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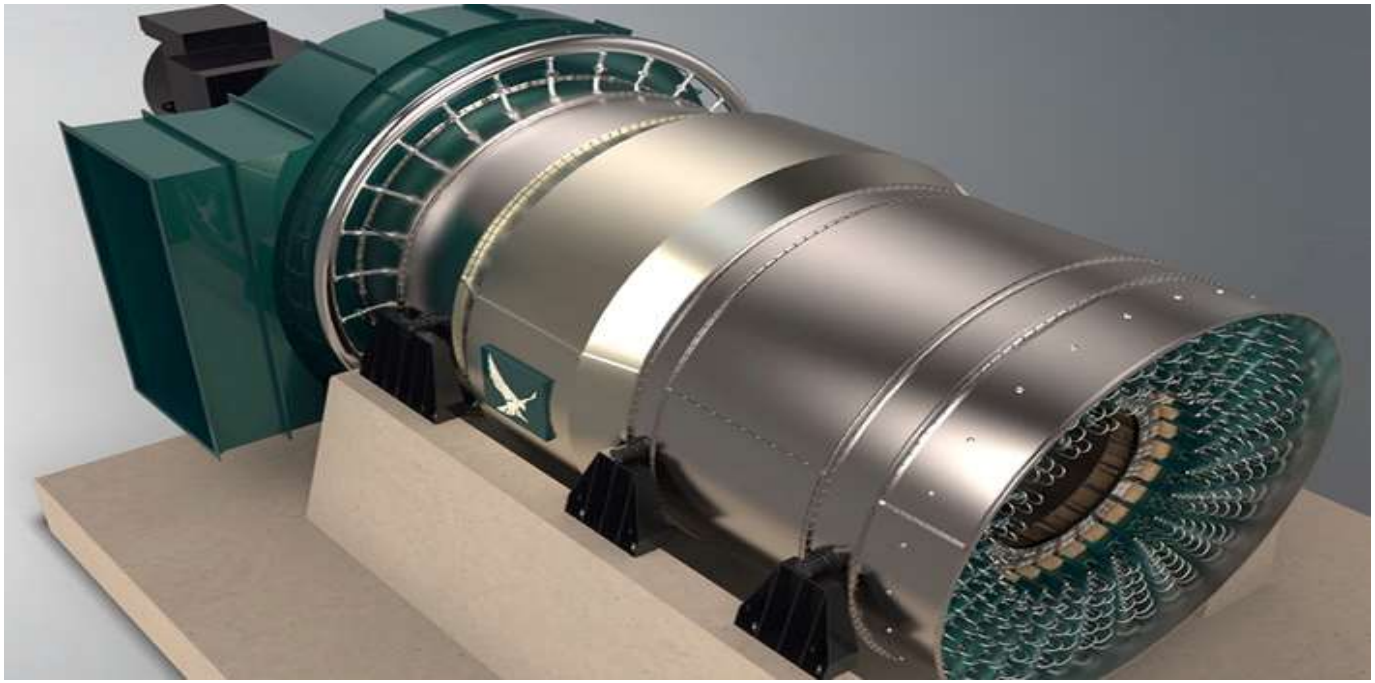
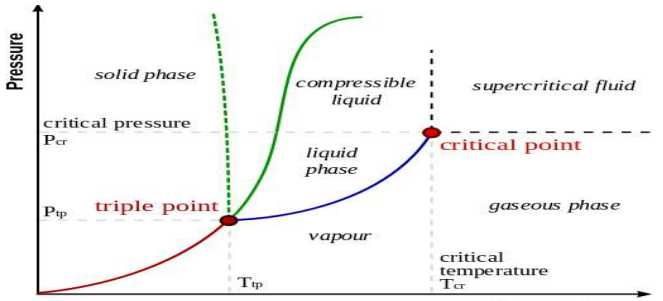


Computational Modeling and Simulation (Task 2)

Joel D. Kress
Laurent Capolungo
Los Alamos National Laboratory



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GOALS

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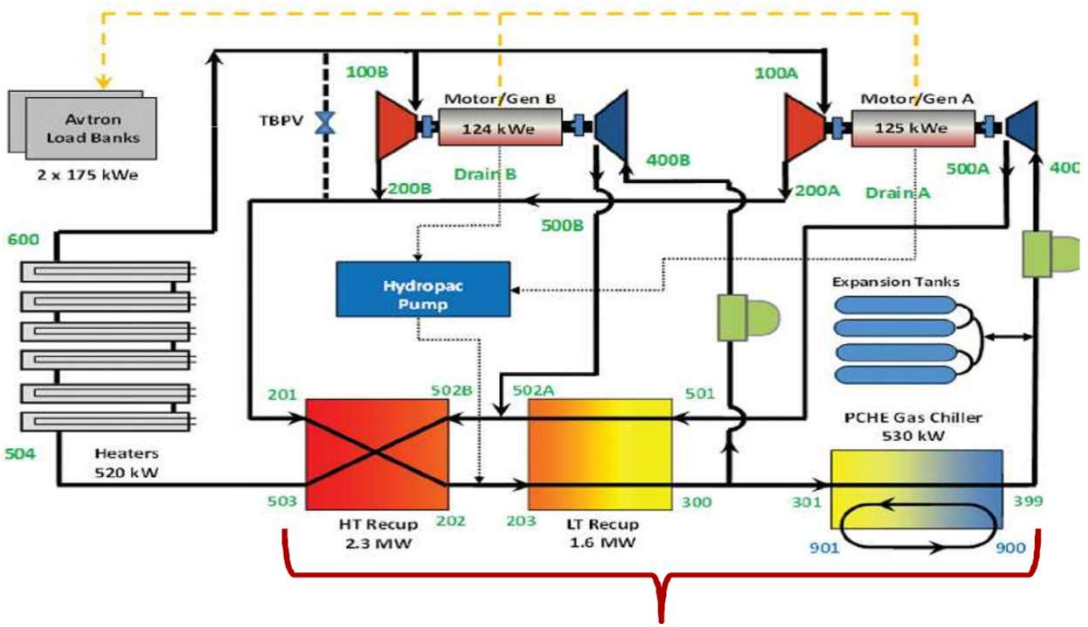
Overall Objective (5 years): demonstrate how modern experimental and modeling tools can be integrated across the National Laboratory Enterprise to accelerate the development and deployment of new Extreme Environment Materials (EEM) for fossil energy applications.

Design austenitic steels that perform as well at 750 C to 800 C as current Fe-based alloys perform at 700 C.

Predict the lifetime of complex components exposed to extreme environments, via an integrated multi-scale modeling approach.



PCHE style units

Priority #1: Alloy design

Priority #2: Lifetime assessment

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State of the art: lessons learned

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Type	Examples	Potential SCO2 Brayton Impacts
Precipitation	Salt Scale (H2O) Oil Transport (CO2)	1. Decreased heat exchanger performance. 2. Cleaning / replacement of heat exchangers. 3. Local thermodynamic property variation.
Particulate	Fabrication Shavings	1. Erosion of surfaces and sharp corners. 2. Sedimentation of piping, headers. 3. Plugging of heat exchanger channels.
Chemical Reaction	Coking	1. Reduced heat exchanger performance 2. Localized hot-spots from high emissivity.
Corrosion	Oxide Formation	1. Reduction of material thickness. 2. Spallation of weak oxide layers. 3. Reduced heat exchanger performance.
Solidification	Vent Line Freeze-up	1. Blockage of vent lines and over-pressurization of other system components. 2. Mechanical failure due to cold temperatures. 3. Stuck mechanisms from material shrinkage.

