Integrated Thermo-mechanical Design of of First Wall Components Under Evolving Chemistry and Microstructure During Fusion Reactor Operation

ThermChem-FW

(An FES/Scidac-5 Center)

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UCLA · Stony Brook University · MIAMI · SciDAC Scientific Discovery through Advanced Computing · Idaho National Laboratory · Oak Ridge National Laboratory · Pacific Northwest National Laboratory

Project senior personnel

Marian (Mat)

Trelewicz (Mat)

- Szlufarska (Mat)
- Morgan (Mat)

Po (Mat)

Cereceda (Mat)

- Permann (Math)
- Spencer (Math)

- Bernholdt (CS)
- Harb (Nucl)

- Cusentino (Mat)
- Sargsyan (Math)

- Setyawan (Mat)

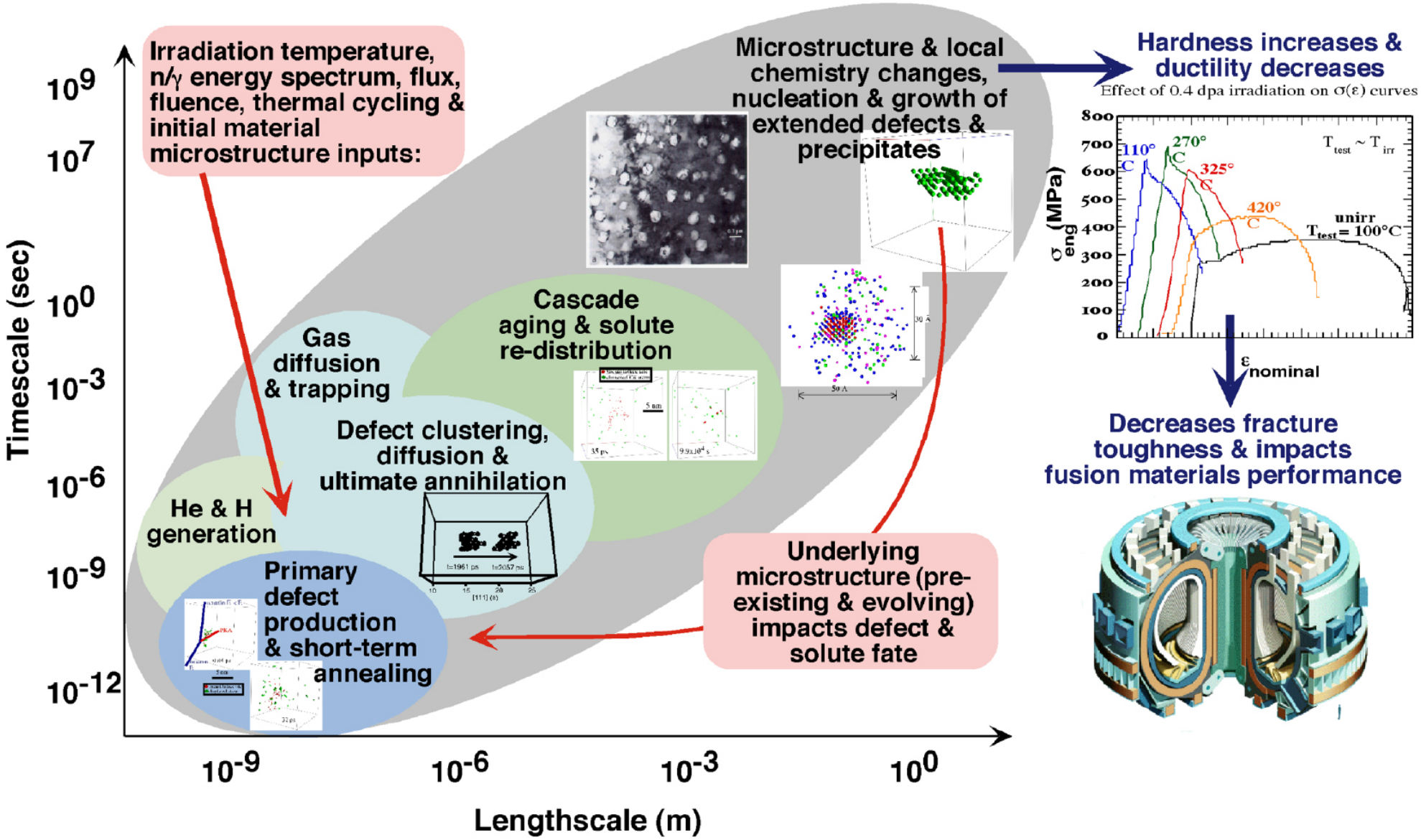
Plus :

- 6 Staff scientists (applied mathematicians, materials scientists, and computer scientists).
- 4 postdoctoral scholars
- 6 PhD students

Multiscale analysis of irradiation damage processes in fusion materials

Modeling paradigm: sequential connection (parameter passing) across scales

Objective: derive ansatz-free, physics-based, predictive models of macroscopic behavior



Solving the mathematical problem embodied by irradiation damage represents a computational grand challenge

Generalized mean-field cluster dynamics PDE based on classical nucleation theory

Golubov, Ghoniem, Odette, Barashev, Stoller, Xu and Wirth

$$\frac{\partial C_i}{\partial t} = \nabla \cdot (D_i \cdot \nabla C_i) + g_i + \left(\sum_j s_j C_j - s_i C_i \right) + \sum_j \left(\sum_k k_{jk} C_j C_k - k_{ij} C_i C_j \right)$$

