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accelerating the development of extreme environment materials

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eXtremeMAT
Development, History & FY2018 Status

Jeffrey Hawk & David Alman

for *eXtremeMAT* Executive Steering Committee & Task Leads

David Teter, Edgar Lara-Curzio, Thomas Lograsso, Ram Devanathan, Sergei Kucheyev, Gabriel Ilevbare, & Laurent Capolungo

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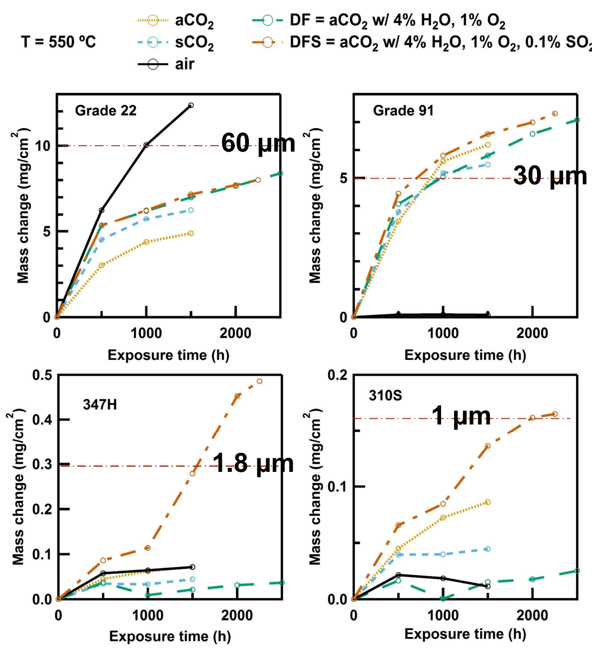
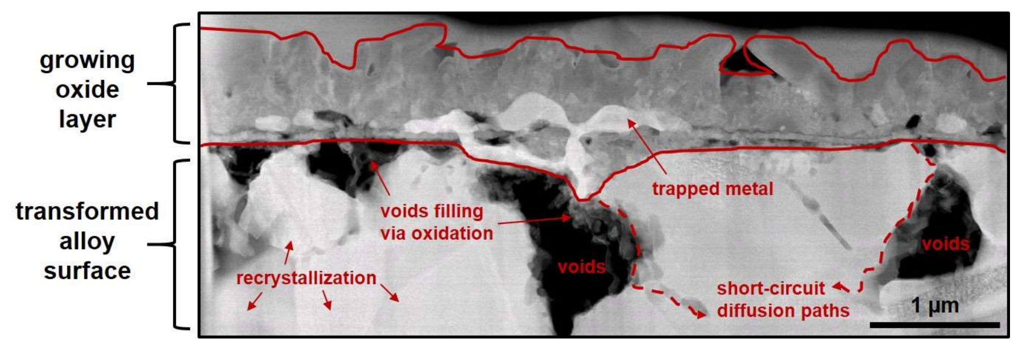
History & Development





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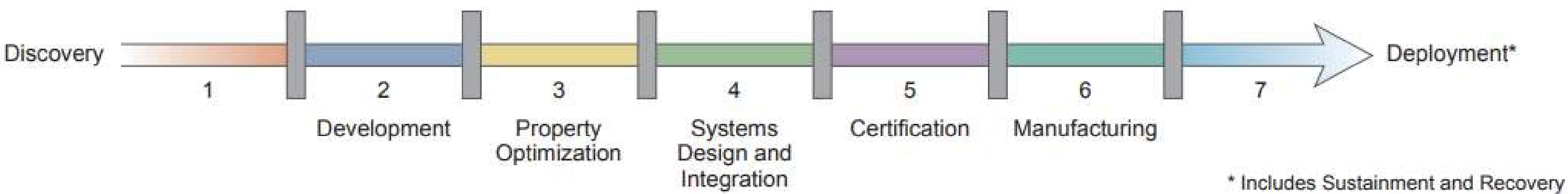
Traditional Empirical Materials Development



Traditional materials development takes 10-20 years (source: OSTP MGI White Paper, 2011)

Empirical **lifetime prediction is unreliable, and it is not transferable to new alloys.**

Solution: Integrate data management and analytics into materials development process.

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- FY 15: FE-HQ commissions Professor Greg Olson of NWU to writer a white paper "Atoms to Metals"
- Nov 30/Dec 01 2015: Special Meeting, "Accelerating Extreme Environment Materials", sponsored by Regis Conrad & Cynthia Powell
- March 22, 2016: R. Conrad requests that V. Cedro III and J. Hawk develop a Roadmap for FE Extreme Environment Materials
- April 22, 2016: Framework, plan and schedule agreed with R. Conrad
  - Input obtained from industry, national labs, universities via meetings and one-to-one phone calls
  - DOE –HQ and NETL strategic documents also reviewed
- First draft of the Roadmap to R. Conrad on 09/30/2016; rev 01 on 12/05/2016. Draft "short version" of Roadmap on 03/30/2017.
- Organizational meeting at DOE Headquarters on 4/5/2017 to lay groundwork for coordinated National Laboratory effort to develop next generation of Extreme Environment Materials for FE Power Systems.
- FWP (FE-785-16-FY17) initiated 4/13/2017 with LANL to develop a program plan for an Extreme Environment Materials (EEM) National Laboratory Consortium. FY2018 start with FY2017 funding.