Materials related failure modes observed in SCO2 High-T HX (SNL Tests):

1. **Corrosion**
2. **Precipitation**

Primary importance: develop a predictive capability (i.e., extrapolation) to quantify microstructure evolution within the material system

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State of the art: material design

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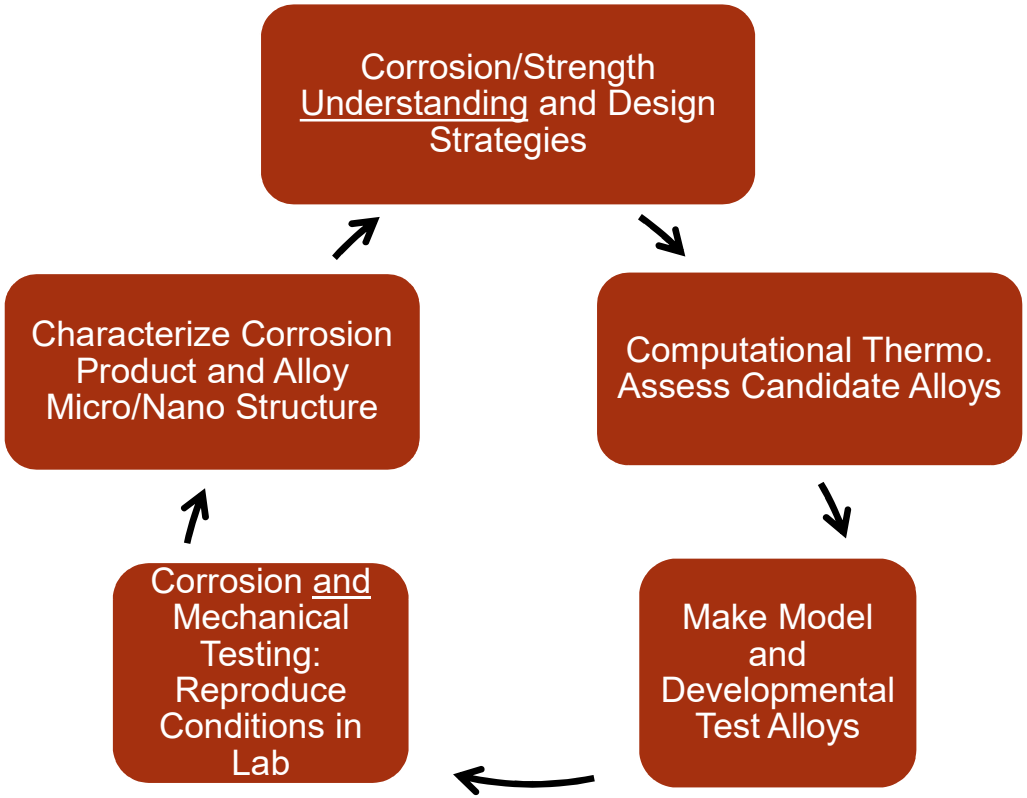

- Alloy design relies on a clear understanding of the relationship between material microstructure, chemistry and its mechanical response (strength), rupture life (damage evolution) and ability to form a continuous oxide layer.

- Task 2 will allow for an acceleration of the design cycle aided by advanced computational models

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Reality check: challenges

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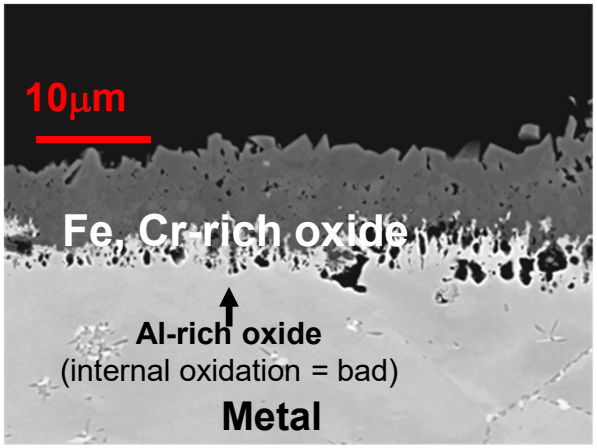
Design a new material system to favor the formation of an alumina passivation layer

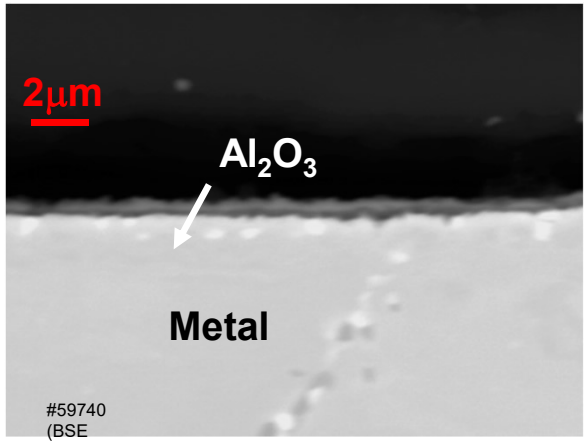
Replace Ti and V with Nb to yield Al_2O_3-Forming Austenitics

Original alloy (V/Ti)



Fe-20Ni-14Cr-2.5Al-0.5V-0.3Ti-0.1C

New alloy (Nb)



Fe-20Ni-14Cr-2.5Al-0.9Nb-0.1C

- Can't just add Al, complex interactions among Al, Cr, Ni, B, C, Nb, Ti, V
- Mechanism(s) not well understood
- Alumina formation lost in this AFA alloy ≥ 850-900°C

Cannot focus on pure systems or proxies; need to tackle the complexity of chemistry.

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State of the art: assessing rupture life

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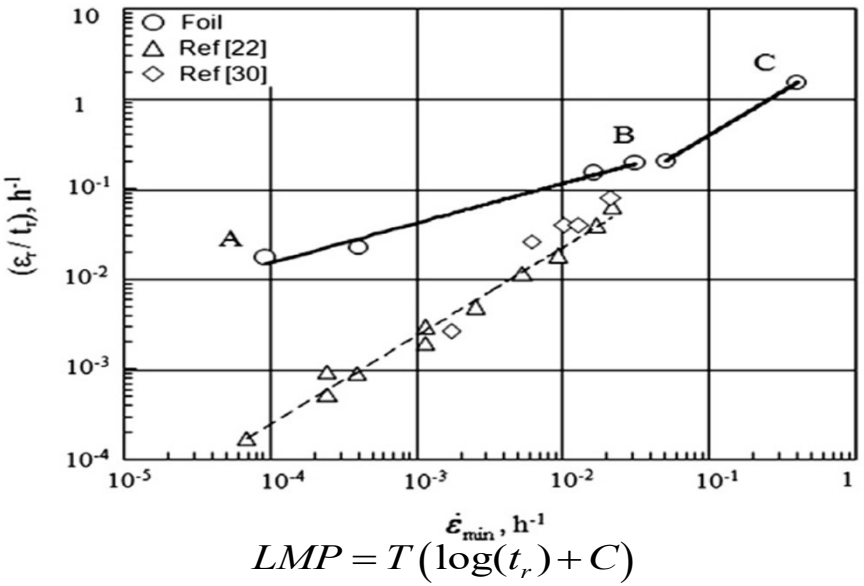

$$LMP = T\left(\log(t_r) + C\right)$$

Larson Miller approach to rupture life

Current engineering criteria to predict the rupture life of a system **can only be used to interpolate** in between empirical data.

