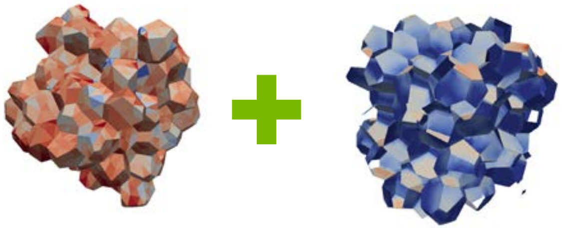
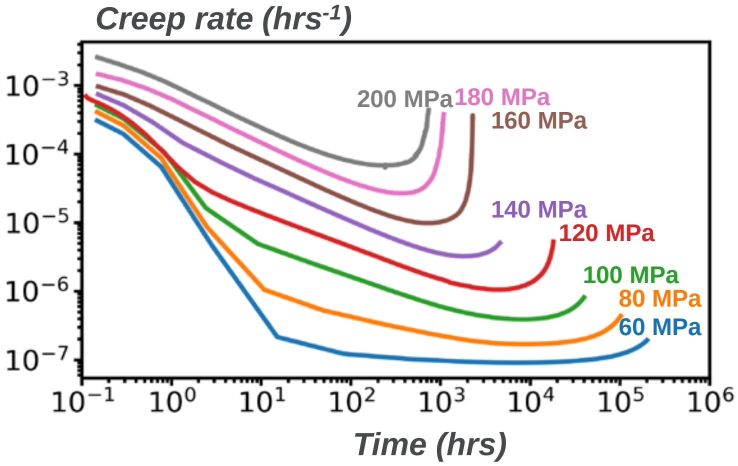
WE START WITH YES.

RAPID QUALIFICATION OF NEW MATERIALS USING MODELING AND SIMULATION





MARK MESSNER
Argonne National Laboratory

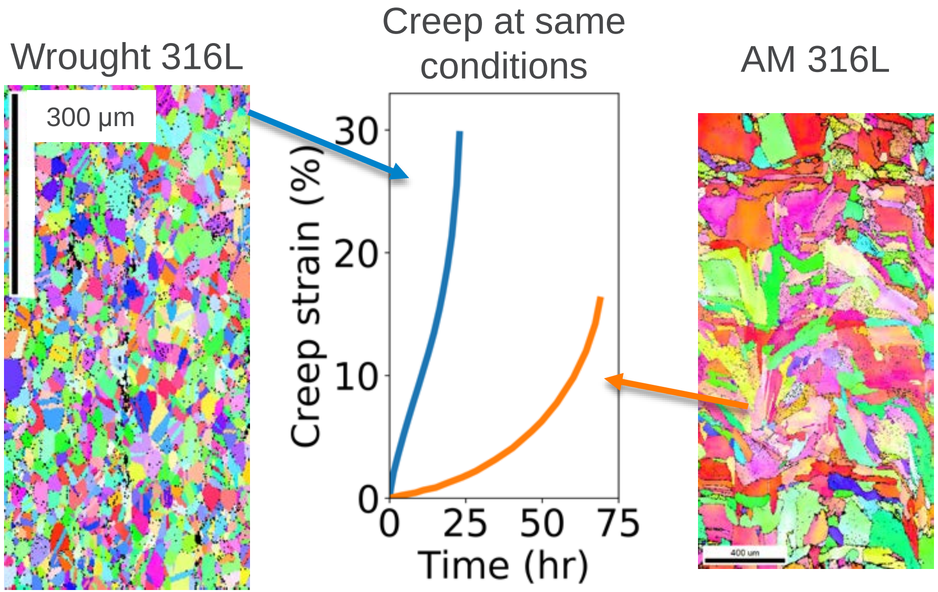
NRC Workshop on Advanced Manufacturing Technologies for Nuclear Applications
December 2020

ACCELERATING QUALIFICATION OF NEW (AMT) MATERIALS

- **Overview** of the key challenges in rapid qualification of new materials and qualifying AMT materials, focusing on high temperature reactors:
  - *AMTs*
    - Expect higher variability compared to conventional processing
    - Manufacturers/vendors have greater control over process
    - Limited data on nuclear materials
  - *High temperature materials*
    - Long-term properties control design, short term tests provide limited information
    - Limited test data on AMT materials
- **Three key tools** for using modeling and simulation to accelerate qualification:
  - *Tool 1*: Physically-based models
  - *Tool 2*: Staggered qualification test programs
  - *Tool 3*: Uncertainty quantification through statistical inference
- **One vision** of how these tools could be used to accelerate the qualification of a new AMT material

WHAT ARE THE CHALLENGES QUALIFYING AM MATERIALS IN GENERAL?