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Extreme Environment Materials Program

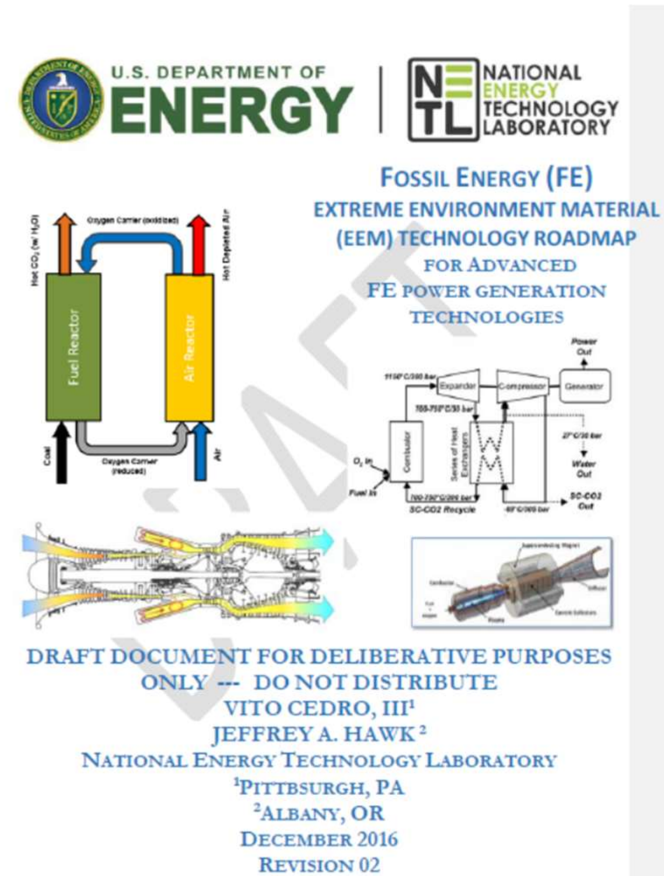
Fossil Energy | National Energy Technology Laboratory

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.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FOSSIL ENERGY (FE)
EXTREME ENVIRONMENT MATERIAL (EEM) TECHNOLOGY ROADMAP
FOR ADVANCED FE POWER GENERATION TECHNOLOGIES

DRAFT DOCUMENT FOR DELIBERATIVE PURPOSES ONLY --- DO NOT DISTRIBUTE

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DECEMBER 2016
REVISION 02

Regis Conrad: Advanced Energy Systems Overview (April 28, 2016)

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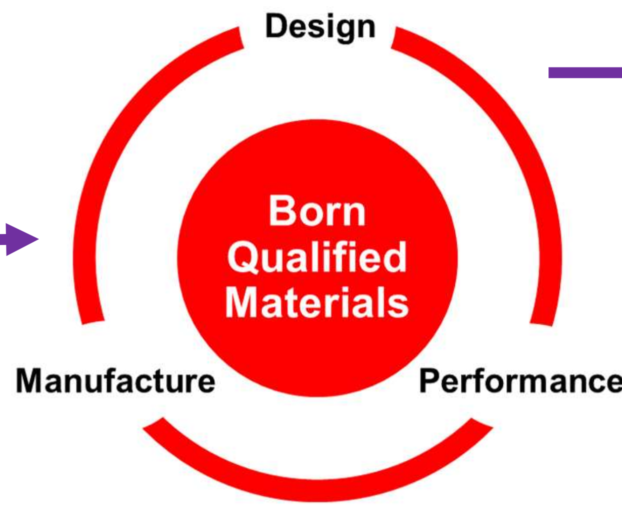
Atoms to Metals
ICME multi-scale computational approaches incorporating best practice manufacturing and focused on performance evaluation and characterization.

Targeted Valdiation 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.

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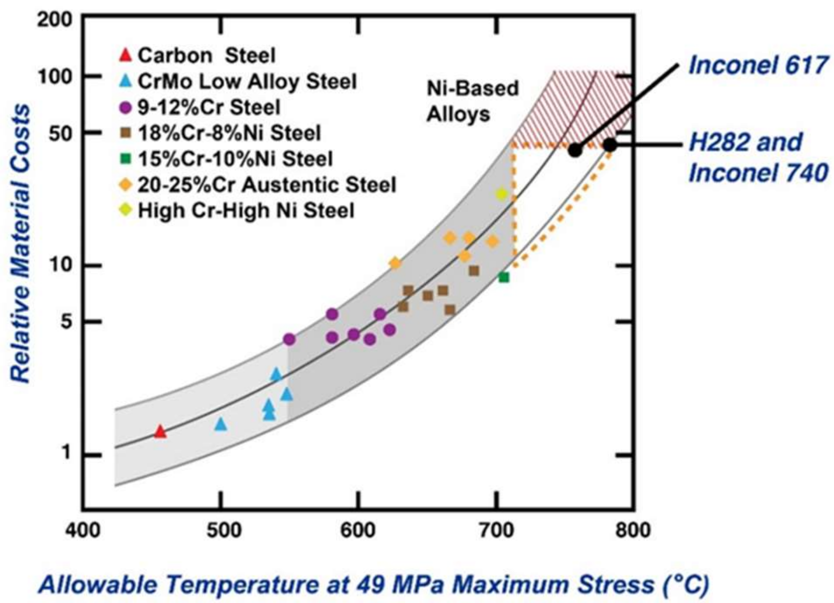
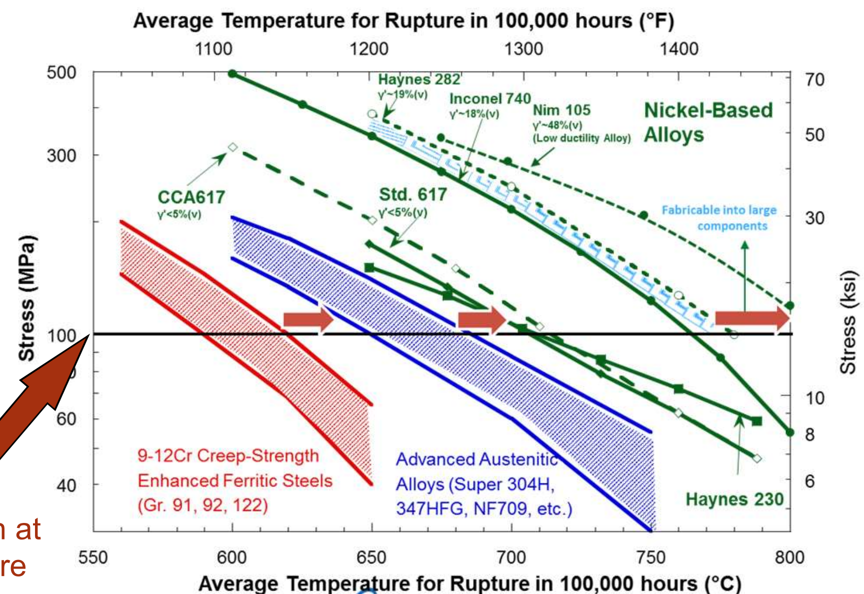