Needed for **in-service conditions**. E.g., there is no stress dependence in the Larson Miller Parameter; multi-axial loading is not considered.

Assumptions:

1. Stage II creep is dominant relative to stage I and III
2. The creep rate in stage II explicitly depends on a single activation energy independent of stress.

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State of the art: rupture life

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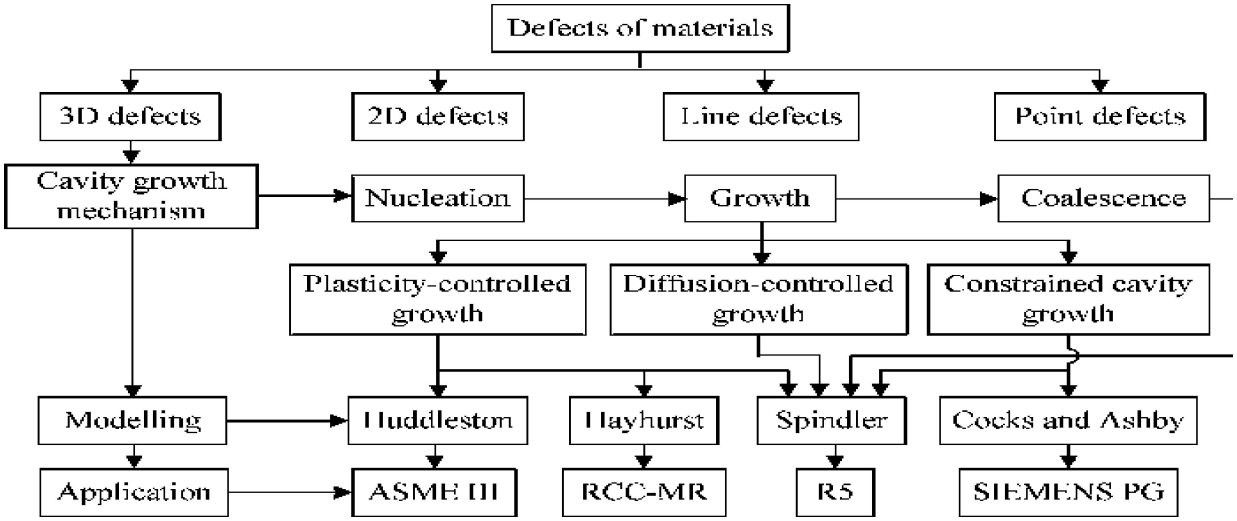

Phenomenological scheme for rupture life

- Damage mechanics has significantly evolved over the past few decades yielding rupture life criteria that relies on the activation of distinct processes (e.g., void nucleation, growth)

- However, both empirical (e.g., Larson Miller) and phenomenological rupture life criteria are significantly disconnected from the materials microstructure and from chemistry

Propose a new rupture life/failure criterion in order to *a priori* predict the lifetime of an actual system subjected to service conditions.

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Reality check: challenges

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Mechanism	Plasticity	Creep
Dislocation mechanisms	Dislocation glide	**Dislocation creep (climb and glide)**
Diffusion mechanisms	No significant role of diffusion mechanisms.	**Diffusion mechanisms relevant.**
Grain boundary sliding	No significant role of grain boundary sliding.	**Grain boundary sliding relevant.**
Damage nucleation	Breakage/decohesion of (intragranular or intergranular) particles	**At grain boundaries, related to dislocation pile-ups, breakage/decohesion of intergranular particles, GBS**
Damage Growth	Accommodated by dislocation plasticity, controlled by stress triaxiality, crystal orientation/ misorientation	**Accommodated by dislocation plasticity and/or diffusional creep, GBS. Depending on temperature and stress, controlled by general stress state/GB orientation.**

In task 2, a rigorous understanding of the activation and contributions of several deformation processes, as a function of chemistry and microstructure, will have to be derived.

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Computational Modeling and Simulation (Task 2)

	Subtask
2.1	Individual defect properties
2.2	Collective effects of defects
2.3	Oxidation, corrosion, and microstructure evolution
2.4	Constitutive modeling and homogenization
2.5	Lifetime assessment

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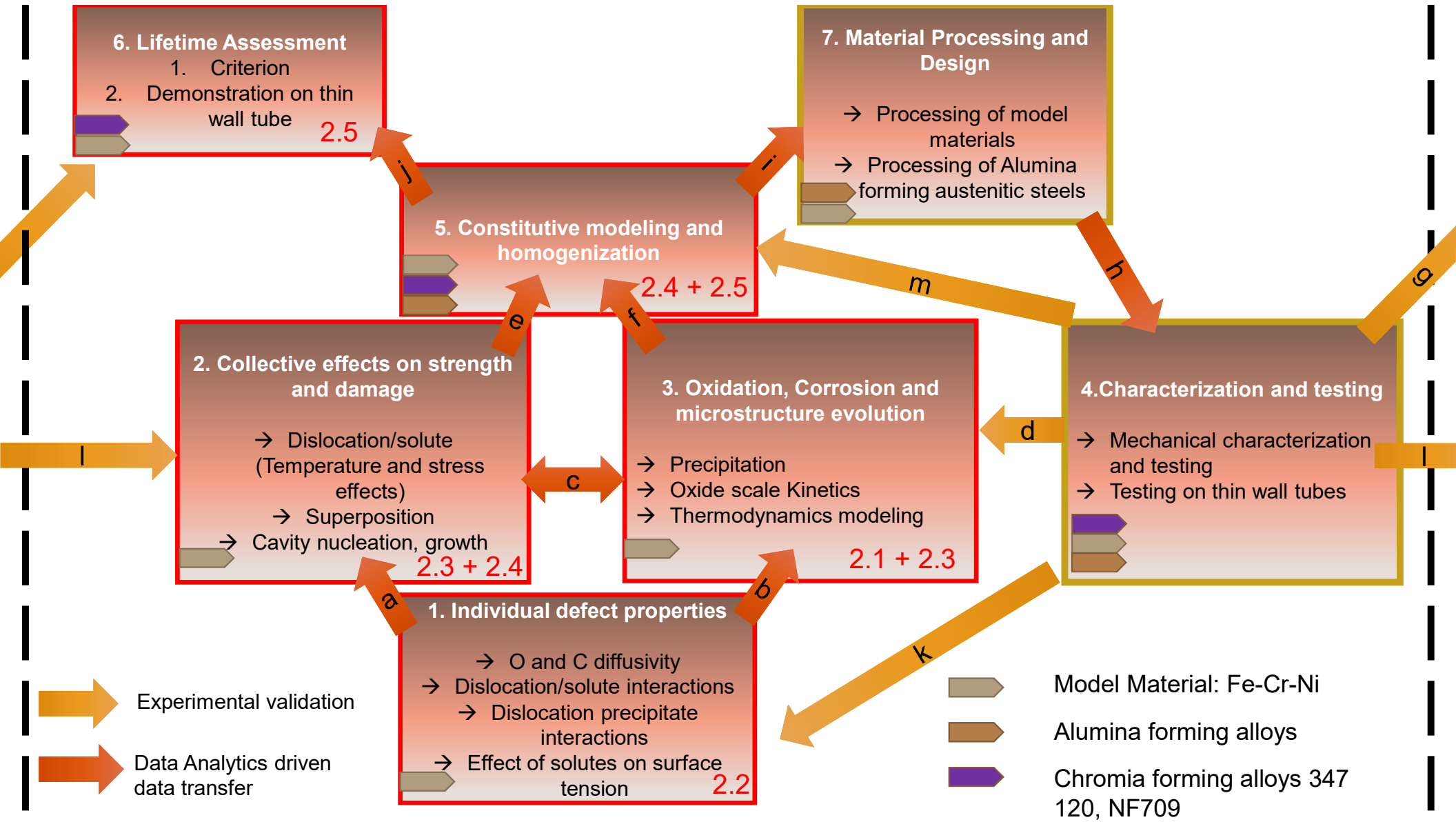
6. Lifetime Assessment
1. Criterion
2. Demonstration on thin wall tube
2.5
7. Material Processing and Design
→ Processing of model materials
→ Processing of Alumina forming austenitic steels
5. Constitutive modeling and homogenization
2.4 + 2.5
2. Collective effects on strength and damage
→ Dislocation/solute (Temperature and stress effects)
→ Superposition
→ Cavity nucleation, growth
2.3 + 2.4
3. Oxidation, Corrosion and microstructure evolution
→ Precipitation
→ Oxide scale Kinetics
→ Thermodynamics modeling
2.1 + 2.3
4.Characterization and testing
→ Mechanical characterization and testing
→ Testing on thin wall tubes
1. Individual defect properties
→ O and C diffusivity
→ Dislocation/solute interactions
→ Dislocation precipitate interactions
→ Effect of solutes on surface tension
2.2
a
b
c
d
e
f
g
h
i
j
k
l
m
l
Experimental validation
Data Analytics driven data transfer
Model Material: Fe-Cr-Ni
Alumina forming alloys
Chromia forming alloys 347 120, NF709

