**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.

**eXtremeMAT’s MODELING FRAMEWORK & APPROACH**

1. **High-Fidelity Constitutive Model**
   - Capturing effects of alloy microstructure and deformation and damage processes.
   - Database of responses with experimental data and synthetic data generated over wide range of conditions.

2. **Surrogate (reduced order) models**
   - Improved component design eliminates over-design and enables predictive maintenance.
   - Data-driven Alloy Life Predictors
   - Engineering Models for embedding in FEM packages

3. **Improved physics-based mechanistic models to inform alloy design; reduce time and cost for alloy development**
   - Extrapolation to regimes where data is absent or scarce.

4. **Stress - Temperature**
   - Operating conditions
   - Experimental data
   - Empirical model
   - Surrogate model
   - High-Fidelity Simulations

- **BENEFITS**
  - Reduce the time and cost for alloy qualification and certification

**APPROACH**

1. Calibrate
2. Populate
3. Emulate

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.
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.

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).