Fickian diffusion

$$D_i = D_0^i \exp\left(-\frac{E_m^i}{kT}\right)$$

Crystal structure, chemistry

Species insertion

Irradiation conditions

Absorption at sinks and thermal dissociation

$$s_i^{\text{diss}} = 4\pi r_i^2 D_i \exp\left(-\frac{E_b^i}{kT}\right)$$

$$s_i^{\text{sinks}} = k_c^2 D_i$$

Microstructure

Production/destruction from binary reactions

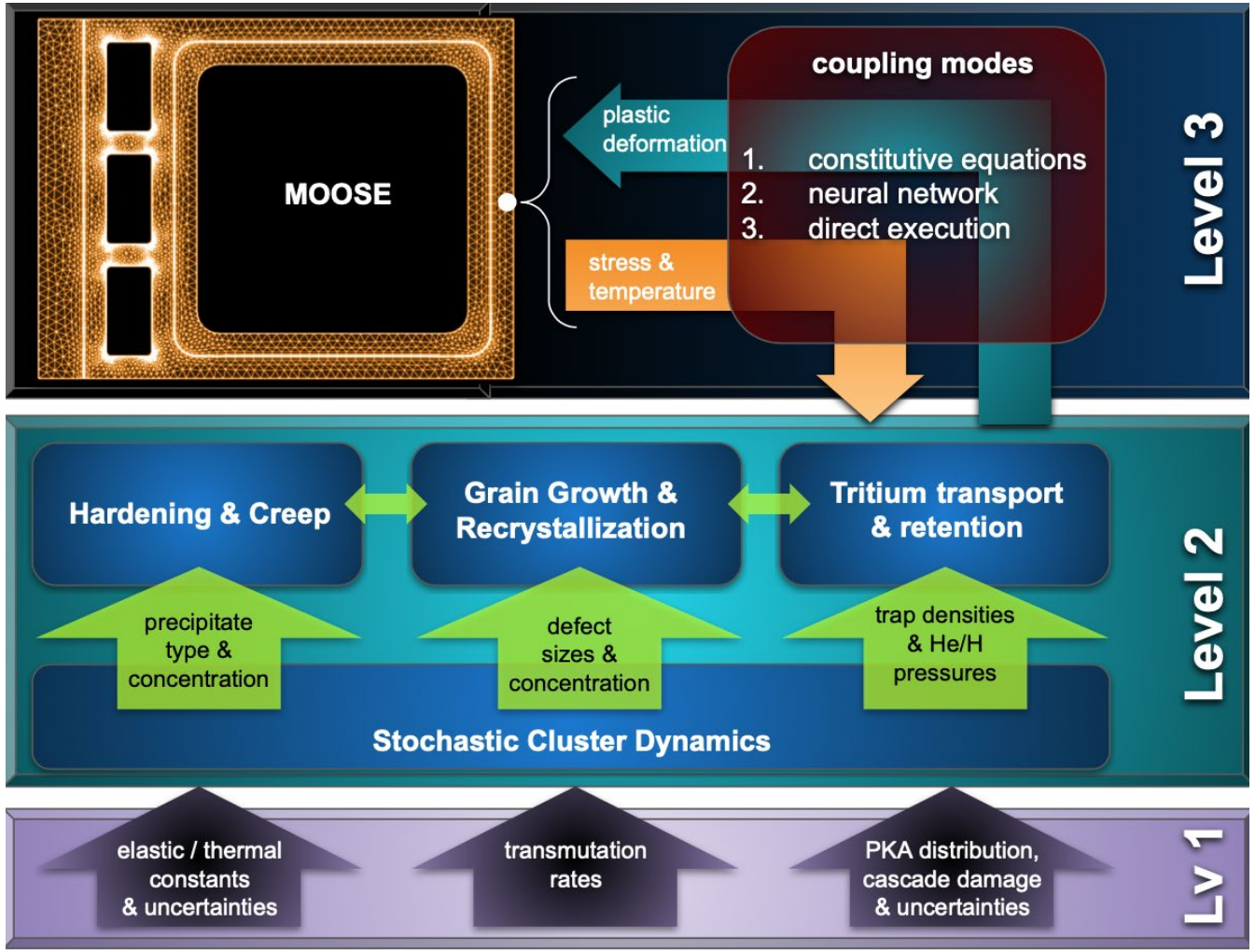
$$k_{ij} = 4\pi(r_i + r_j)(D_i + D_j)$$

Materials physics

All these coefficients give information about the physics of the process, the host material, and the microstructure

Damage accumulation models must incorporate all our latest knowledge on irradiation effects coming from MD, cascade damage, irradiation phenomena (RIS, RED, RIP), multispecies chemistry, etc. → this can lead to ~10^6 coupled equations

The project has been structured as a connected multi-level workflow



Level 3 involves time-dependent simulations (using the finite element code MOOSE) of the thermomechanical evolution of the full FW/B structure. These models will capture the entire geometric complexity and diversity of the multi-material FW/B and will furnish component lifetime prediction and design recommendations based on stress distributions and material property degradation.
INL, ORNL, Miami

Level 2 operates at mesoscopic scales where microstructural evolution occurs, including irradiation hardening, irradiation creep and swelling, thermal fatigue, precipitation, recrystallization (grain growth), and tritium permeation and retention.
UCLA, Miami, ORNL