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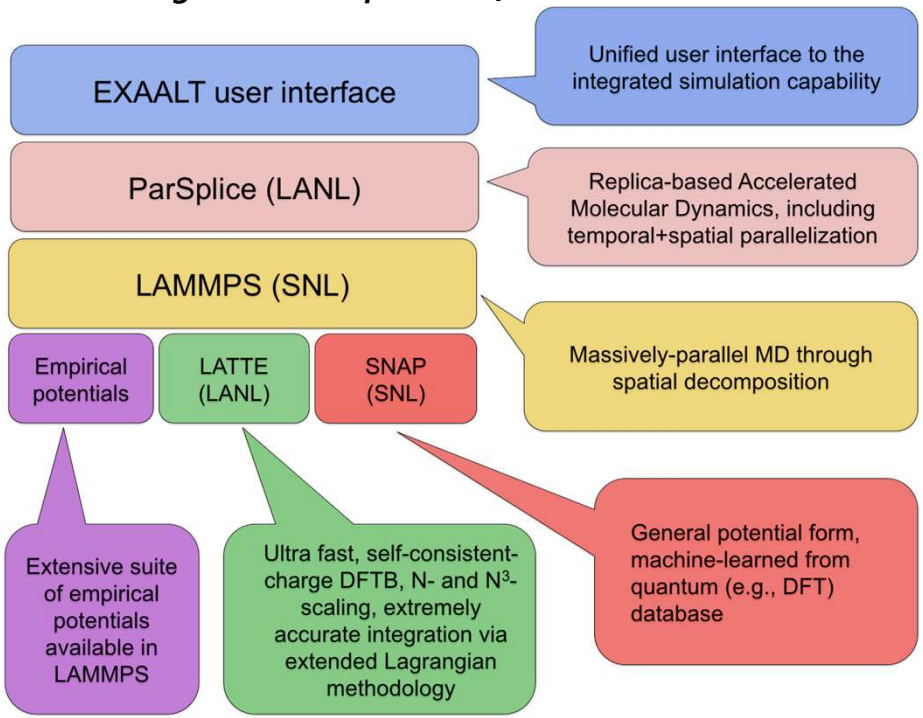

ECP EXASCALE COMPUTING PROJECT

Exascale Atomistic capability for Accuracy, Length, and Time

Task 2.1: Individual defect properties

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The overall mission of Task 2.1 is to provide critical information to Tasks 2.2 and 2.3 associated with individual defect properties.

Questions to be addressed

- → Interatomic potential development
- → Solute-Dislocation interactions
- → C and O diffusivities
- → Strengthening due second phase particles
- → Effect of chemistry on cavity nucleation and growth kinetics (diffusive regime)
- → Carbide and metallic/intermetallic kinetics

A series of MD and DFT based approaches will be used to (1) enrich thermodynamics and kinetic databases such as to accelerate alloy design and (2) to assist in the quantification of solute and precipitates to strength and damage

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Task 2.1: Individual defect properties

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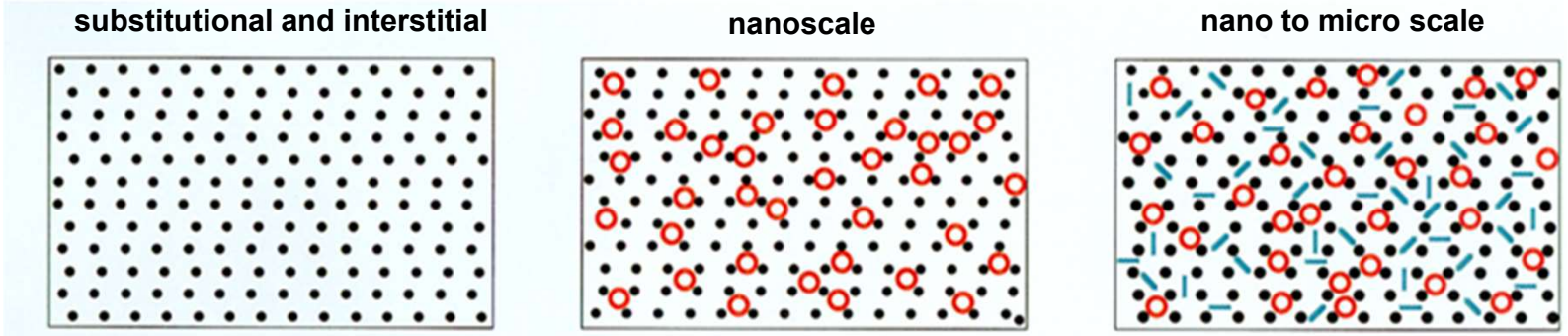
Strength Improvement: Synergies Across Multiple Length Scales/Mechanisms

Solid solution + **Carbides/Nitrides** + **Intermetallics**



→ Solid solution impact: use computational thermodynamics to predict composition of FCC matrix, other approaches to predict strengthening potentially gain?