- *Variability in AM material properties is much greater than for conventional wrought/cast material – more akin to welds*
  - Less understood processes
  - Many processing parameters controllable by users
  - Wide variety of technologies
  - Manufacturing likely to occur at a number of smaller sites, rather than at large, central production facilities
- *AM methods often result in significant material property variations within a single build*
- *We want a process that can take advantage of the flexibility of AM processes – not trying to simply 3D print conventional material*



AM material good, bad, or just different?

AM creep specimens courtesy UW Madison

WHAT ARE THE CHALLENGES QUALIFYING MATERIALS FOR HIGH TEMPERATURE SERVICE?

- At high temperatures long-term, time-dependent material properties control design:
  - Creep strength and ductility
  - Creep-fatigue life
  - Thermal aging characteristics
  - Environmental degradation
- Short-term tests might tell you very little about important long-term properties
- Statistical variation in mechanical properties tends to be high, even for well-controlled traditional wrought material processes
- Weld resilience can be challenging
- Very little long-term mechanical test data on AM material for properties relevant to high temperature design

Seam pipe failure at coal power station (Viswanathan and Stringer, 2000)

Creep cavitation (INL)

HRSG tube failure (EPRI, 2005)

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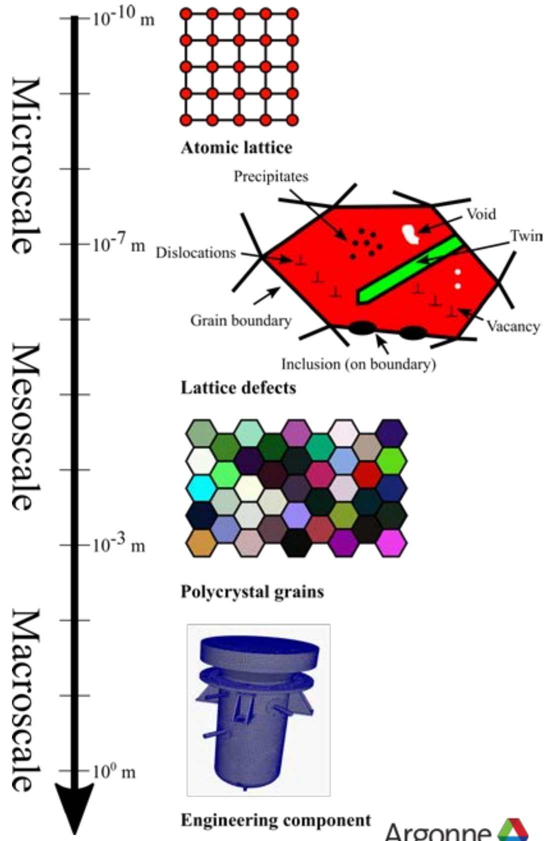
TOOL #1: PHYSICALLY-BASED MODELS

- **Physically-based model:** model the physical mechanisms that underlie a process
- Opposed to an **empirical model** correlating data to outcome
- **Types of physically-based models:**
    - Microstructural model: (some of) the model parameters are measurable microstructural characteristics
    - Multiscale model: hierarchical model propagating physical descriptions of processes on smaller length scales to higher length scales

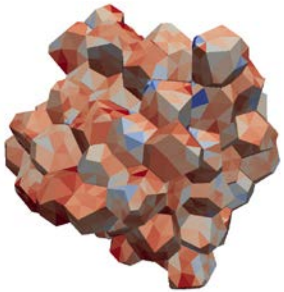
How physically-based models can improve property predictions and accelerate qualification:

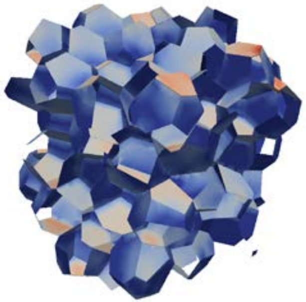
1. Direct link to microstructure: connection to *in-situ process monitoring* and *process models*
2. Better chance of accurate extrapolation: physics remains the same regardless of lengths scale, time scale, environmental conditions…



