eXtremeMAT | Accelerating the Development of EXTREME ENVIRONMENT MATERIALS

eXtremeMAT — Physics-based models coupled with data analytics and machine learning

eXtremeMAT is an NETL-led U.S. Department of Energy National Laboratory effort harnessing the DOE's unparalleled breadth of world-leading materials science and engineering expertise and capabilities to realize affordable and durable materials needed for extreme environment applications. eXtremeMAT is developing and demonstrating advanced computational tools to accelerate the development cycle of cost-effective alloys needed to enable the production, transportation, and utilization of hydrogen with carbon capture.

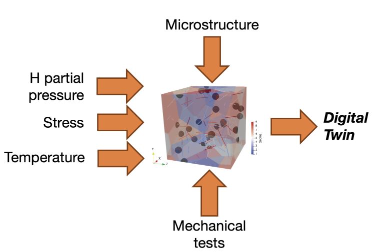
eXtremeMAT's Advances

Mechanistic model can simulate 10 years of creep behavior in 5 hours

Incorporation of complex stress states representative of real service conditions

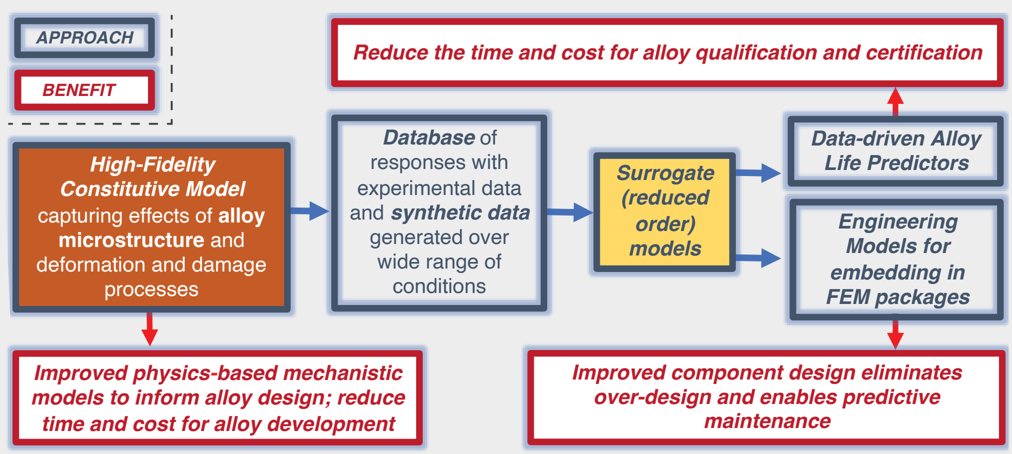
Incorporation of alloy chemistry and microstructural evolution (coarsening) during service in predictive models

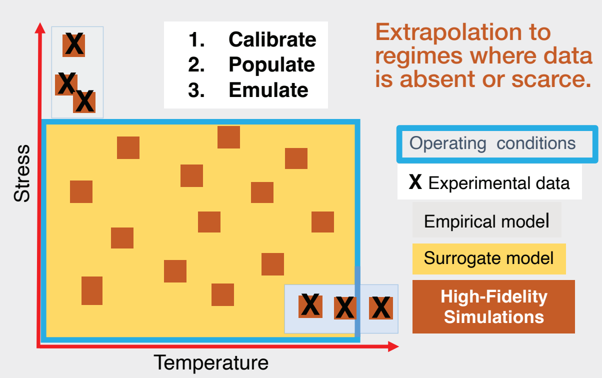
Current Focus: Extending tools to predict long-term performance in hydrogen



U.S. DEPARTMENT OF ENERGY

eXtremeMAT's MODELING FRAMEWORK & APPROACH





The eXtremeMAT models are intended to be predictive in arbitrary loading conditions, sensitive to microstructure and composition, and account for operative alloy deformation and damage processes. The model framework is applicable to multiple alloys.