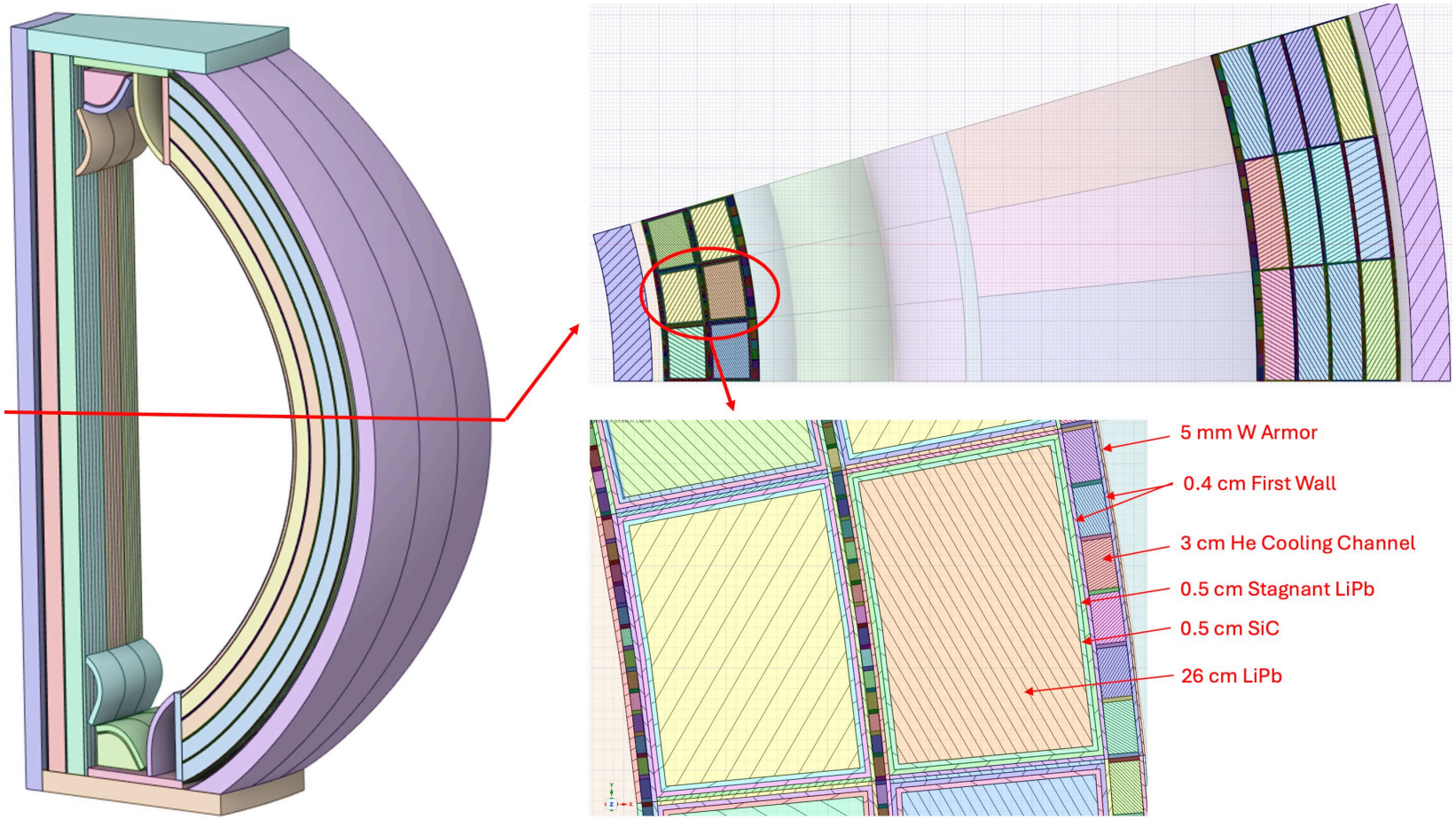
Level 1 captures atomic-level physical processes representative of fusion reactor operation in the FW/B structure, such as (i) transmutation, primary knock-on atoms (PKA) distributions, (ii) cascade damage, (iii) interactions of defect clusters, and (iv) tritium uptake, trapping, and diffusion.
Stony Brook, Wisconsin, Villanova, SNL

Model Description

Harb, Yakubov, Bernholdt

- Neutronics model contains He cooling channels in FW, SW, and breeding zone ribs, as well as SiC FCI.

- Material and neutron source definitions are taken from ARIES conceptual design (https://doi.org/10.1016/j.fusengdes.2017.06.008)
- CAD-based neutron transport was used via OpenMC v0.15.0 (https://docs.openmc.org/en/stable/index.html)
- Materials:
  Structures: W, SiC, RAFM steel
  He and LiPb colling/breeding channels



Level 1: ML Potential Development Workflow

Cusentino, Sargsyan

Model Form

- Energy of atom i expressed as a basis expansion over N-body ACE descriptors

$$E = \sum B^{(N=1)} + \sum B^{(N=2)} + \sum B^{(N=3)} + \cdots$$

The ACE descriptors are generalizable

Regression Method

- β vector fully describes an ACE potential
- Decouples MD speed from training set size