Materials Challenges

Extreme Service Conditions (temperatures, pressures, cycling, corrosion, oxidation, erosion, etc.)

Long Services Life Spans (>100,000 hours)

Large components (materials & manufacturing costs)



Minimum Desired Strength at Application Temperature

Affordable, Durable Alloys are Needed

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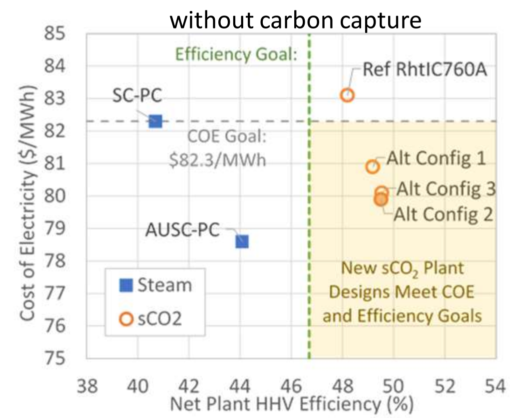
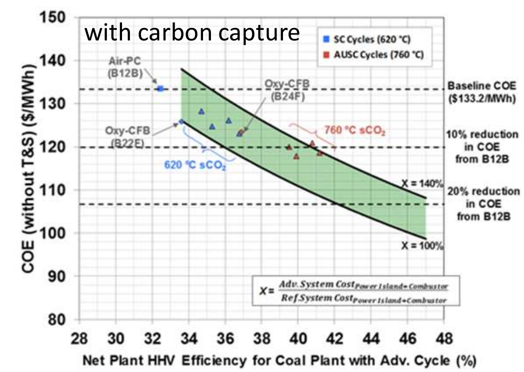
- The EEM Roadmap is consistent with:
  - The DOE Quadrennial Technical and Environmental Reviews, the technical elements of the NETL Lab Plan - FY16, and the NETL Strategic Plan
  - The current sCO_2 and Advanced Turbines Programs development schedules (to 2025)
- The Roadmap starts from the high level DOE-FE goal of more efficient, lower cost FE power generation, and works backward with respect to EEMs as a key enabler for that DOE-FE goal.
- The Roadmap provides a cascading set of supporting enabling technologies to achieve the goal of cost effective EEMs for FE power generation cycles.





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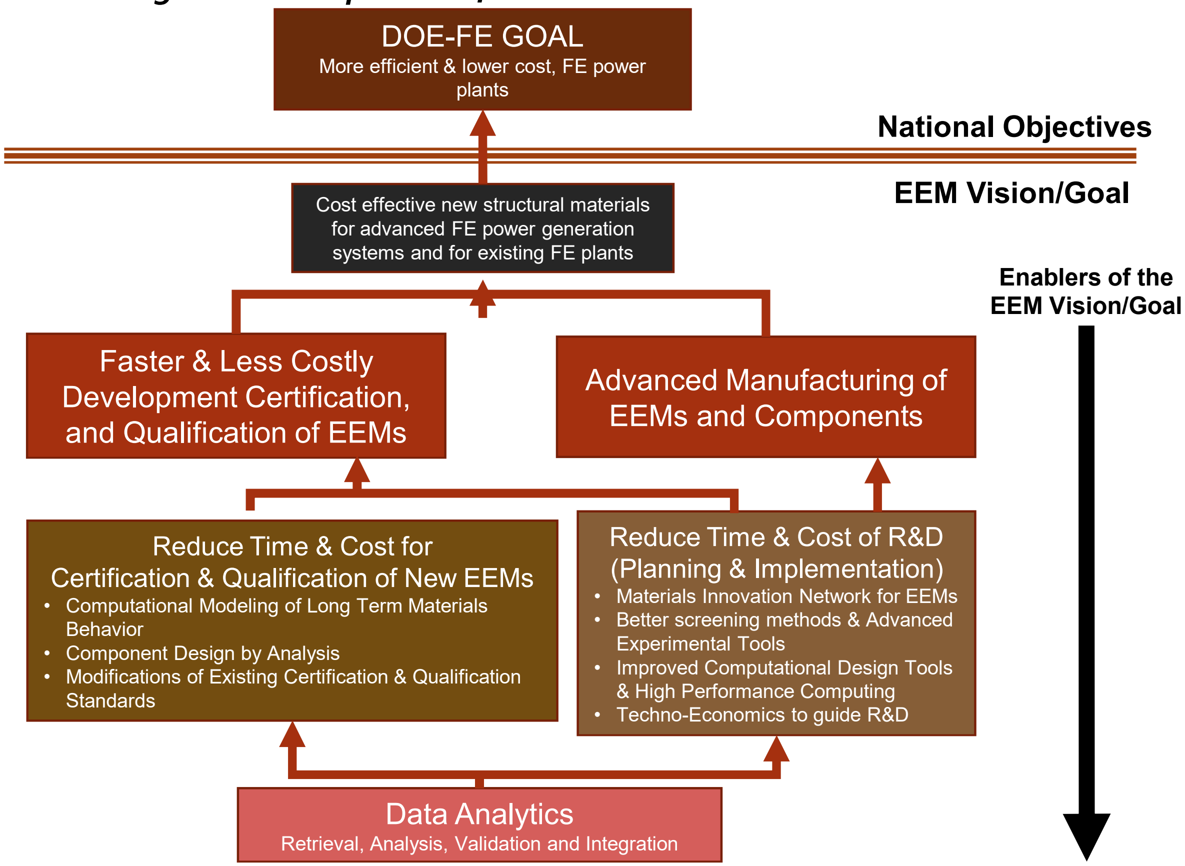