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National Energy Technology Laboratory · Ames Laboratory · Idaho National Laboratory · Lawrence Livermore National Laboratory · Los Alamos National Laboratory · Oak Ridge National Laboratory · Pacific Northwest National Laboratory

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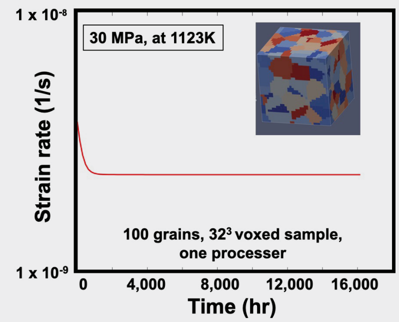
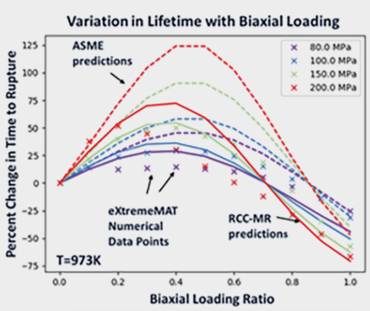
Advancing Materials Discovery and Qualification

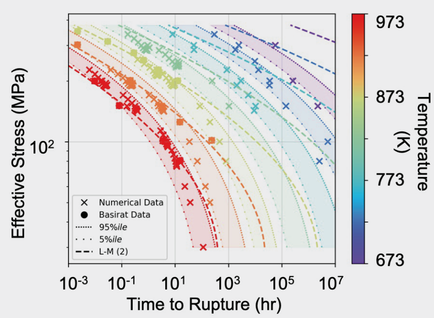
CONSTITUTIVE MODEL

The mechanistic model— initially developed for alloy P91 and implemented in a finite element solver— has been extended to account for second phase strengthening, to predict primary secondary and tertiary creep, and implemented in a numerically efficient Fast Fourier Transform (FFT)-based formulation. The code can simulate the response of an alloy subjected to creep loading conditions for a time period of 10 years in approximately 5 hours. The model has been successfully calibrated for alloy 347H and is being used to produce a database of expected rupture life as a function of stress and temperature.

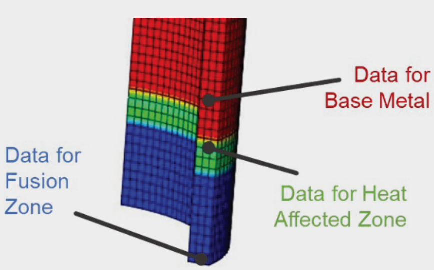


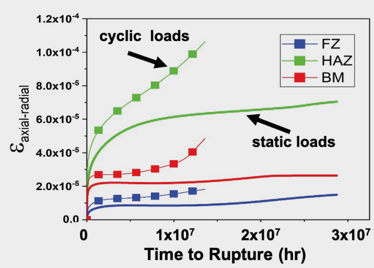
PERFORMANCE PREDICTORS





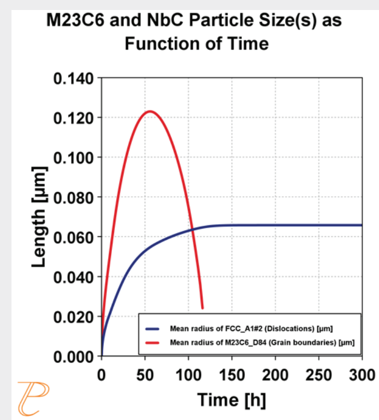
As demonstrated above for alloy P91, a rupture life criterion that considers uncertainty and is applicable to multi-axial loading was derived using limited experimental data.

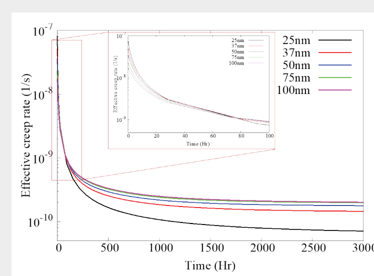




Using LaRomance (Los Alamos Reduced Order Models for Advanced Nonlinear Constitutive Equations), a surrogate model was developed for embedding into commercial finite element packages and can account for cyclical loading (demonstrated above for an idealized weld).

INCORPORATION OF MICROSTRUCTURE





Simulation of carbide phase growth and dissolution during service and impact of carbide size on creep of type 347H stainless steel.