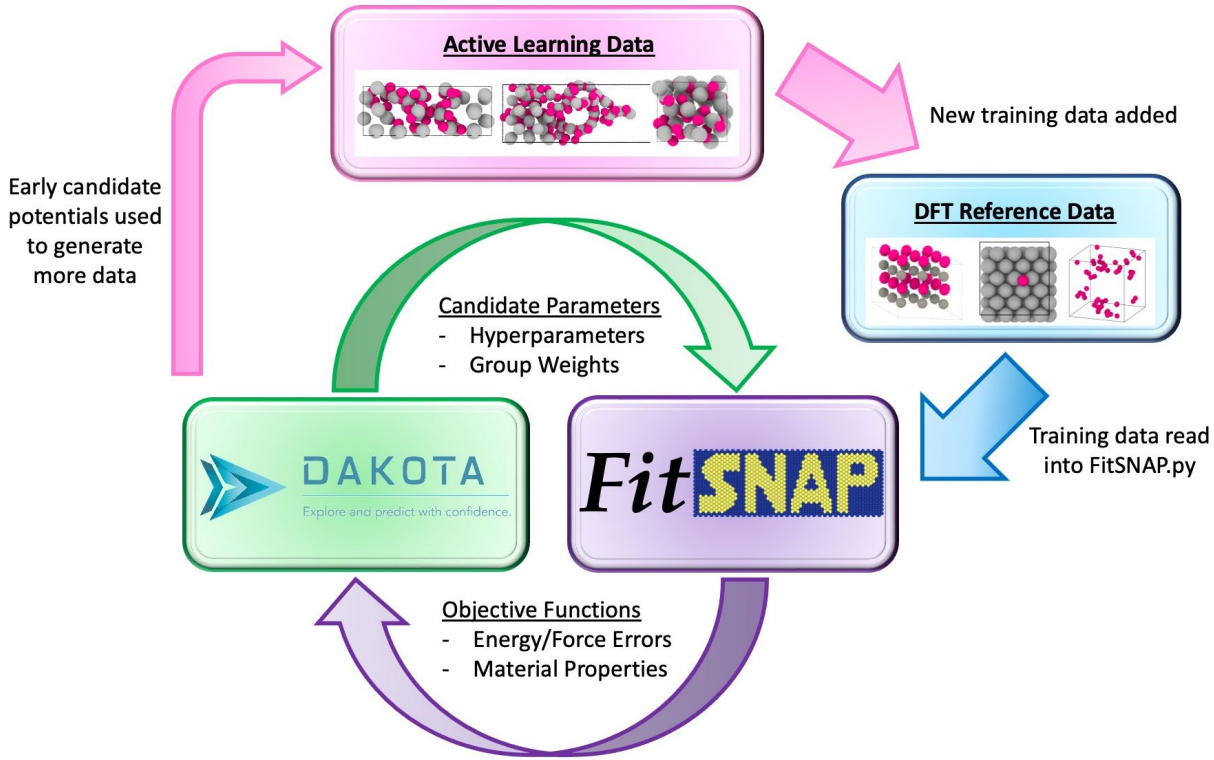
$$\min(||\mathbf{w} \cdot D\boldsymbol{\beta} - T||^2 - \gamma_n \, ||\boldsymbol{\beta}||^n)$$

Weights — Set of Descriptors — DFT Training

Focus of this project:

W-Re-Os SiC-Mg Fe-Cr-Mn-W

ACE Development Workflow



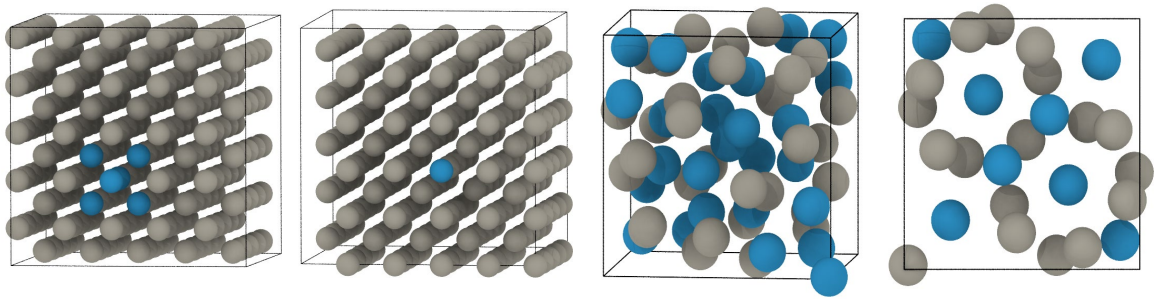
Code available: https://github.com/FitSNAP/FitSNAP

Rohskopf et al., (2023). FitSNAP: Atomistic machine learning with LAMMPS. Journal of Open Source Software, 8(84), 5118