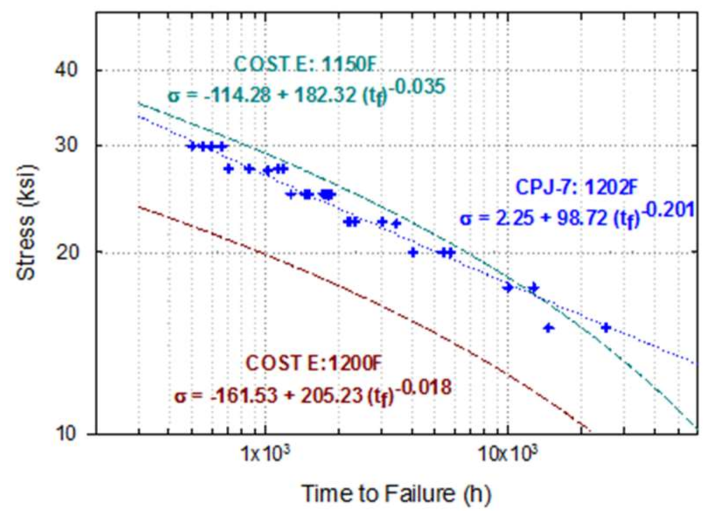

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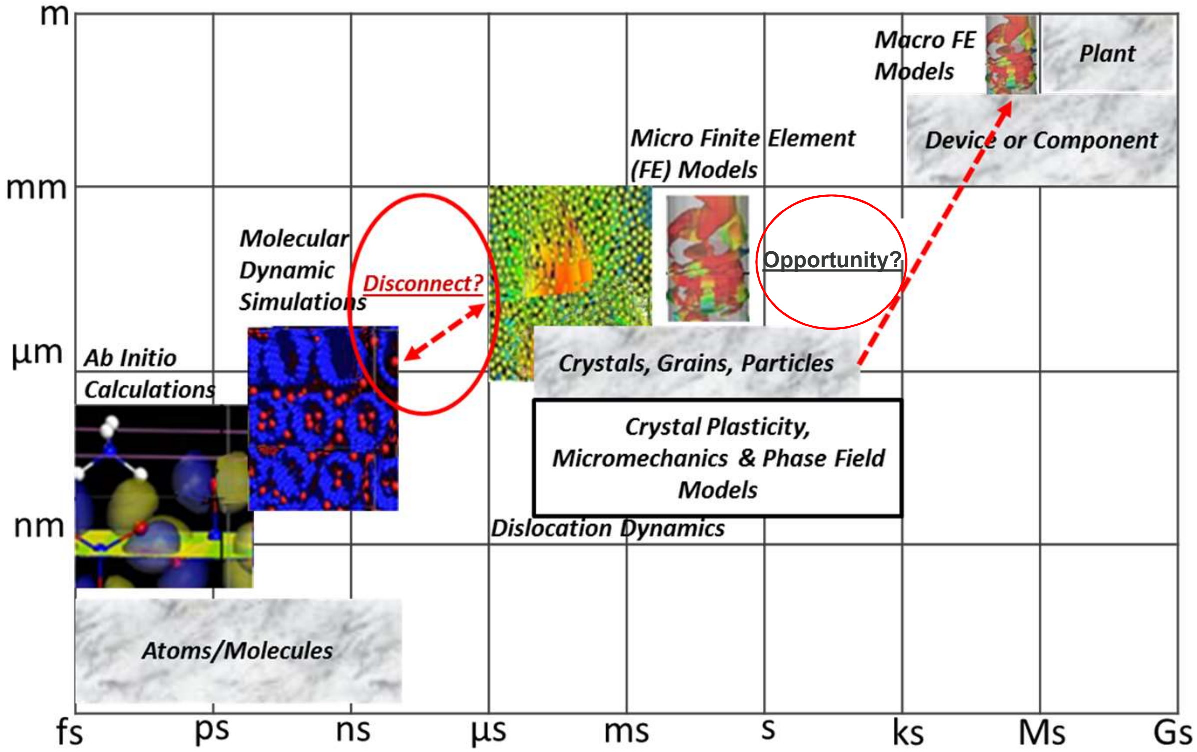
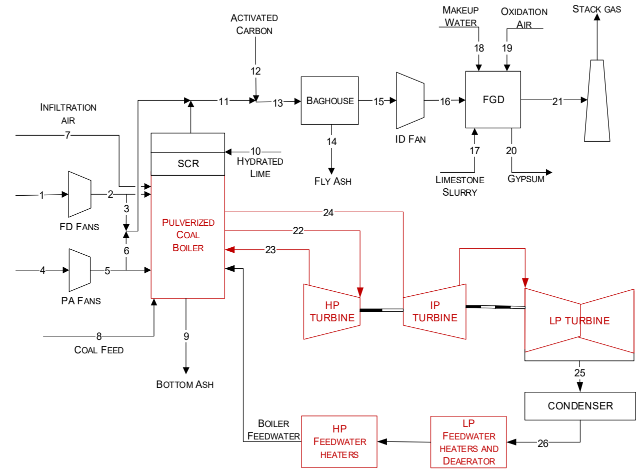


General Requirements for Computational Tools and Analysis in Multi-time & Multi-dimensional Scales.



Note: Block Flow Diagram is not intended to represent a complete material balance. Only major process streams and equipment are shown.