→ Predict number density, size, location, coherency, dislocation interactions, etc. of potential carbide/nitride/intermetallic 2nd phases. Impact of phase chemistry?

→ Multi scale: How multiple strengthening mechanisms interact, synergistic benefits which yield greatest strength? What is optimum mix of strengthening mechanisms?

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Task 2.2: Collective effects of defects

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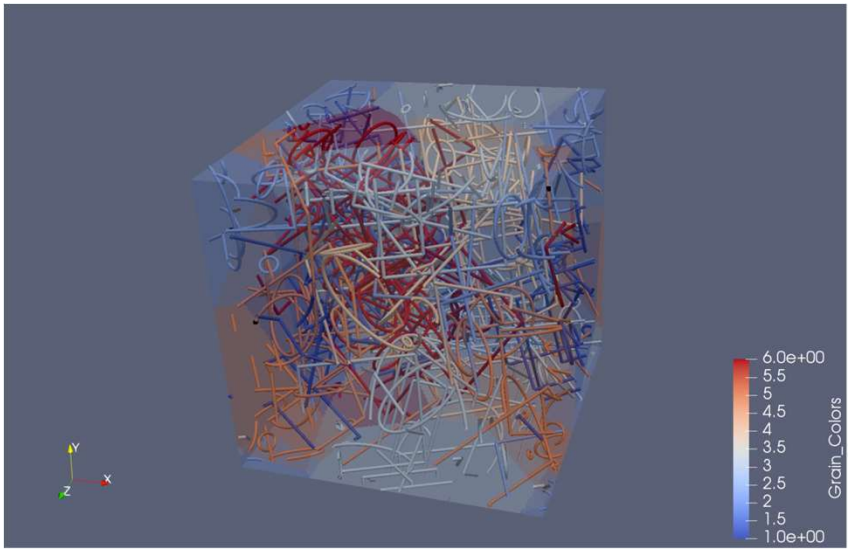
Derive laws that quantify the correlation between material chemistry, microstructure and damage nucleation, strength and chemico-mechanical dissipative processes (e.g., climb).



Problem statement: Plasticity is governed by the short and long-range interactions between defects (i.e., V, I, dislocations). Atomistic scale simulations alone cannot quantify the long range interactions.

Solution: Discrete dislocation dynamics

Questions to be addressed:

- **Effect of Solute-Dislocation interactions on strength**
- **Effects of Carbides on strength**
- **Superposition law (i.e., how to quantify strength when several strengthening processes are use simultaneously)**
- **Damage evolution**

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Discrete dislocation dynamics (DDD) is a method that simulates plasticity in microstructures by tracking the evolution of individual dislocations within the system.

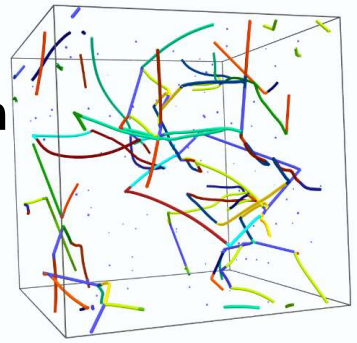
DDD allows for the quantification of the collective effects of defect interactions on strength. It is used to validate/correct/devise constitutive models.

DDD can be combined with reaction diffusion models to track the evolution of chemical species on the system.

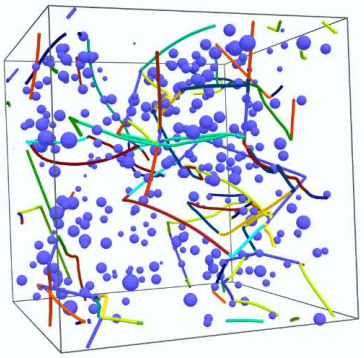
By combining discrete dislocaton dynamics with cluster dynamics we will simultaneously predict microstructure evolution due to plasticity and due to damage evolution.

Example: reaction/diffusion model for vacancy evolution (taken from work on Radiation Damage)

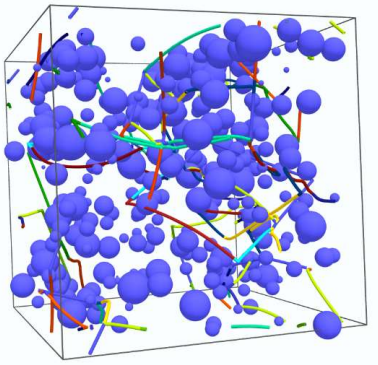
0.01 dpa



1. dpa



10 dpa



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Task 2.3: Oxidation, corrosion and microstructure evolution

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- Predicting the relationship between composition and as-processed microstructure and kinetics of microstructure evolution.
- Propose designs for new alloys.
- Two key questions will be addressed:
  - Material thermodynamics (i.e., likely microstructure as per the phase diagram)
  - Material kinetics (boundary mobility, coarsening of precipitates).
- A series of tools will be used: CALPHAD, DICTRA, Phase Field modeling

Phase Field, Thermodynamics modeling (DICTRA, CALPHAD)

Questions to be addressed:

- Second phase precipitation (Coarsening of carbide, metallic, and intermetallic strengthening phases)
- Transition from internal to external oxidation
- Establishment and maintenance of protective oxide scale: oxygen diffusivity/oxidation kinetics across protective oxides

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Task 2.3: Diffusion Modeling

