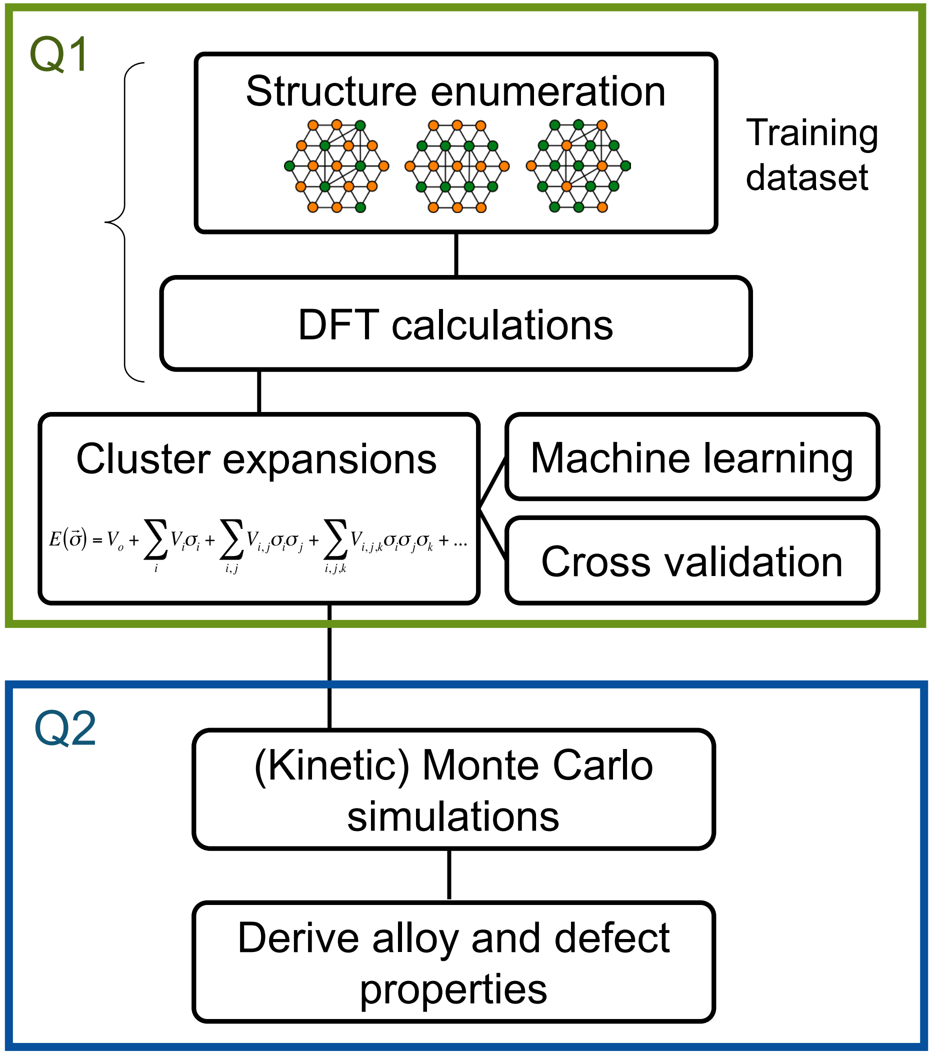
Computational Scientist, C650

Machine learning and atomistic modeling to predict thermo-kinetic properties of nuclear structural materials

Introduction to atomistic modeling + machine learning workflow

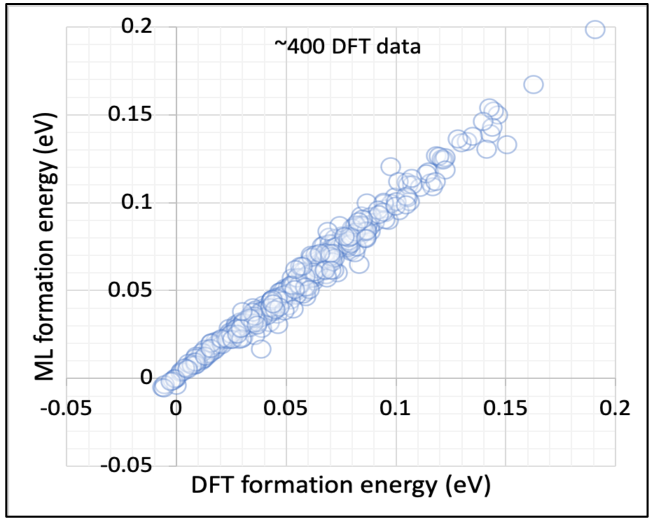
- **Long term goal**:
  Develop a workflow to predict thermo-kinetic and defect formation properties of multicomponent nuclear alloys

  Q1: High throughput DFT setup and data analytics
  Q2: Workflow to derive thermo-kinetic properties (kMC)
  Q3: Multicomponent and concentrated alloy extension
  Q4: Workflow to derive solute-defect formation properties