AN EXAMPLE OF HOW PHYSICALLY-BASED MODELING CAN SPEED QUALIFICATION

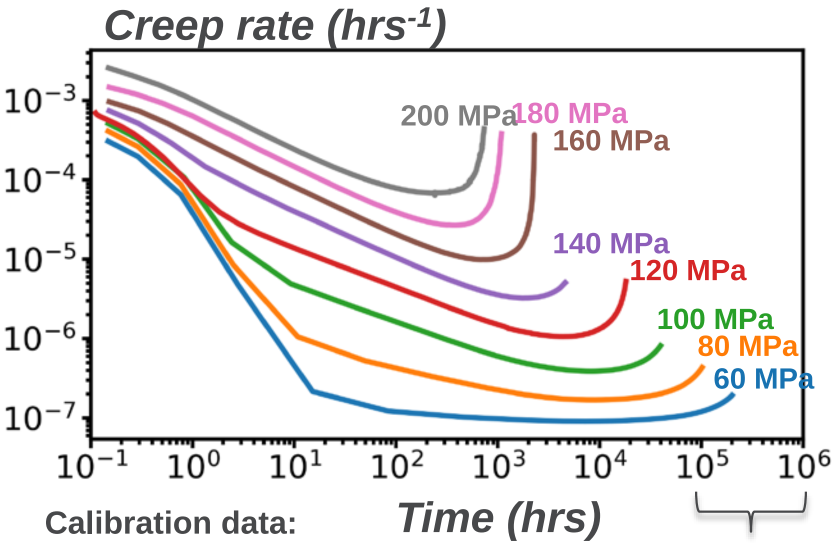
Wrought Grade 91





Grain bulk:
- Solid finite elements (tet10)
- Constitutive model captures:
  - Dislocation-mediated creep on BCC slip systems
  - Isotropic diffusion-mediated creep

Grain boundaries:
- Interface-cohesive formulatio (DG method)
- Constitutive model captures:
  - Cavity nucleation
  - GB diffusion mediatec void growth
  - Bulk plasticity (=dislocation) mediated void growth
  - Viscous GB sliding



Calibration data:
Kimura (2009) at 160, 140, 120, and 100 MPa

Experimentally inaccessible, >100,000 hours life

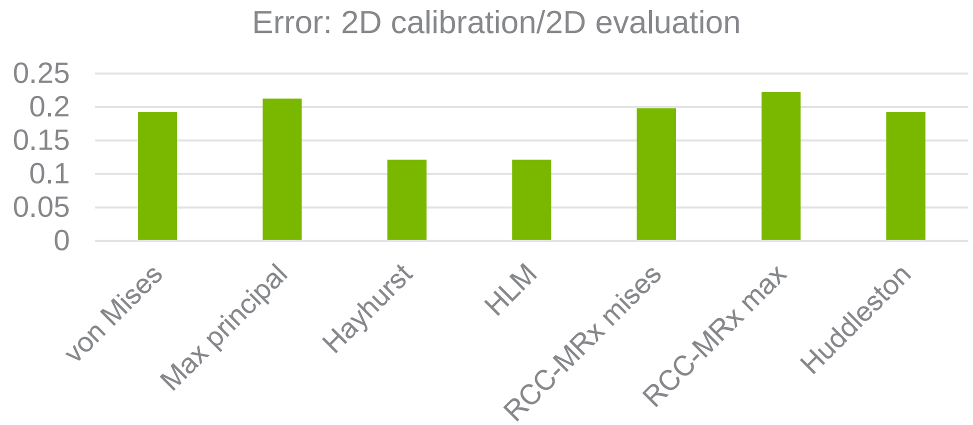
Model predicts full creep curves, including rupture time