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Manufacturing Science	Modeling and Simulation	*In situ* Characterization	Data Analytics
Pilot Scale Manufacturing Facility Process Modeling and Control Process Science	Integrated Computational Materials Engineering (ICME) Scale Bridging Theories and Codes Code Validation Methods	Capture Kinetic Response Incipient Failure (multi-axial, cyclic/dwell) Showcase Multiple Condition Environments	Flexible Open-Access Databases Materials Properties Data for Extreme Environments Analytical Tools

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Applications	Cost Analysis Engine				
	Design for Resilience	Modeling & Reliability Validation	Manufacturing & Scalability	In Situ & Operando Characterization	Failure Analysis & Data Analytics
Advanced Steam/CO_2 Turbines/Thick Wall Components	Increase operating temperature range of current candidate austenitic and martensitic-ferritic steels, e.g., alloy 347, by 50°C.				
Waste Heat Recuperators/ Heat Exchangers	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.				

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❑High Strength, High Temperature Austenitic Steels

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 50°C above 650°C, 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 700°C by designing the size, morphology, distribution, and composition of precipitates (i.e., mesoscale microstructure development).

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❑Low Cost, High Performance Nickel Alloys

Supports EEM Technology Roadmap goal of enabling supercritical CO_2 (sCO_2) 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, sCO_2 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).

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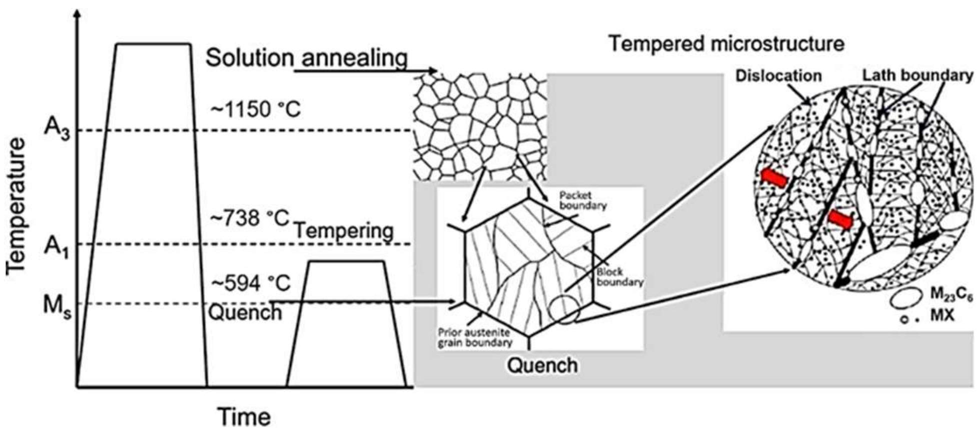
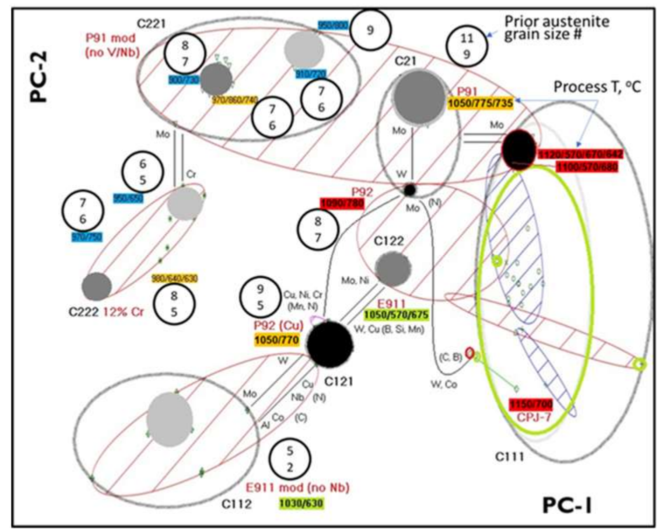
Current Status





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- **Dec. 12-13, 2017 *eXtremeMAT* Workshop**
  - Industrial Advisory Board Development: Contact list prepared for potential invitees as members, including materials suppliers, OEMs, end users, etc. Future webinars planned as an introduction to project.
- ***eXtremeMAT* Roadmap, Version 0 prepared**
  - Complied by Laurent Capolungo, LANL. Input from all NLs.
  - Gap analysis of computational methods.
  - Identified FY2019 research plan moving forward.
  - Provided to Regis Conrad & Briggs White in March 2018 for consideration and comment. Review comments from Vito Cedro. Once comment/review process complete, Version 1 will be sent out for peer review.
  - Potential basis for peer-reviewed archival research articles on approach.

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- **March 16, Meeting in Phoenix (after TMS)**
  - Technical team meeting for Task 2, Computational Materials Development. Fifteen (15) key researcher from NLs identified. Refined FWP17 research plan based on *eXtremeMAT*, V.0 Roadmap.
  - Executive Steering Committee meeting.
- **IP Agreement between NLs discussed. Circulated CCSI, IDEAS and Critical Materials Institute IP Plans for analysis for use in *eXtremeMAT*.**