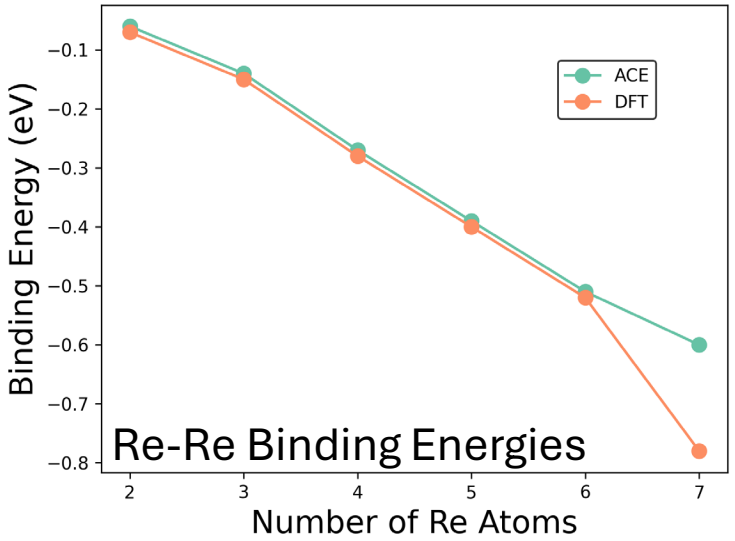
Level 1: Development of ACE W-Re ML-IAP

Cusentino, Sargsyan

Training Data Includes Defects and Intermetallic Structures

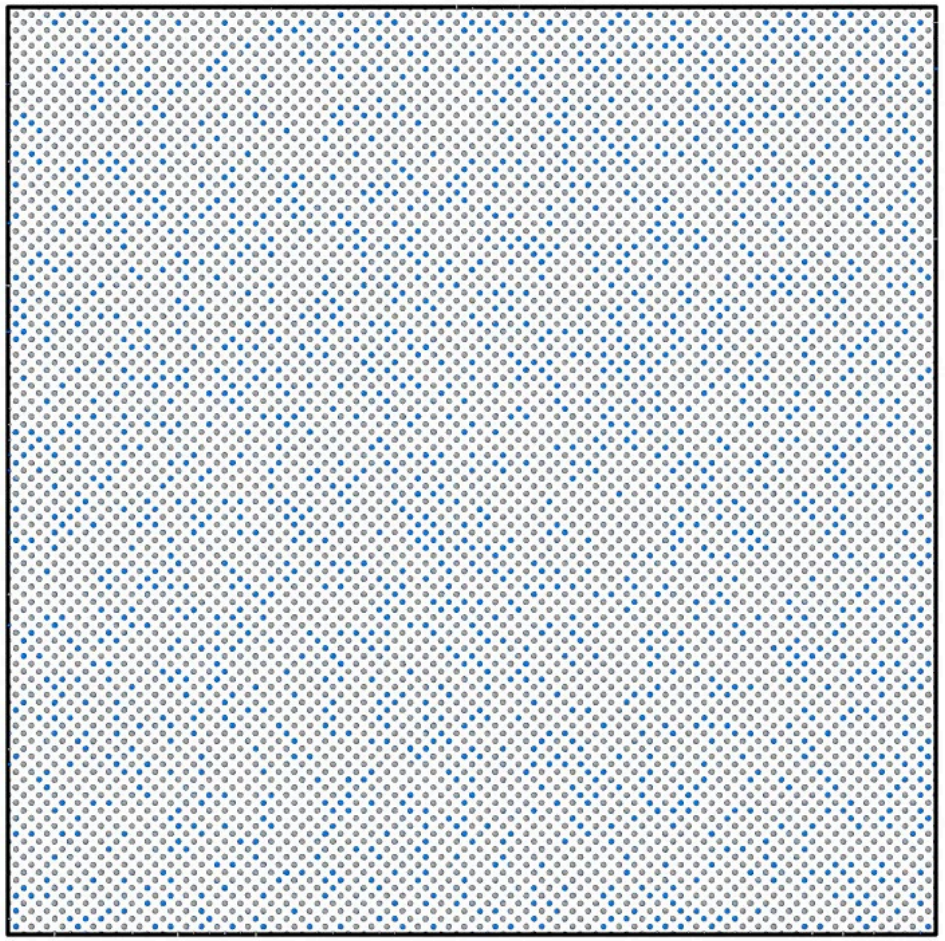


ACE W-Re Reproduces Key Properties



Migration Barriers (eV)	DFT	ACE
Vac	1.69	2.29
W SIA	0.003	0.02
Re	0.12	0.13

ACE W-Re Stable for 10 KeV PKA Simulations



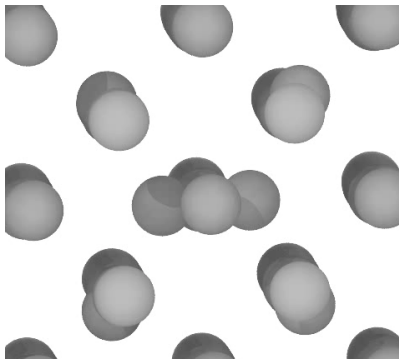
Level 1: Development of Fe and SiC-Mg ACE ML-IAPs