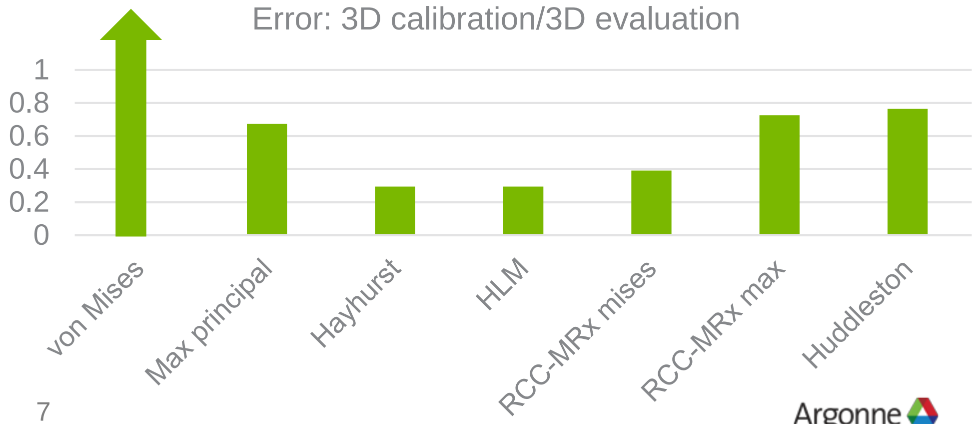
EVALUATING CREEP UNDER TRIAXIAL LOAD

- We typically test creep specimens with uniaxial stresses
    - Occasionally we have biaxial test data (pressure tubes)
    - Notched tests are difficult to interpret
- **Key question: how to extrapolate this data to realistic 3D states of stress?**
- Usual engineering approach: find an effective stress measure that converts 3D → 1D so that the 1D rupture correlation predicts 3D rupture
- But we don’t have 3D creep test data or long-term 2D data
- We can use the physical model to predict triaxial rupture and assess different engineering models (or develop new ones!)

Key outcomes of study:

- All the effective stress measures are about equally accurate when calibrated and compared to biaxial rupture data
- ***Some are much better than others when calibrated and evaluated against 3D data***





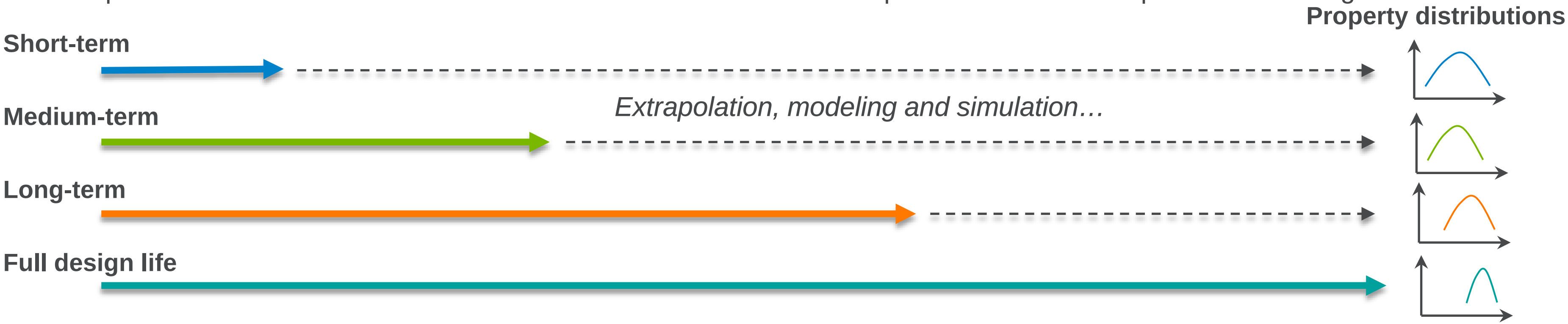
TOOL #2 STAGGERED QUALIFICATION APPROACHES

How would this work?

1. Initiate long-term property tests on many candidate materials (you can terminate the tests for the materials that don't pan out)
2. Use the short-term test results, the best available processing information (in-situ process monitoring, advanced characterization), and material simulations to predict long-term properties *with uncertainty*
3. As tests from #1 conclude, updated models in #2 to provide new best estimates and uncertainties