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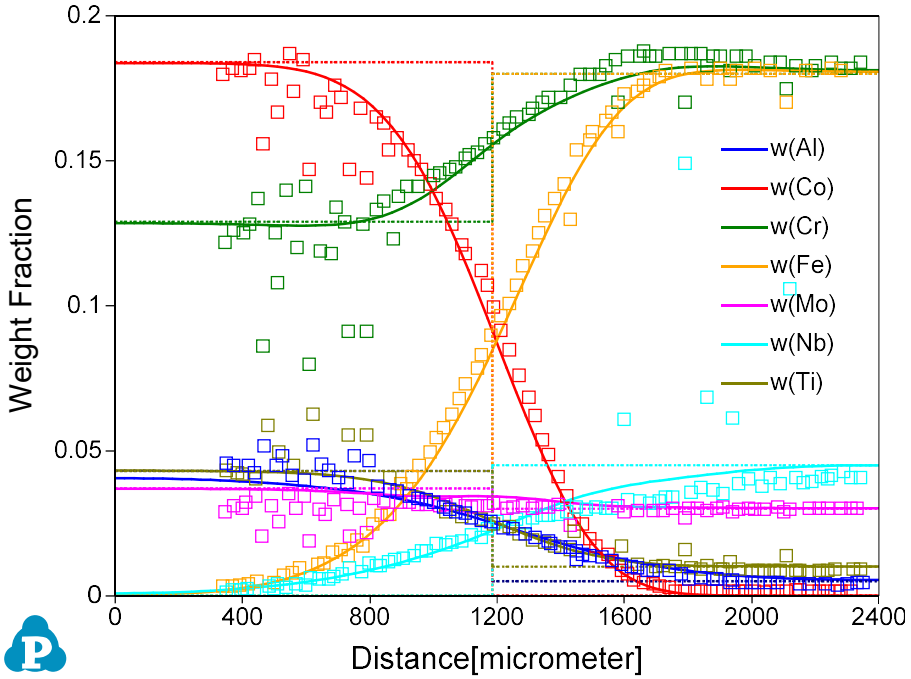
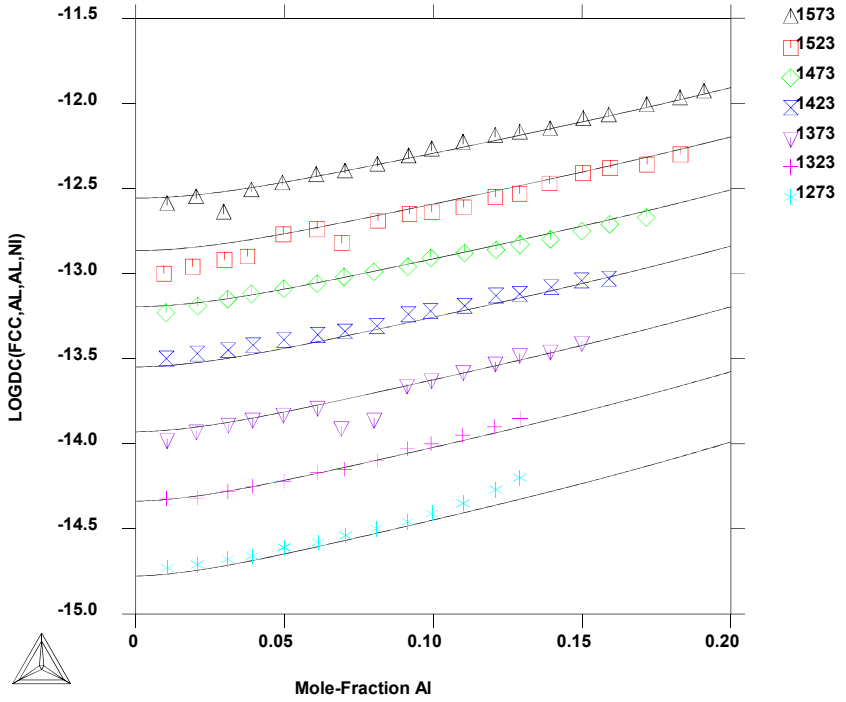


Diffusion between IN100 and Alloy 718 at 1150 °C for 1000 hours, experimental data are from Campbell et al., Mater. Sci. Eng. A **407** (2005), 135-146.
(Courtesy of Fan Zhang of CompuTherm)



Symbols are experimental data taken from Yamamoto et al, Trans. Jpn. Inst. Met. **21**(1980), p. 601.
(Courtesy of Paul Mason of ThermoCalc)

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Task 2.4: Constitutive modeling and homogenization

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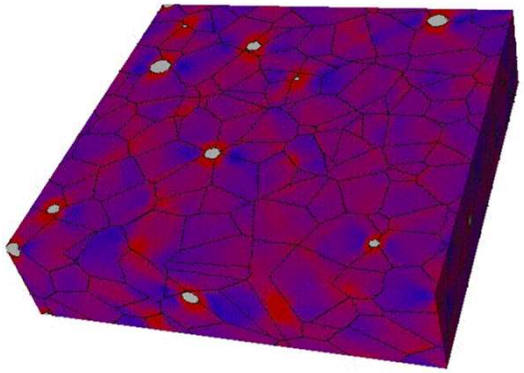
- Predict the mechanical response and damage kinetics of austenitic steels (e.g., 347, 316 etc.) as a function of material chemistry and microstructure.
- Focus on a full-field description of the polycrystalline microstructure.
- Kinetics of microstructure evolution and strength models will be provided by Tasks 2.2 and 2.3.
- Use a numerically efficient Fast Fourier Transform method for rapid simulation (100x faster than finite element methods)



- **Constitutive model development for single crystals**
- **Prediction of mechanical response in the absence of oxide scale**
- **Reduced order modeling for mechanical response in the absence of oxides**

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Task 2.4: Constitutive Modeling & homogenization

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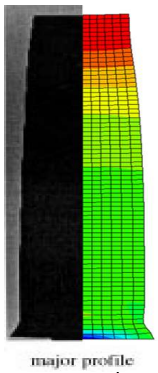
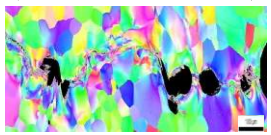
1

Tasks 2.2 and 2.3 will provide an enhanced constitutive modeling approach (i.e., strength models and damage nucleation and growth laws) and microstructure evolution kinetics

2

Tasks 2.4 will be used to derive simple reduced order models that can be used within FEM (i.e., Task 2.5) in order to predict the rupture life of a system

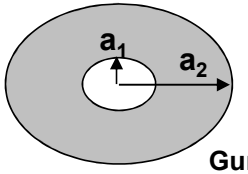




FEM: A *voided* PX in each material point

MACROSCALE (specimen)

MESOSCALE polycrystal (PX)



$$\left(\frac{\sigma_{eq}}{\sigma_o}\right)^2 + 2\phi\cosh\left(\frac{3\sigma_m}{2\sigma_o}\right) - 1 - \phi^2 = 0$$

Semi-analytical methods

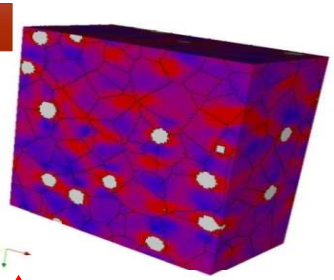
Gurson-type with anisotropic matrix and porosity

validation/calibration

Polycrystal models

full-field

2

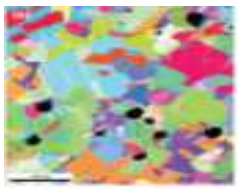


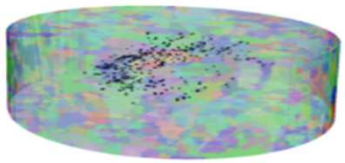
validation

1

Tasks 2.2 and 2.3

Mesoscale experiments





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Task 2.5: Lifetime assessment

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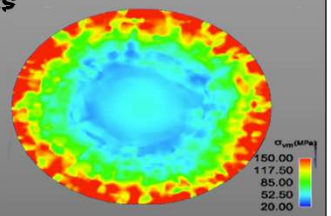
MOOSE, MAMBA

MOOSE

- MOOSE: a finite element, multiphysics framework that simplifies the development of advanced numerical applications.
- MAMBA: a 3D adaptive mesh framework that solves coupled transport and chemistry encountered in the corrosion and oxide growth in alloys.