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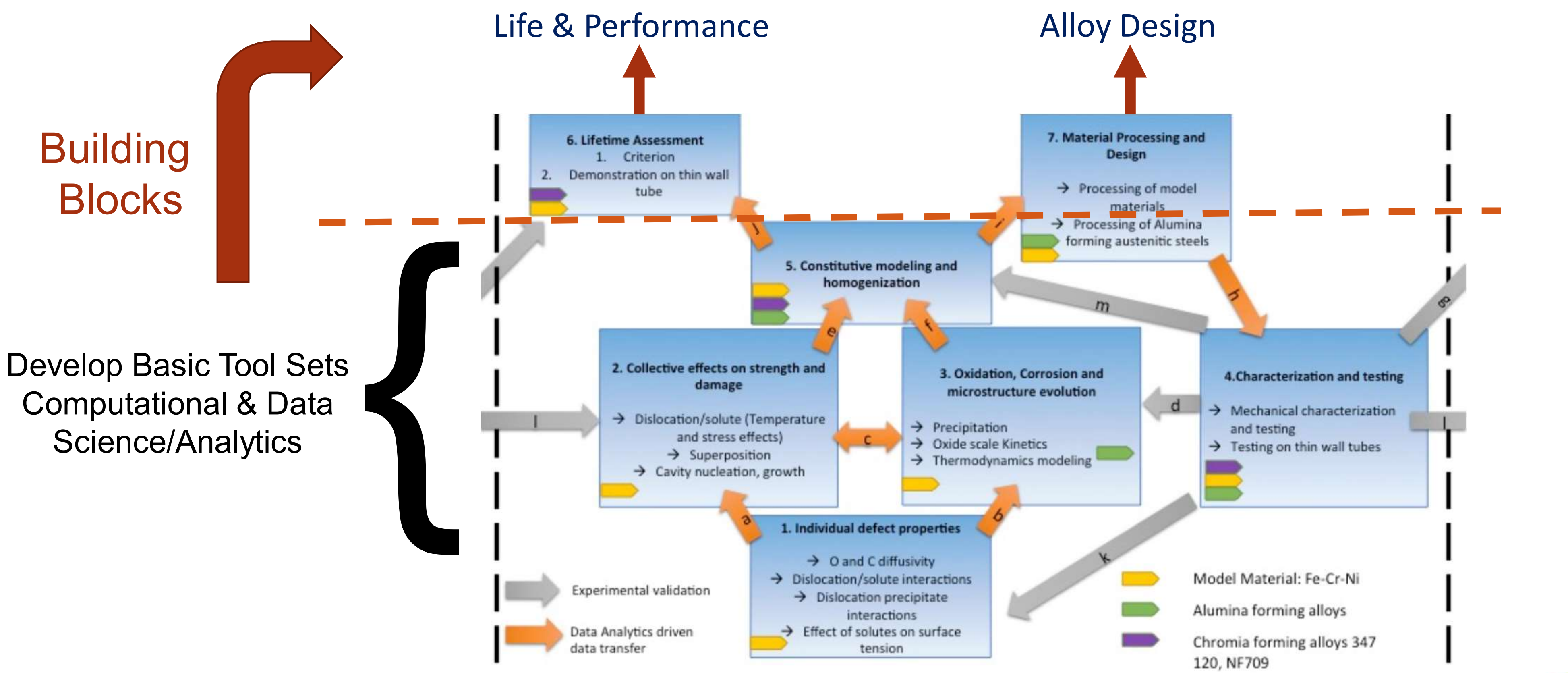

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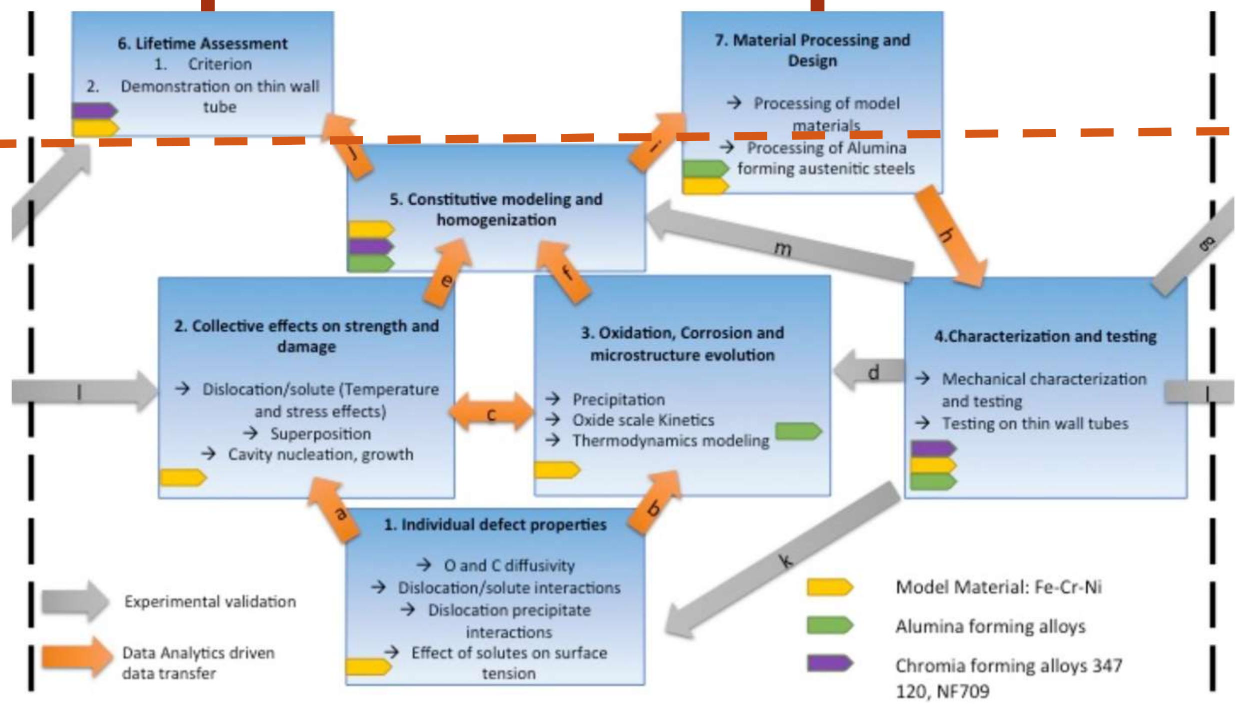
Life predictions, including thin sections