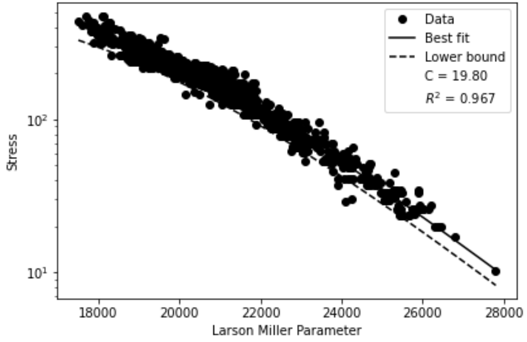
Key questions

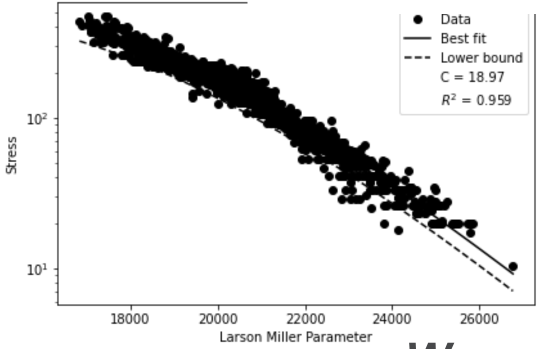
1. Can vendors/designers work like this? You won't have "certain" design data in the beginning and the mean of the property distribution might change.
2. Can regulators work like this? You'll be asked to assess designs with uncertain design data and/or accept designs configured for alterations if long-term testing results change the design assumptions.
3. Can codes and standards bodies work like this? It may require a move towards probabilistic design.

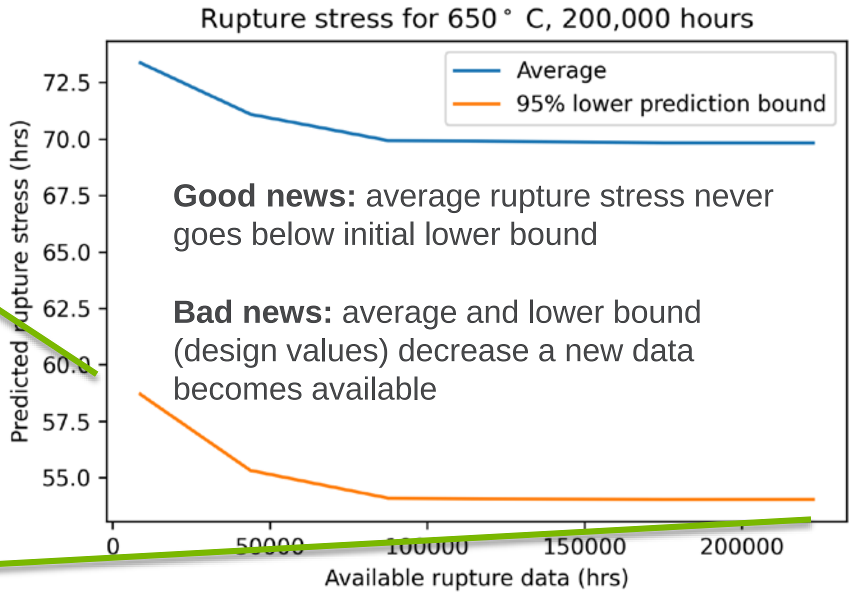


ARE STAGGERED QUALIFICATION APPROACHES FEASIBLE?

"What if" analysis pretending that 316H is a new material. Targets 200,000 hours life because we have actual rupture data for this time







Good news: average rupture stress never goes below initial lower bound

Bad news: average and lower bound (design values) decrease a new data becomes available

We need a better way to quantify uncertainty

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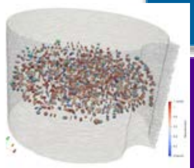
TOOL #3: UNCERTAINTY QUANTIFICATION THROUGH BAYESIAN INFERENCE

Challenges applying staggered, probabilistic approach with conventional modeling:

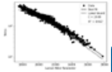
- Mechanisms not present in short-term data!
- Little opportunity to take advantage of improved processing (data stays in database…)
- Doesn't take advantage of all available data to narrow/improve statistical estimates
  - Processing data
  - Microstructural characterization

Physical models have a better chance of accurately capturing long-term properties from short term data

Bayesian inference provides a framework feeding in *incomplete* processing and microstructure information to yield better predictions

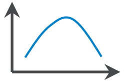


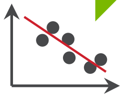
Current process



Available rupture data

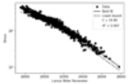
Predicted rupture strength





Empirical model + frequentist statistics

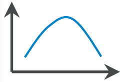
Improved process using microstructure data

