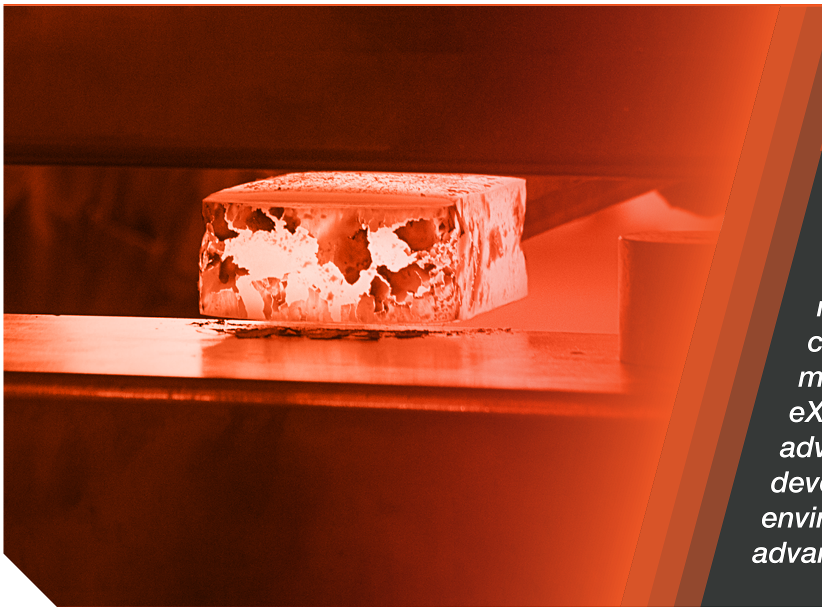
# eXtremeMAT | Accelerating the Development of EXTREME ENVIRONMENT MATERIALS



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

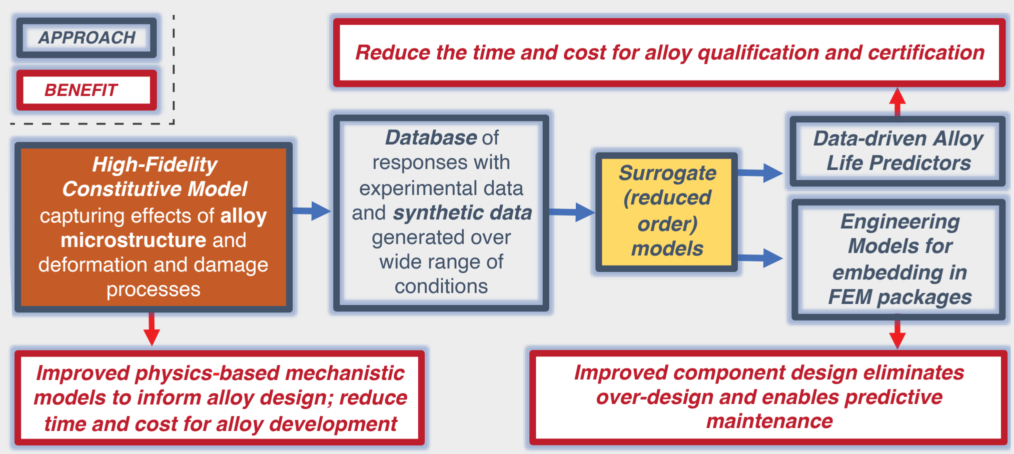
*eXtremeMAT is an NETL-led U.S. Department of Energy National Laboratory effort harnessing the DOE's unparalleled breadth of world-leading materials science and engineering expertise and capabilities to realize affordable and durable materials for fossil energy applications. eXtremeMAT is developing and demonstrating advanced computational tools to accelerate the development cycle of cost-effective alloys for harsh environments needed to enable highly efficient advanced energy systems.*