Cusentino, Sargsyan

Focus on Point Defect Properties

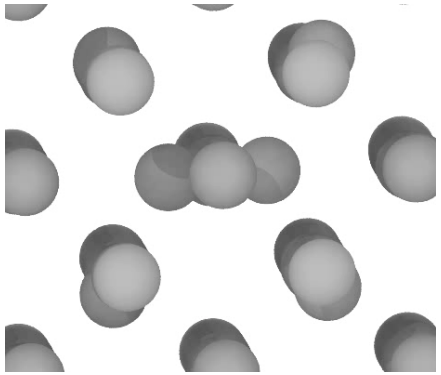
NEB Barriers

110-111 Rotation



DFT: 0.67 ACE: 0.57

110-011 Rotation



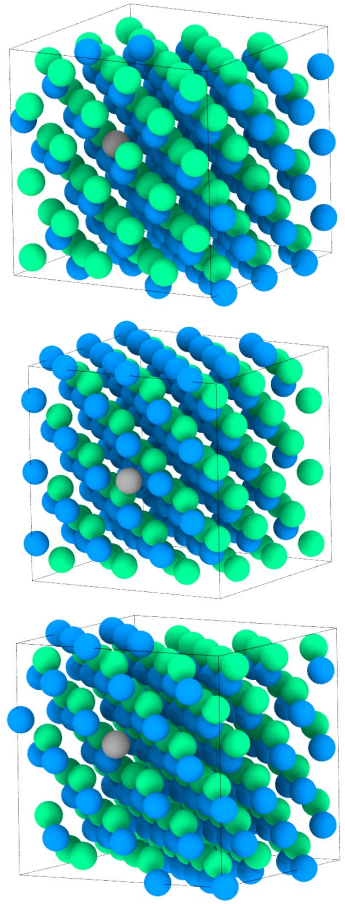
DFT: 0.58 ACE: 0.48

Vacancy Binding Energy (eV)	DFT	ACE
1 NN	0.13	0.13
2 NN	0.21	0.21
3 NN	-0.16	-0.09

More Complex Defect Landscape

Mg Defect Structures in 3C SiC

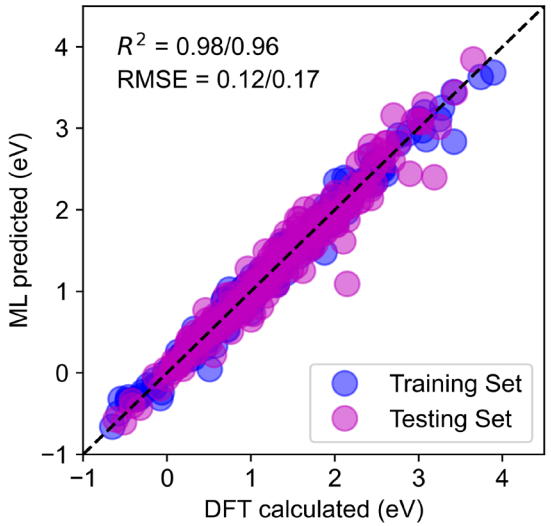
Mg Defect Formation Energies (eV)	DFT	ACE
Mg_{Si}	0.74	0.77
Mg_{Si}-V_C	1.52	1.55
Mg_{TC}	5.53	5.22
Mg_{TSi}	6.95	5.91
Mg_{Si}-V_{Si}	7.75	6.18
Mg_C	8.92	8.81
V_C	4.08	4.16
V_{Si}	5.26	4.65