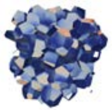


Available rupture data

Processing/ microstructure characterization

Predicted rupture strength





Physical model + Bayesian inference

A HIGH LEVEL DESCRIPTION OF BAYESIAN INFERENCE

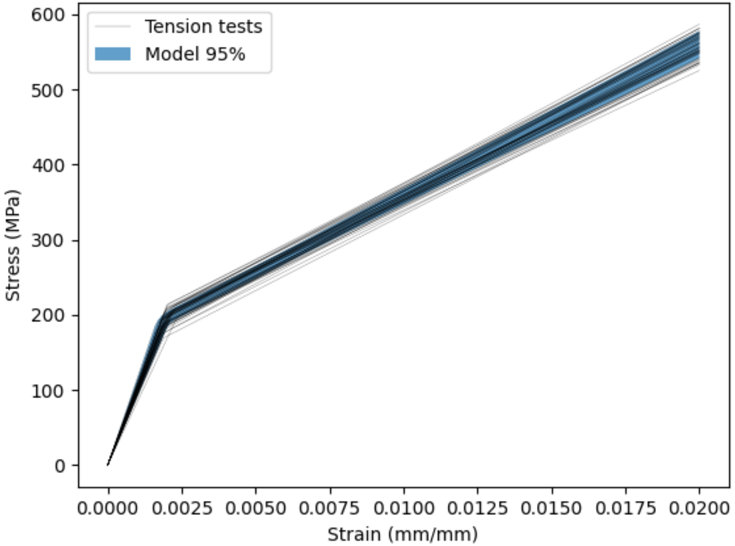
Statistical inference: deduce properties of a underlying probability distribution, often one that is difficult to sample directly

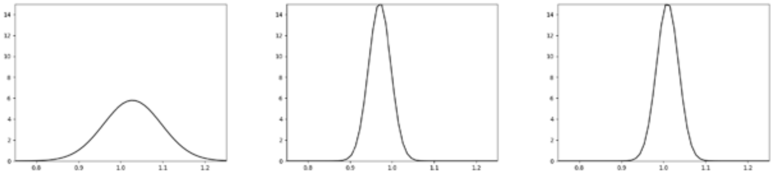
Example:

- Traditional approach: fit a deterministic model to the average response of several tension tests
- Inference: infer the distribution of the model parameters that explains the variation in the test data

Importance:

- Quantify uncertainty in model predictions – not just a predicted material property + a confidence interval, but an understanding of what causes the variation in the property
- A method for understanding microstructural variation from limited characterization data, but lots of high throughput property measurements





Young's modulus Yield stress Hardening modulus

COMBINING INFERENCE WITH PHYSICALLY-BASED MODELS

Linking microstructural statistics to the corresponding material property statistics

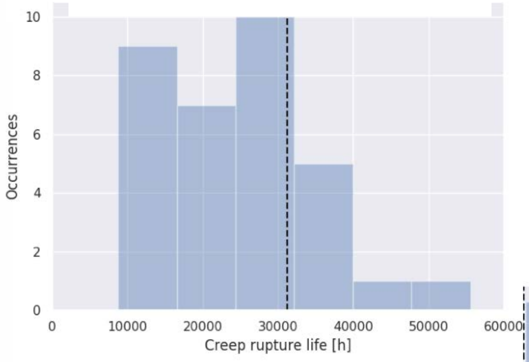
Why?

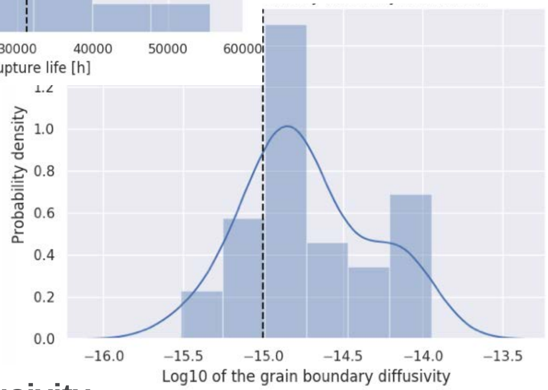
- If we can characterize the microstructure coming out of the process we can translate that directly to (long-term?) property predictions
- We can tune the process (via experimentation or process modeling) to produce better materials

Example

- Back to wrought Grade 91
- Grain boundary diffusivity is a key property controlling rupture life
  - What distribution of GB diffusivity explains distribution of Grade 91 rupture life?
  - How could we control GB diffusivity (via GB energy) to improve the rupture life of the material?

