

NEAMS Structural Materials & Chemistry Overview

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MSR Program Review Meeting

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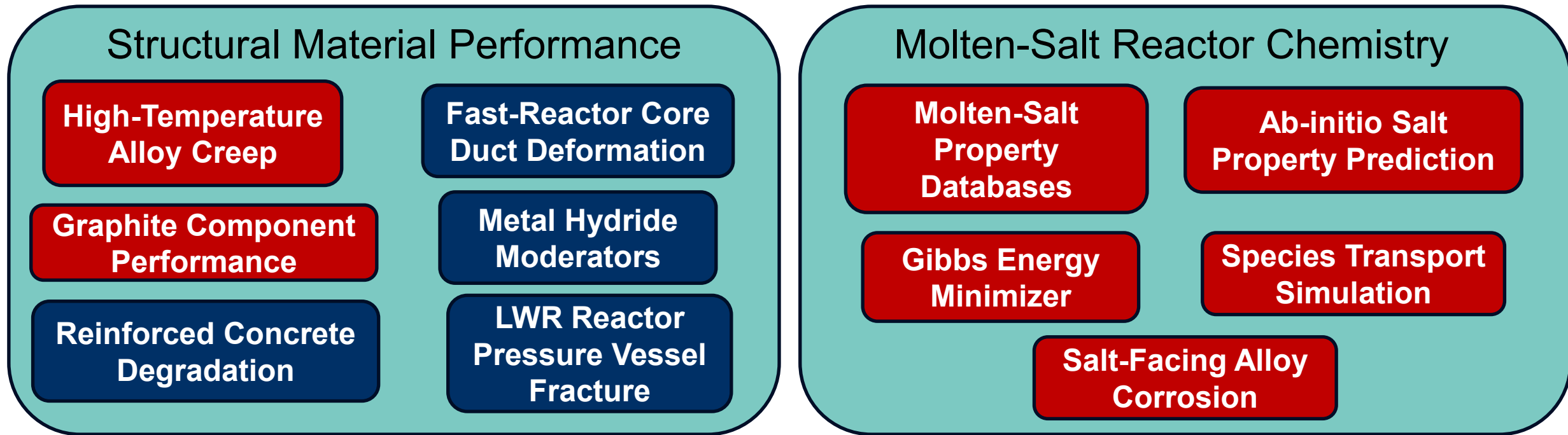


