Initiated in October 2018, the US DOE-FE/NETL eXtremeMAT collaboration leverages the unparalleled materials science & engineering expertise and capabilities available within the US-DOE National Laboratory complex to accelerate the development of affordable and durable materials for extreme environment service.

Lower cost, higher temperature alloys reduce the cost of advanced power cycles. Improved life prediction for critical components under complex service conditions (e.g. plants undergoing cycling conditions, thin sheet for heat-exchangers).

**YEAR ONE OUTCOMES**

**Improved predictive capability of a polycrystal model describing the mechanical response of steels to complex states of stress.**

A data schema and data quality tool have been developed and deployed to assess the quality of the data and other associated information based on selection criteria.

Reliable prediction of the yield stress of Fe-9Cr steels from eXtremeMAT’s alloy database. (Random forest (RF) with top 20 features and normalized scaler. PCC = Pearson correction coefficient, MIC = Maximal information coefficient.)

Constitutive model developed, applicable to both ferritic and austenitic steels, to predict mechanical failure due to void nucleation growth and coalescence. Demonstration of applicability - new rupture life criterion for Grade 91 steel.
Harnessing the unique, world-leading National Laboratory resources in a focused and coordinated effort:

- Materials design
- High Performance Computing (HPC) power
- Advanced processing and manufacturing
- In-situ characterization
- Performance assessment at condition

MULTISCALE MODELING FROM DFT TO FINITE ELEMENTS

INPUT DATA & KNOWLEDGE

EXPERIMENTAL VALIDATION

DATA MINING, OPEN FRAMEWORK, & MACHINE LEARNING

VISUALIZATION & ANALYSIS

HPC RESOURCES