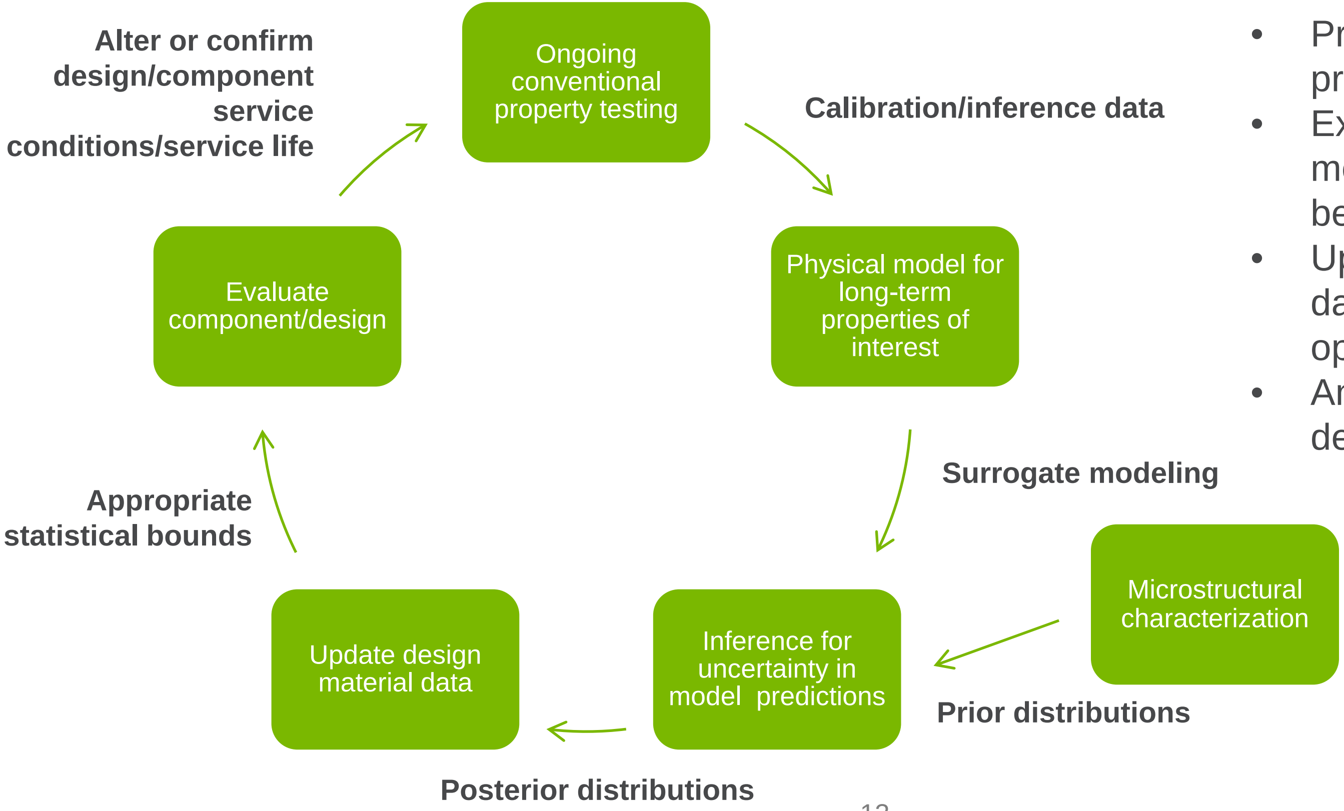
Experimental rupture distribution





Inferred GB diffusivity distribution

ONE ROUTE TOWARDS RAPID QUALIFICATION



- Provides initial, uncertain predictions for initial design
- Extrapolates with physical model, hopefully providing better long-term design data
- Updates design material data to ensure ongoing safe operation
- Amenable to probabilistic design methods

SUMMARY

- **Modeling and simulation can play a role in accelerating the qualification of new AMT materials**
- **Key gaps:**
  - Building regular, owner, and codes/standards confidence in new approaches
  - Benchmark studies to test out rapid qualification approaches
    - Low hanging fruit: try with well-characterized wrought material
    - Round robin benchmarks for nuclear materials + AMTs
  - Improved data-driven methods for material science problems and ways to combine data-driven and physically-based modeling
    - Comparatively sparse datasets
    - Physical constraints on model predictions
  - Better ways to bridge length scales and time scales in multiscale modeling

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