Overview of the Fossil Energy (FE), NETL, & NL Extreme Environment Materials (EEM), *extremEmat*, Program

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**DOE-FE Champion:**
Regis Conrad
Extreme Environment Materials Program

Goal:
Develop modeling methodology tools and manufacturing processes that can provide a scientific understanding of high-performance materials compatible with the hostile environments associated with advanced Fossil Energy (FE) power generation technologies.

Objective:
Materials R&D focused on structural and functional materials that will lower the cost and improve the performance of fossil-based power-generation systems.

Regis Conrad: Advanced Energy Systems Overview (April 28, 2016)
“Born Qualified” EEMs

Atoms to Metals
ICME multi-scale computational approaches incorporating best practice manufacturing and focused performance evaluation and characterization

Targeted Validation Experiments
Conducted in industrial relevant environments and scales

Data Informatics and Analytics
Analyze the large volume of data generated from materials testing incorporate leaning to improve predictive capability of simulations and reduce uncertainty.

Validated simulations linking structure, processing and performance.

Accelerate the identification and deployment of cost effective materials by 2X for extreme environment applications.
Long-term extremEmat Capability Theme Areas

**Manufacturing Science**
- Pilot Scale Manufacturing Facility
- Process Modeling and Control
- Process Science

**Modelling and Simulation**
- Integrated Computational Materials Engineering (ICME)
- Scale Bridging Theories and Codes
- Code Validation Methods

**In situ characterization and test beds**
- Capture Kinetic Response
- Incipient Failure (multi-axial, cyclic/dwell)
- Showcase multiple condition environments

**Data Analytics**
- Flexible Open-Access Databases
- Materials Properties Data for Extreme Environments
- Analytical Tools
Developing cross-cutting “tool sets” focused on accelerating discovery & scale-up for reliably manufacturing materials at scale.

<table>
<thead>
<tr>
<th>Applications</th>
<th>Cost Analysis Engine</th>
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<tbody>
<tr>
<td>Advanced Steam/CO₂ Turbines/Thick Wall Components</td>
<td>Increase operating temperature range of current candidate austenitic and martensitic-ferritic steels, e.g., alloy 347, by 50°C.</td>
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<tr>
<td>Waste Heat Recuperators / Heat Exchangers</td>
<td>Reduce the costs (at least 30% over the life cycle) of a nickel-based alloy, e.g., H282 or IN-740 capable of 760°C, 25 year service in corrosive environment.</td>
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High Strength, High Temperature Austenitic SS Alloys

• FY17-FY18 Challenge & Technical Effort
Supports EEM Technology Roadmap goal of enabling supercritical CO$_2$ (sCO$_2$) technologies through development of High Yield Strength, High-Temperature Austenitic Stainless Steels for extended high temperature service in demanding environments.

**Challenge:** Increase the yield strength of austenitic SS above current state-of-the-art commercial SS alloys to enable long-term operation at temperatures, at least 50ºC above 650ºC, while maintaining low cost and fabricability, making use of NL complex computational tools integrated with experimental validation.

**Benefit:** While targeting austenitic SS, the computational methodologies & validation procedure developed in this project will benefit other lower cost alloys such as 9-12% Cr steels. Modeling framework & informatics/analytics development tools should benefit more difficult/complex materials issues in gas turbines, direct energy extraction, etc.

**Leverage Opportunity:** In addition, there is interest in improving the creep strength of ferritic alloys at 700ºC by designing the size, morphology, distribution, and composition of precipitates (i.e., mesoscale microstructure development).
Low Cost, High Performance Ni-based Alloys

• FY17-FY18 Challenge & Technical Effort
Supports EEM Technology Roadmap goal of enabling supercritical CO₂ (sCO₂) and gas turbine (limited) technologies through development of high performance, low(er) cost nickel superalloys for extended high temperature service in demanding environments.

Challenge: Develop nickel superalloys with higher creep strength than H282 and IN740H at no, or minimal additional alloy, cost while maintaining the favorable fabrication and welding properties of both alloys. (1) Lower cost by element substitution approach; (2) Improve high temperature mechanical strength overall, and creep life in particular, by optimally stabilizing microstructure relative to H282/IN740H.

Benefit: Nickel alloys are expensive and to facilitate use they must be affordable on a cost to performance basis. Their use can guarantee optimum efficiency design goals for A-USC, sCO₂ and other FE systems needing performance at this level. (Ditto: Modeling framework ...)

Leverage Opportunity: Achieving similar performance through element manipulation, and/or improving microstructure stability leading to improved creep life, can in principle be used on other alloy system classes (e.g., high γ′ fraction nickel superalloys).
FY17: Gap Analysis of Computational Techniques

**DOE-FE Program Leadership**

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  Brandon Wood, LLNL
  Ram Devanathan
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- **2.5 Continuum Models**
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- **3.2 Data Analytics Machine**
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