Tensor Mechanics

- Linear elasticity
- Eigenstrains
- J2 Plasticity
- Crystal plasticity
- Power-law creep
- Rate-dependent damage models



Generic Multi-species Diffusion-Reaction Module

- Full reaction networks: both equilibrium and kinetic reactions
- Examples:
  - H diffusion and hydride formation in nuclear claddings
  - Chemical degradations of concrete structures in nuclear power plants
  - All coupled with thermo-mechanics modules

Questions to be addressed:

- Component level modeling of corrosion (outside)
- Component level modeling of microstructure evolution
- Mechanistically-based multiscale/multiphysics modeling
- Component level modeling of system performance

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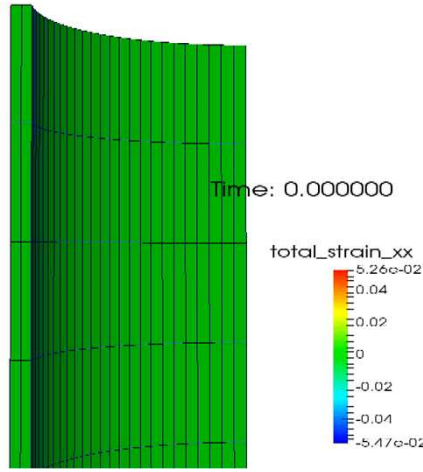
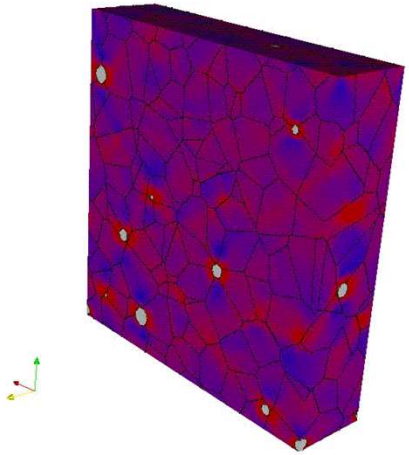
Task 2.5: Lifetime assessment





The MOOSE framework will predict the mechanical response and failure of components as a function of alloy chemistry and microstructure

microns

Mesoscale (Task 2.4)

- Predict microstructure evolution
- Determine impact on properties:

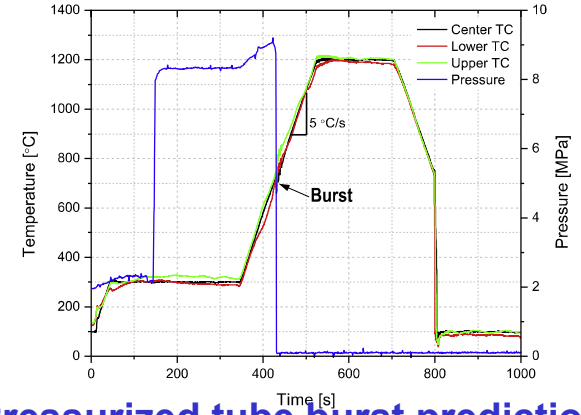
Reduced order models (ROM) at the FEM integrations points

- Tangent stiffness matrix sensitive to chemistry, composition and conditions
- Oxidation rate

ROM via data analytics, mutliscale experiments

millimeters and up

Engineering scale (Task 2.5)



Pressurized tube burst predictions due to temperature ramp

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Computational Modeling and Simulation

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FY18 Deliverable (28Sept18): A report that captures the team's assessment of existing modeling and simulation code capabilities identifying gaps, a pathway to fill gaps, and an integrated frameworks for multi-scale modeling of extreme environments allow design and performance. **On track.**

Subtask	FY19 Accomplishments (Proposed)
2.1	Interatomic potentials developed for Fe-Cr-Ni-O-C system
2.2	Development of coupled chemico-mechanical tool
2.3	Initial thermodynamics analysis for the Fe-Cr-Al-Ni-O system
2.3	Initial phase field alloy design tool for oxides
2.4	Initial framework for elasto-plastic and unified constitutive models
2.5	Implementation of constituitive models in the MOOSE framework
2.5	Demonstration lifetime FEM simulation using MOOSE multiphysics

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Thank you

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Summary

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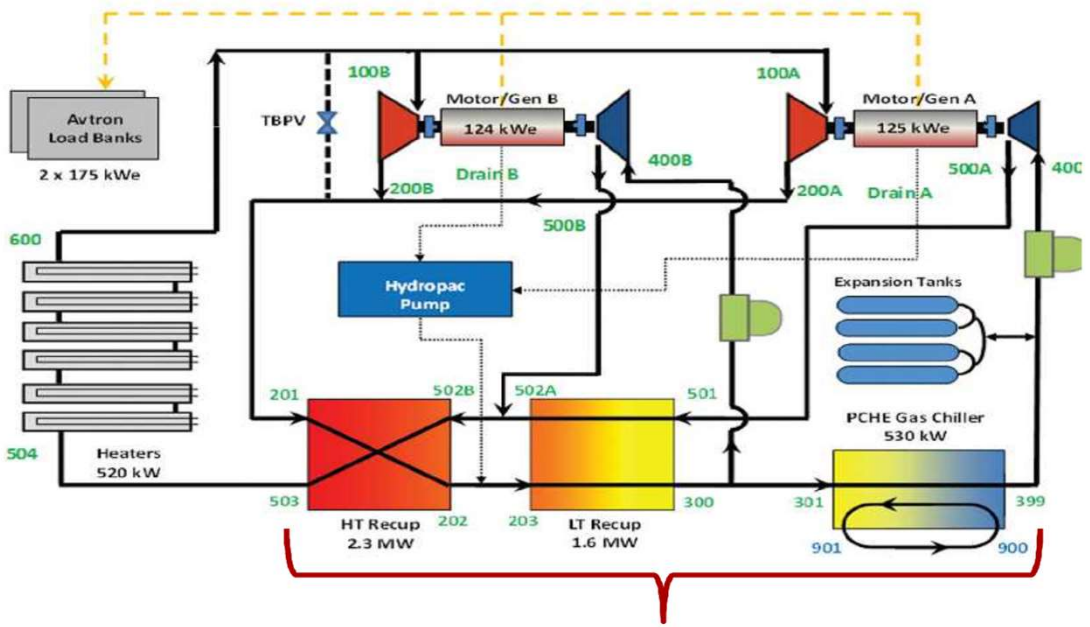
Task 2. Computational Modeling and Simulation

- ***EEM will design austenitic steels that perform as well at 750 C to 800 C as current Fe-based alloys perform at 700 C.***
- ***Further, throughout the integrated multi-scale modeling approach to be pursued EEM will allow for the prediction of the lifetime of complex components exposed to extreme environments.***