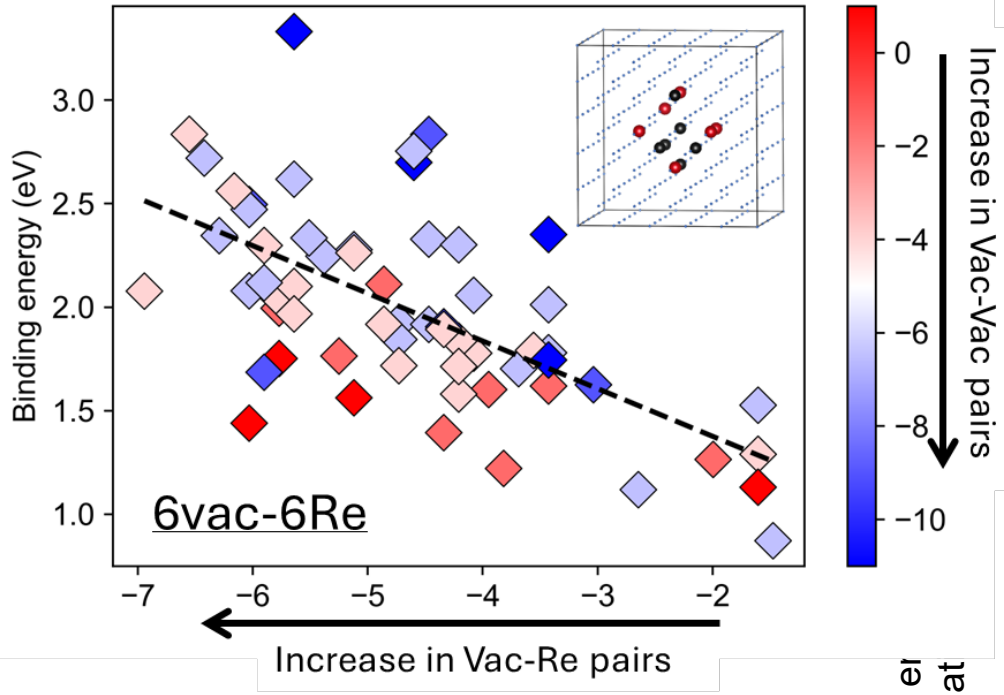


Application of the ML Model for Binding Energy

Manzoor, Jin, Thomas, Trelewicz

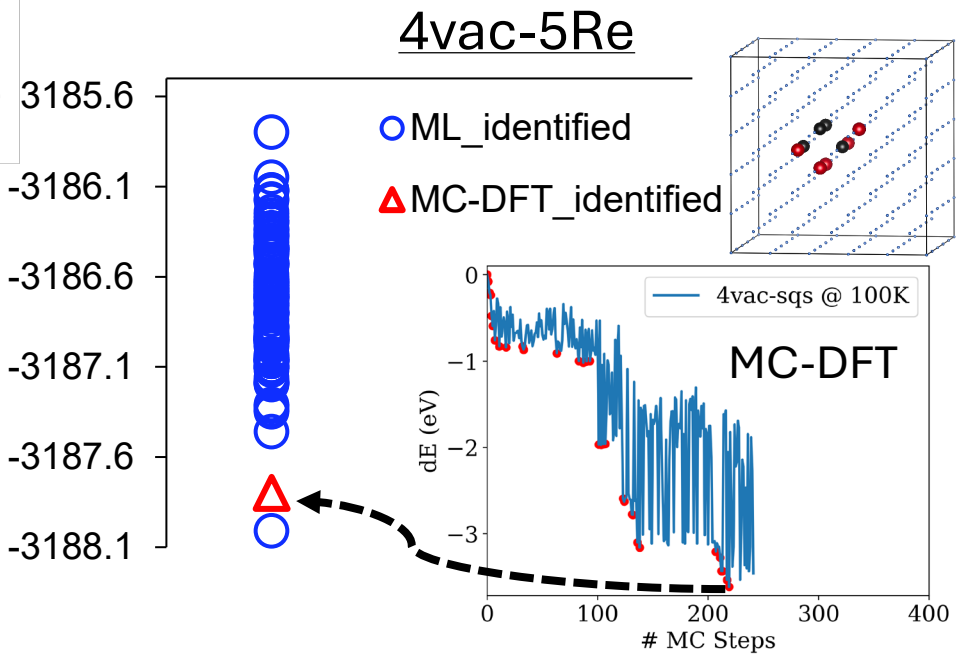
- Trained on 10 configurations for each composition
- Every random configuration is unique





Identical binding energy trend as observed in DFT

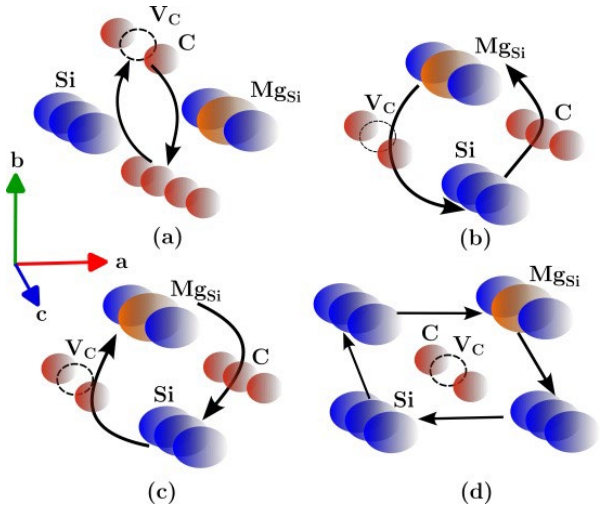
- Low energy configurations are comparable between ML and DFT
- ML significantly less computationally expensive, i.e., 10 vs. 300 DFT calculations for a given composition



Mg interactions with native defects in SiC

Ullah, Morgan, Szlufarska

- 3C-SiC – a candidate structural material for the future fusion reactors.
- Radiation exposure causes damage and burns-in transmutants.
- Transmutants interact with native defects.
- 3C-SiC is a wide bandgap semiconductor – defects can be charged, and their energies depend on Fermi level μ_F.



transmutant	burn-in rate (appm/efpy)	after 6.5 efpy (at. %)
He	6384	4.2
H	2307	1.5
Mg	1630	1.1
Be	632	0.4
Al	469	0.3
P	146	0.1

[1] R.H. Jones, […], W. J. Weber, *Journal of Nuclear Materials* **307–311**, 1057 (2002)
[2] Rafi Ullah, Dane Morgan, Izabela Szlufarska, J. Phys. D: Appl. Phys. 58 (2025) 265302

Level 2: Calculation of material properties using mesoscale simulations

Marian, Szlufarska

Ray-tracing Monte Carlo model of electronic dynamics to calculate the **thermal conductivity** of tungsten and its alloys under changing microstructure

Computational cost and error estimation

Calculated vs experimental in pure W

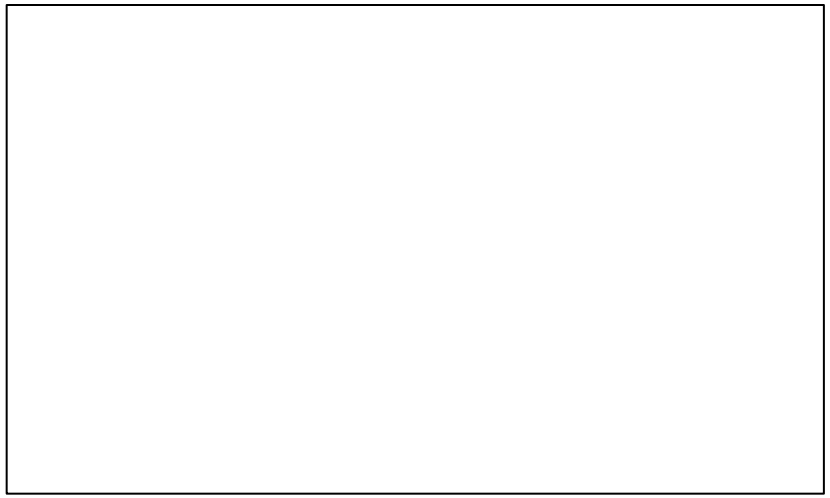
Calculated vs experimental in W-Re

Calculated thermal and concentration dependence

Level 2: Simulations of helium-defect interactions in irradiated RAFM steel

Marian, Po

Cluster dynamics simulations using grouping methods to reduce the number of ODEs from 10^8 to 10^4, and reach dpas ~50 dpa.