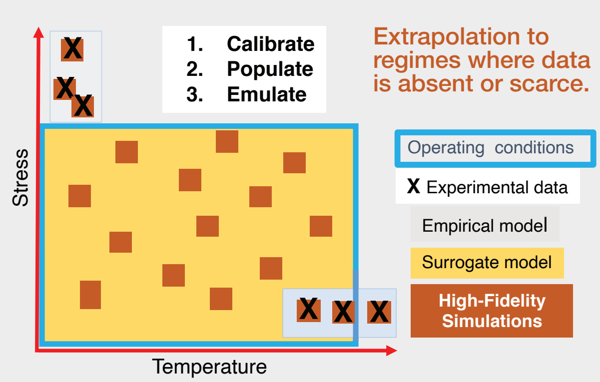
## THRUSTS

1. Materials Lifetime & Performance Predictors
2. Component Lifetime & Performance Predictors
3. Data Science & Analysis Tools
4. Guidelines for Designing New Alumina Forming Alloys

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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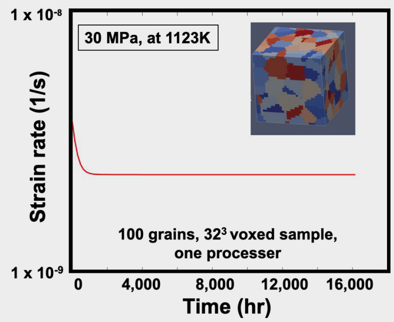
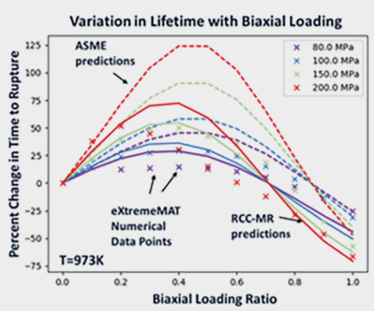
## Advancing Materials Discovery and Qualification

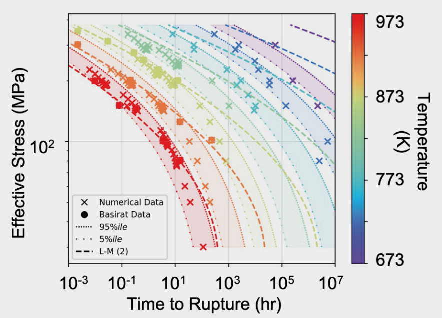
## CONSTITUTIVE MODEL

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.

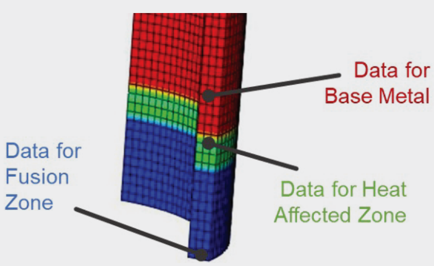


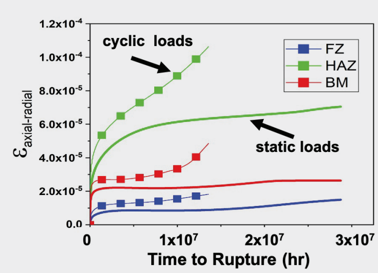

## PERFORMANCE PREDICTORS




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).

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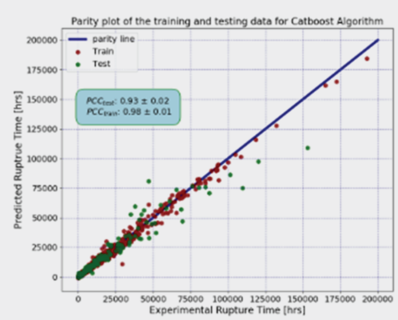
## DATA SCIENCE

Using NETL EDX's® data curation and collaboration tools, eXtremeMAT has developed a Materials Database capable of continuous data analysis and assessing data quality. The database continuously evaluates datasets as new data points are added to enhance materials-analysis conclusions and inform and verify material performance predictions. To ensure high-quality data for use, eXtremeMAT developed a methodology to assess and characterize materials data quality.

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