Apply to optimize or improve 347/316 type alloys

Building Blocks

Develop Basic Tool Sets Computational & Data Science/Analytics



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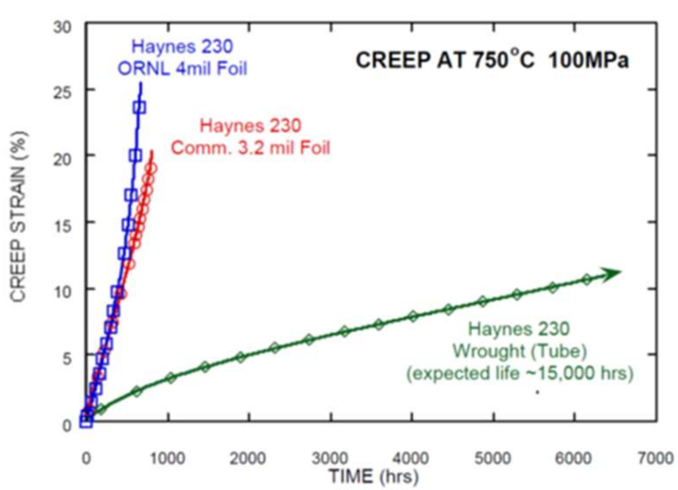
Importance

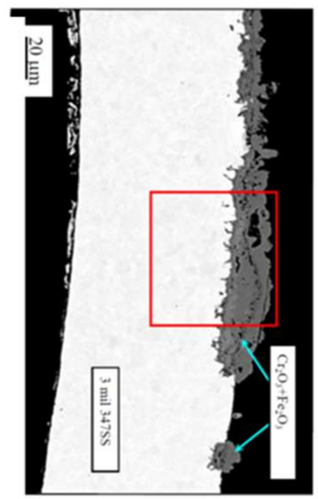
- Low cost alloys for >650°C
- Thin sections

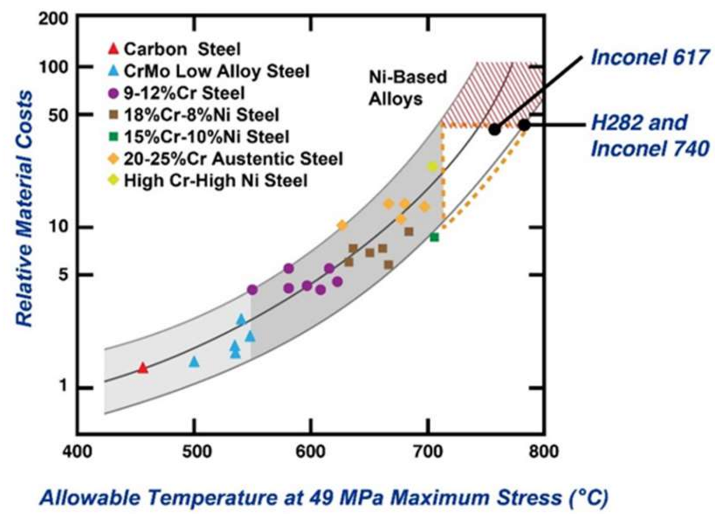
eXtremeMAT Targets

- Cost effective, heat-resistant materials
- Reliable life prediction models based on actual PP operation parameters

✓critical for sCO_2 power cycles, but valuable for <u>existing</u> FE power plants







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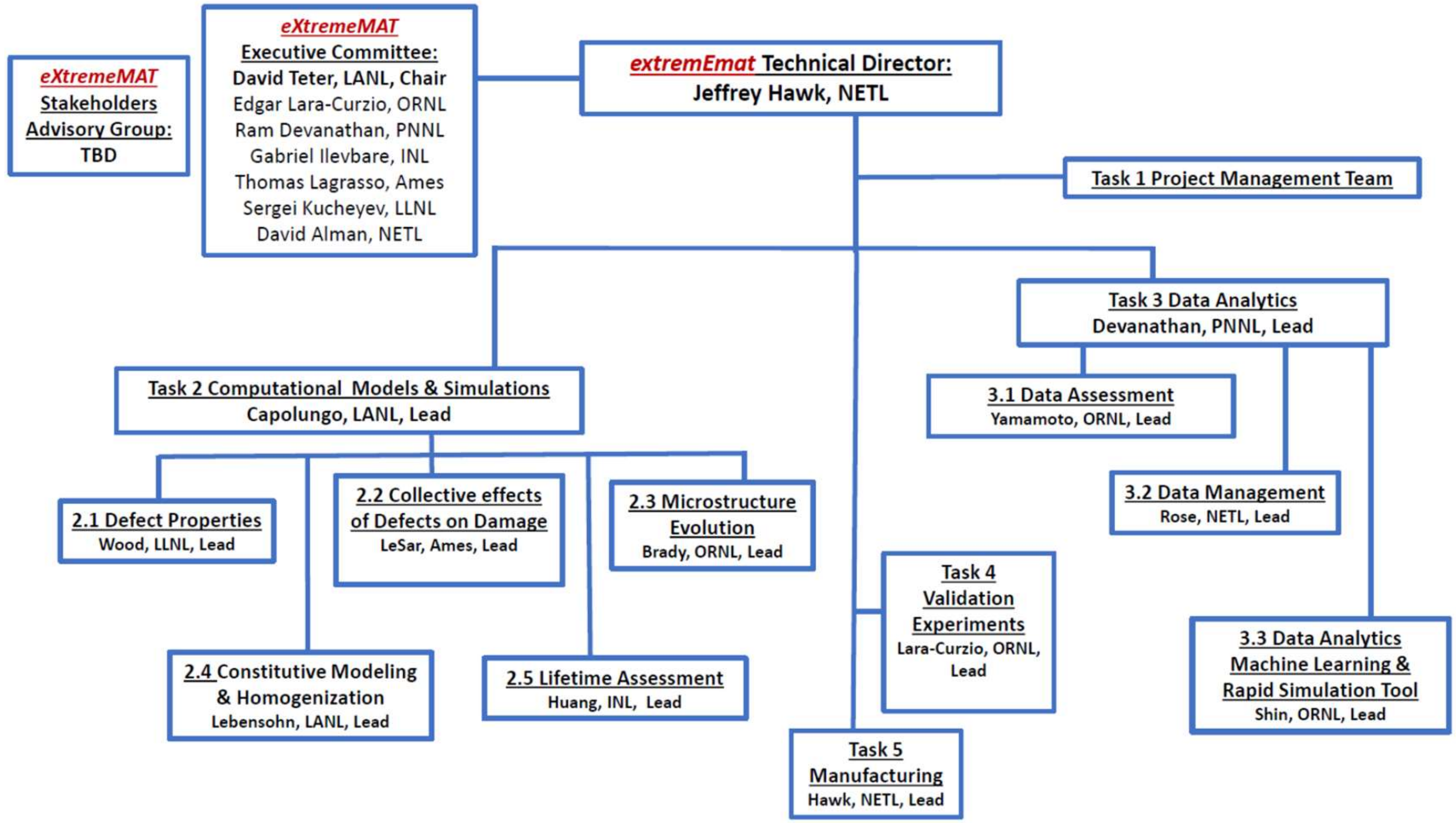
Structure