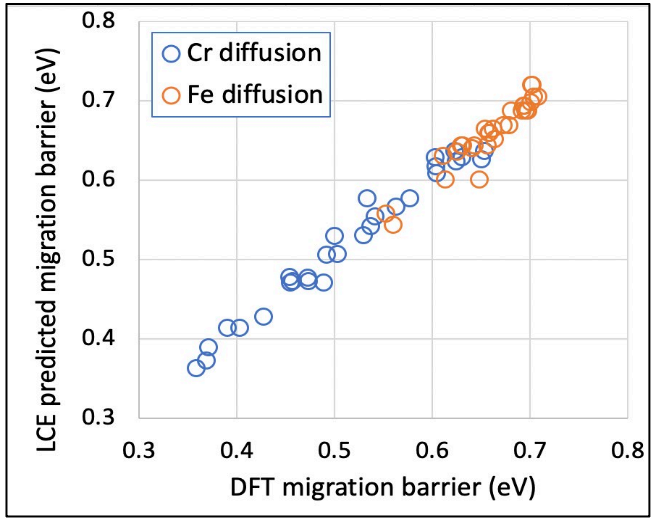


DFT vs ML prediction for Fe-Cr baseline system (Q1)

Formation energy (thermodynamics)



Migration barrier (kinetics)

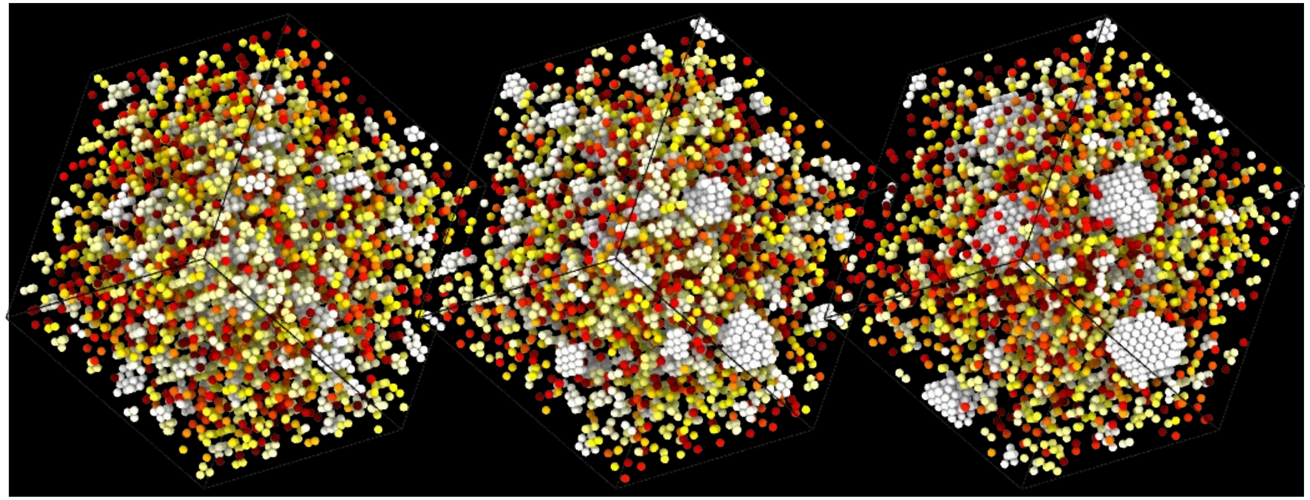


Update on (kinetic) Monte Carlo modeling

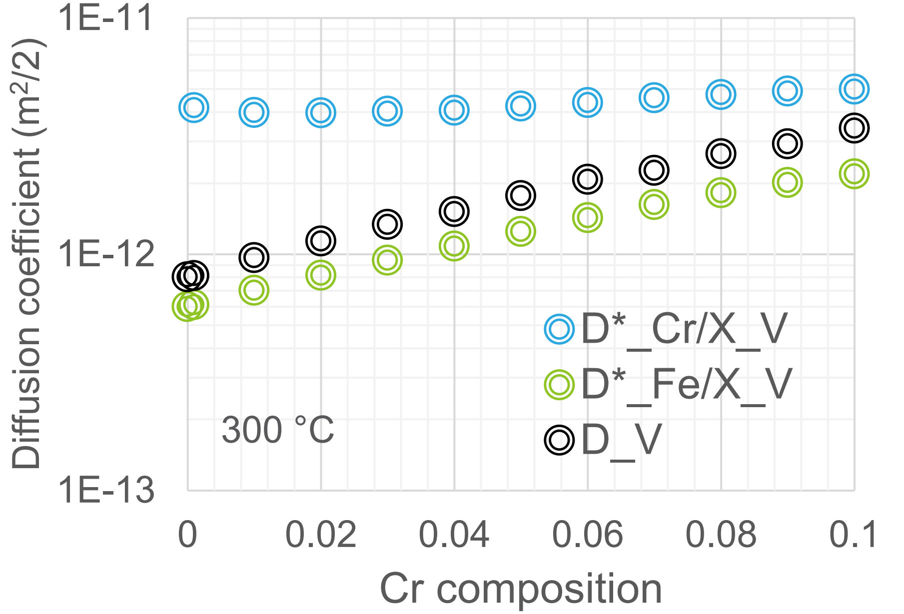
Completed the following workflow (Q2)

- Kinetic properties (diffusivities, Onsager coefficients)
- Microstructure evolution (binary cluster nucleation, precipitation, and phase stability)

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



Nonlinear trend of Cr effect on atom transport



Experimental comparison and validation of high temperature data are in progress

Next steps in FY21

- Extend to multicomponent system
- Derive defect formation/binding energies by coarse graining

This coding work was done in collaboration with Prof. Anton Van der Ven and Sanjeev Kolli (UCSB)