U.S. DEPARTMENT
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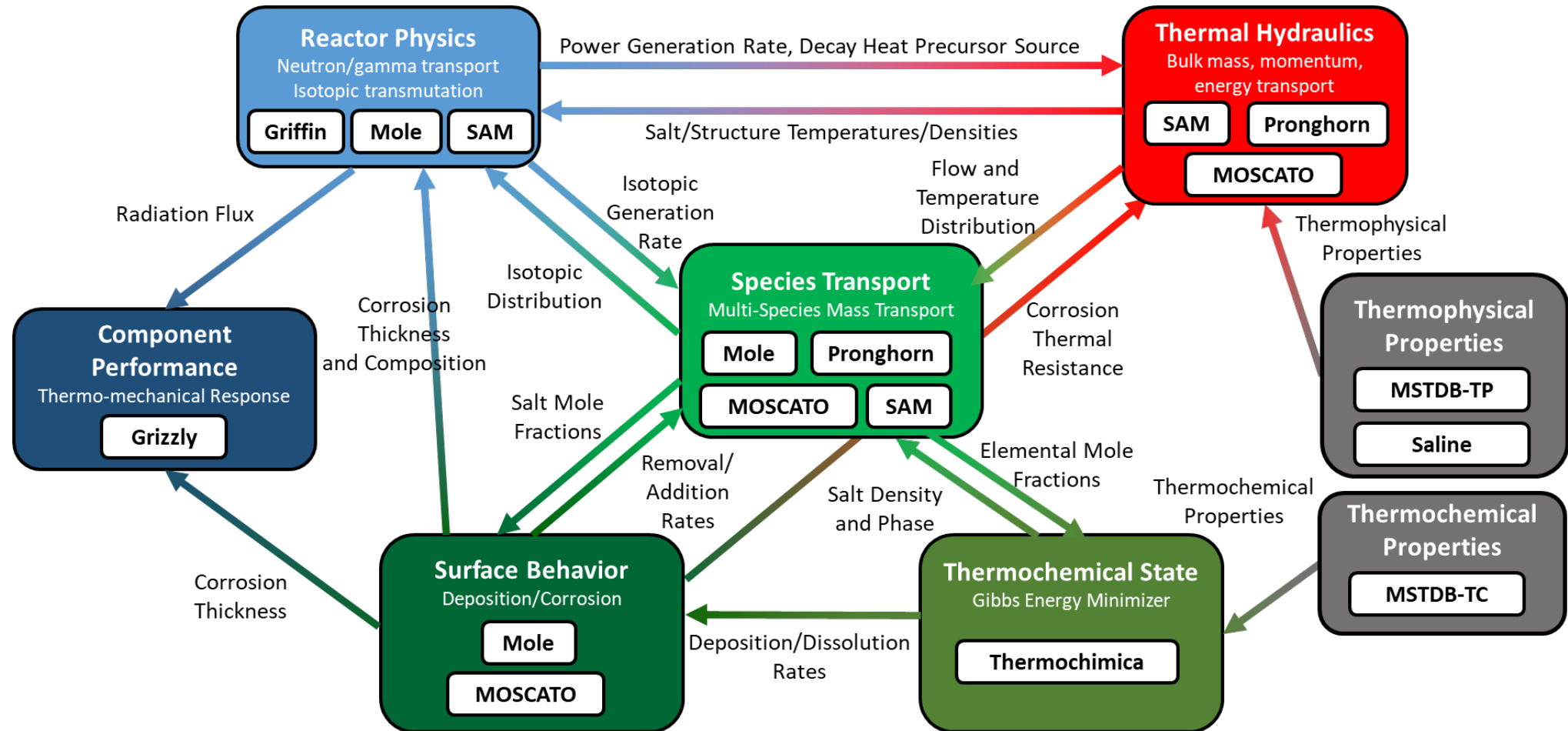
Office of
Nuclear Energy

High-Level Overview of Technical Area

Focus: Developing simulation tools for modeling structural component degradation in light-water reactors and advanced reactors, the chemistry in molten-salt reactor (MSR) coolant systems, and interactions between coolants and coolant-facing structural components



Code Coupling/Exchange for Representing MSR Behavior



Current NEAMS MSR-Related Projects/Activities

- **Databases**

- MSD-TP: Development of new property relations; SALINE code for interfacing NEAMS codes and related GUI for accessing MSD-TP thermophysical relations
- MSD-TC/Thermochemica: Development of applications utilizing MSD-TC; and uncertainty and its propagation in multi-component systems

- **Computational thermal property determination**

- Developing machine learning potentials for the LiF-BeF₂-UF₄ and LiF-BeF₂-ZrF₄ systems
- Performing ab-Initio Molecular Dynamics (AIMD) simulations of NaF-ZrF₄-UF₄ molten salts
- Creating analytical expressions to fit thermo-physical property data from molecular dynamics simulations
- Large Language Models application for literature searches for properties of halide salts

- **Codes**

- SAM: System-level species transport
- Mole: Migrating developed mass transfer coefficients to MOOSE for use across codes
- Pronghorn: Modeling electrochemical corrosion mechanisms and noble metal plating
- MOSCATO: Multiphase flow code implementation and V&V; computing mass transfer correlations for MSR geometries
- MOOSE/Phase Field: Mesoscale modeling of corrosion and dealloying in salt-facing alloys

Agenda

NEAMS Structural Materials & Chemistry Overview	Ben Spencer (INL)
Atomistic Simulations for Thermophysical Properties of Molten Salts	Gaoxue Wang (LANL)
Reactive Multiphase Flow Modeling with MOSCATO	Nathaniel Hoyt (ANL)
Phase-Field Modeling of Corrosion in Alloys	Chaitanya Bhave (INL)