PCHE style units

Priority #1: Alloy design

Priority #2: Lifetime assessment

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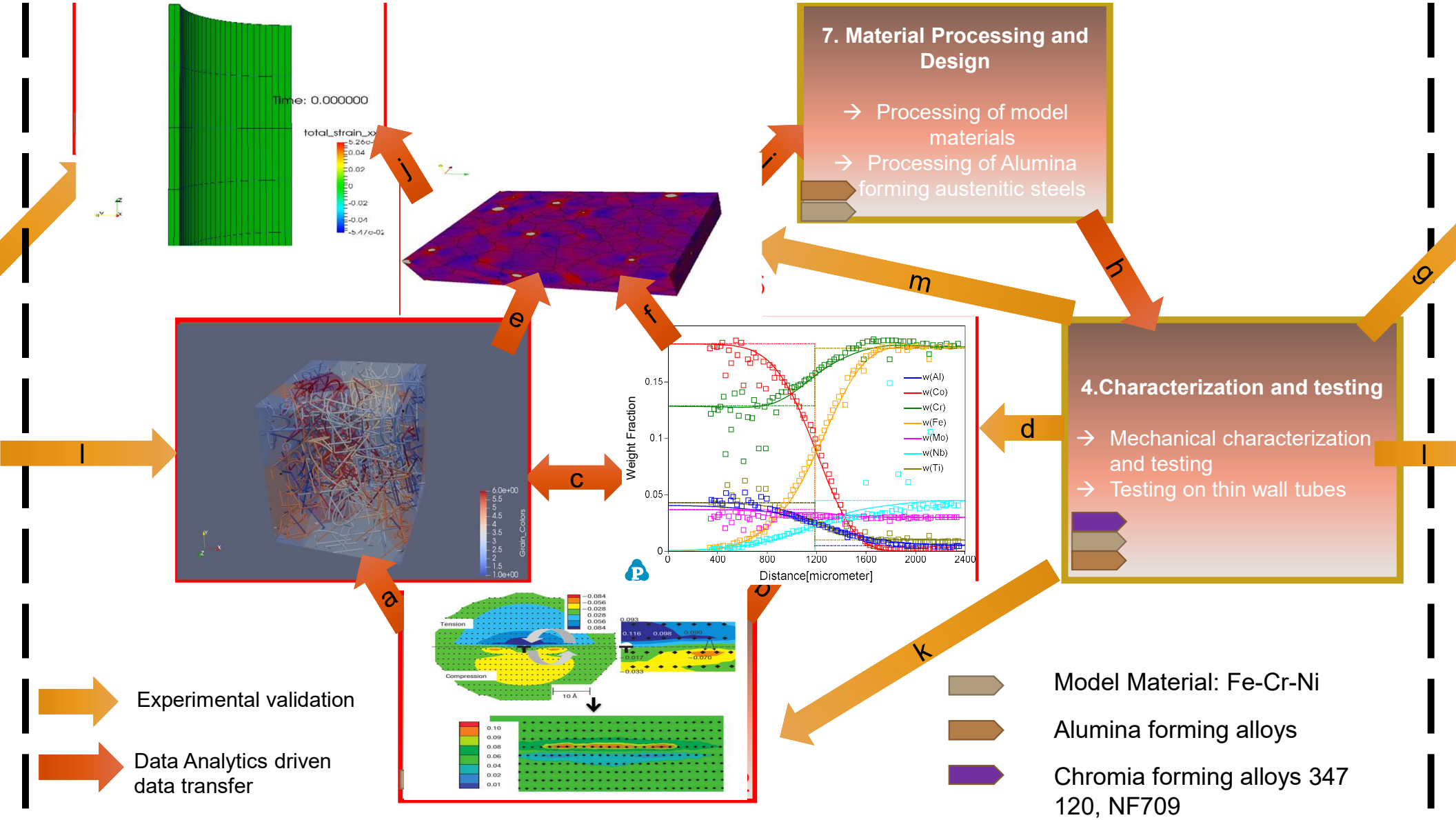
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total_strain_xx
Grain_Colors
Weight Fraction
Distance[micrometer]
w(Al)
w(Co)
w(Cr)
w(Fe)
w(Mo)
w(Nb)
w(Ti)
Tension
Compression
7. Material Processing and Design
→ Processing of model materials
→ Processing of Alumina forming austenitic steels
4.Characterization and testing
→ Mechanical characterization and testing
→ Testing on thin wall tubes
a
b
c
d
e
f
g
h
i
j
k
l
m
Experimental validation
Data Analytics driven data transfer
Model Material: Fe-Cr-Ni
Alumina forming alloys
Chromia forming alloys 347 120, NF709

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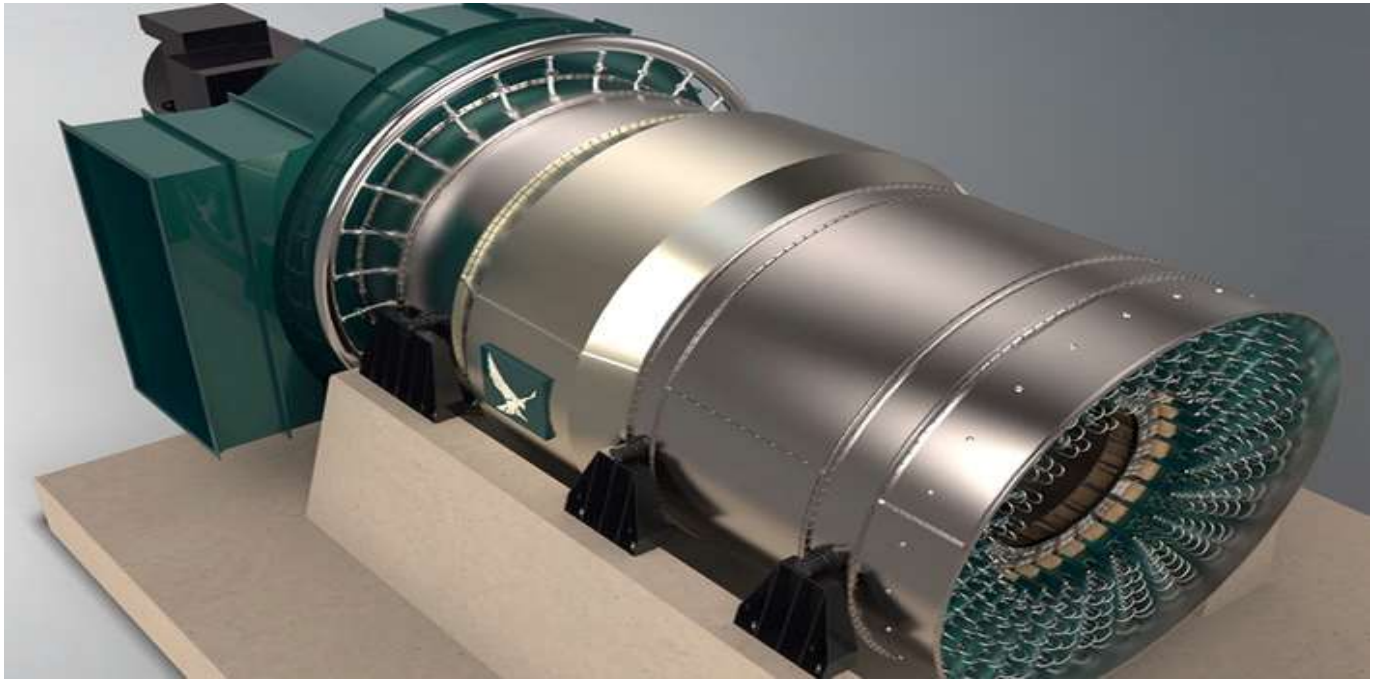

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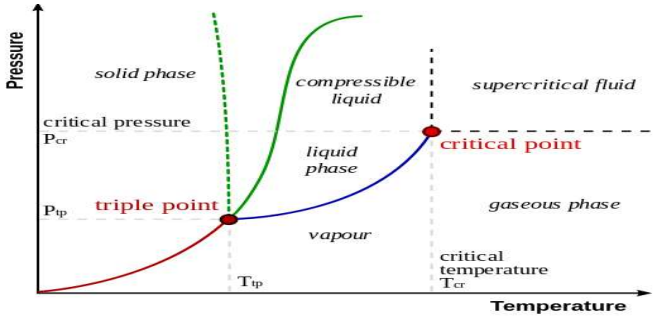

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