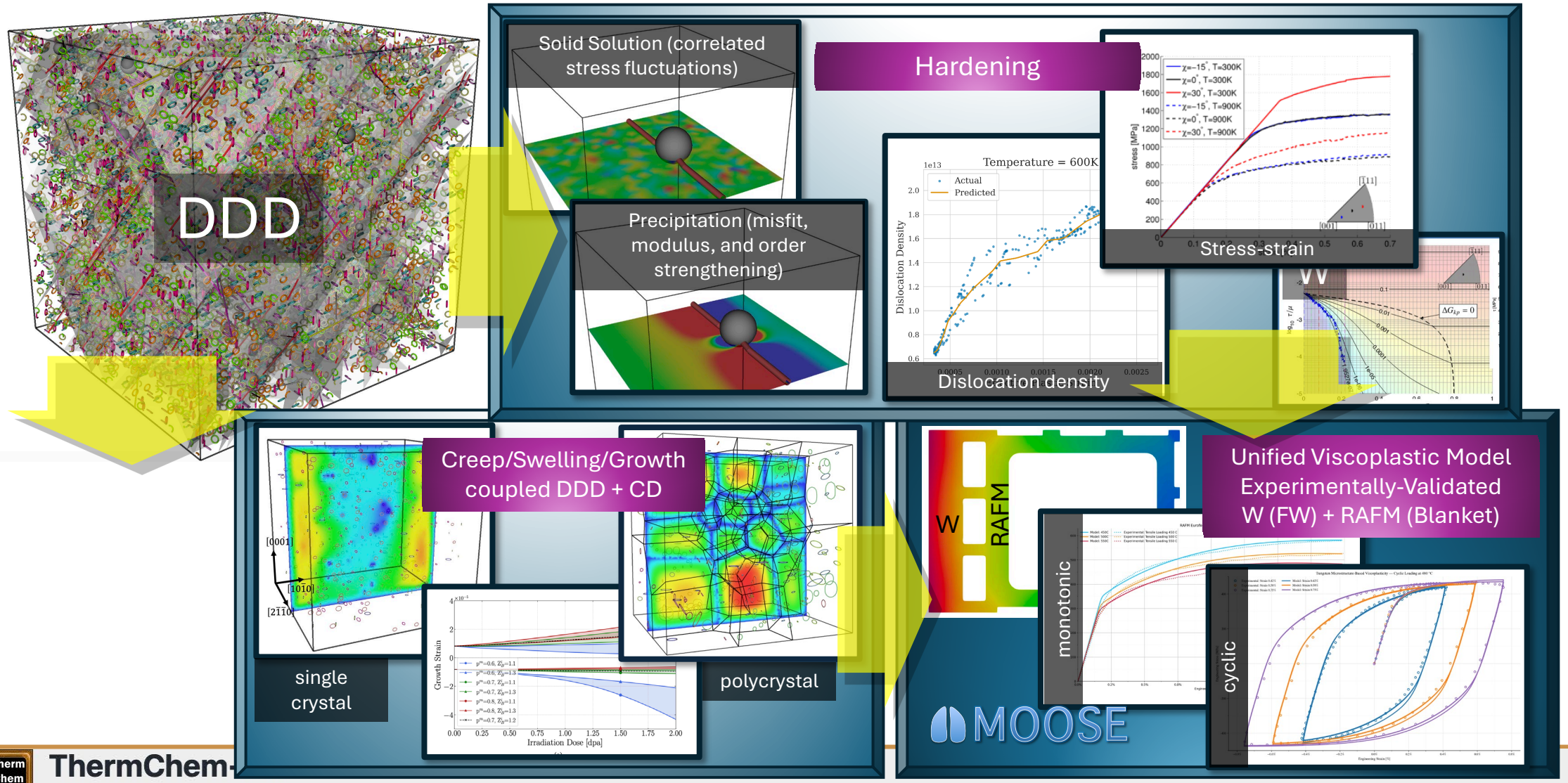
Inclusion of heterogeneous nucleation of bubbles in irradiated RAFM steels

Equation of state for V-He clusters (bubbles) used to obtain the critical He-to-vacancy ratio

Using grouping methods reduces the number of ODEs to tractable numbers, allowing reaching 50 dpa and enabling comparison with experiments

Level 3: Integration of mesoscale models with engineering design codes

Po, Spencer



Collaboration resources

- The project mailing list (thermchem-fw@email.ornl.gov)
- The Box workspace we use for internal file sharing (https://ucla.box.com/s/o2unb7df1ep12g1lefdwsm7e0fmttf49)
- The Slack workspace we use for informal communications (https://thermchem-fwscidac.slack.com/home)
- The GitHub team(s) associated with our GitHub organization (https://github.com/ThermChem-FW)

- Our website: https://thermchem-fw.github.io/
  - Which uses the Jekyll static site generation tool and is hosted in this repository: https://github.com/ThermChem-FW/thermchem-fw.github.io
- Information on accessing various computing facilities here: Computer Access.boxnote

Nuclear Hearing

- Nuclear heating was obtained over a 1x1x1-cm cartesian mesh.
- Figures below show nuclear heating [W/cc] - at vertical slice (left) and horizontal (middle) slices – and neutron flux [n/cm^2/s] (right).
- Cylindrical mesh could be considered to align better with the structural zones.