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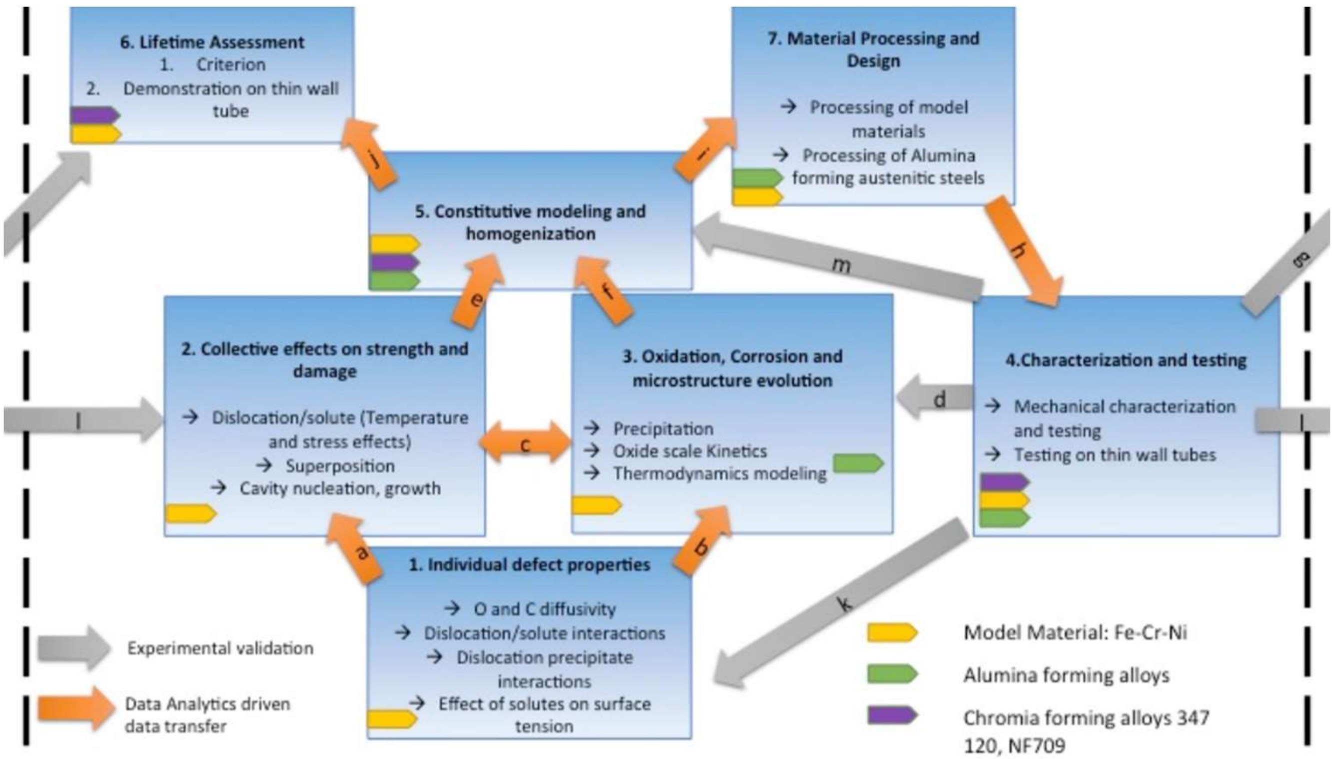
Research Plans

- Execution Year FW2019, w/FY2018 Funds
- Computational Tasks & Data Analytics (ongoing)
  - Develop & Optimize Computational Frameworks
  - Establish Targeted Validation Experiments
  - Construct & Implement Data Science Resource for FE Materials



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❑Data Science Resource for Existing & Transformational FE Materials

Alloys	Descriptors/Features	Properties/Performance
Chromia-forming	**Thermochemistry**	**Physical Properties**
316H	Elemental Composition	Mechanical Strength
347	Phase Stability	Creep Rupture Time
347H	**Diffusion Kinetics**	**Chemical Properties**
Alumina-forming	Atomic Mobility	Corrosion/Oxidation
AFA-HP	**Crystalography**	Open Circuit Voltage
AFA-low Ni	Lattice Parameters	**Thermal Properties**
Nickel-based	Polyhedra	Thermal Conductivity
	Atomistic	ΔH_f, ΔS_f, C_p
	Atomic Radius	
	Electronegativity	

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eXtremeMAT
Overarching Goals for Existing & Transformational Power Plants

- **Change the existing paradigm on how materials are conceived and developed.**
- **Introduce, and continuously improve, a *schema* of materials design, manufacture, and performance built on computational formalism, and utilizing best practice and targeted validation.**

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