INL/CON-21-61741-Revision-0

# Overview of Nuclear Materials Discovery & Qualification initiative (NMDQi)

March 2021

Changing the World's Energy Future

Robert Allen Roach

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# Overview of Nuclear Materials Discovery & Qualification initiative (NMDQi)

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**March 2021**

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March 2021

R. Allen Roach

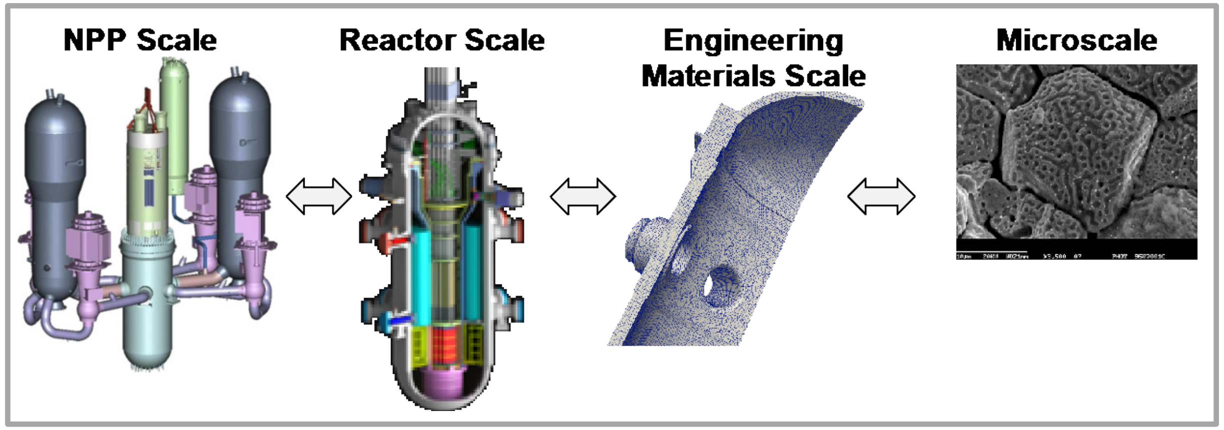
# Overview of Nuclear Materials Discovery & Qualification initiative (NMDQi)

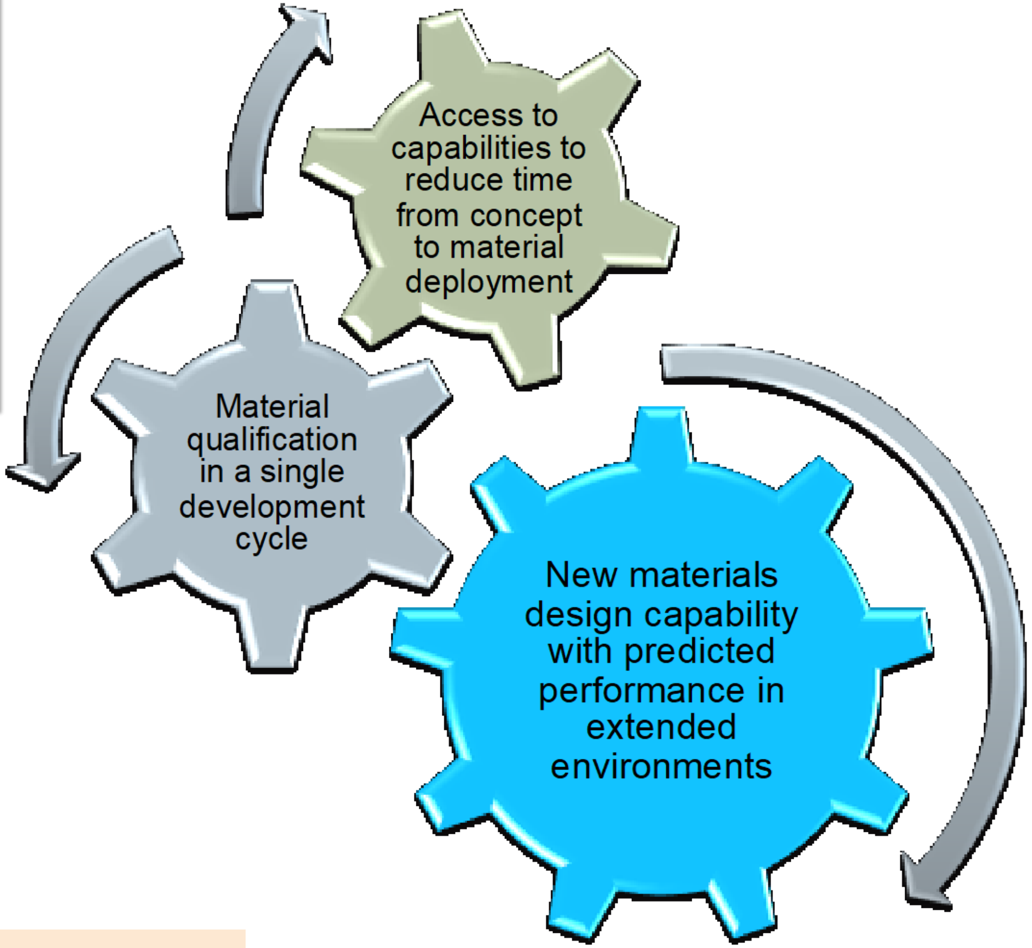
Idaho National Laboratory

NMDQi Nuclear Materials Discovery and Qualification Initiative

**NMDQi takes a Grand Challenge R&D approach to establish the prediction of material performance in their service environment before creation.**

**Allows materials discovery and qualification to become conjoined, accelerating development and qualification of new nuclear materials for future reactor technologies.**




***Ultimate R&D objective is materials-structure-based qualification of new, designed materials***

# Background

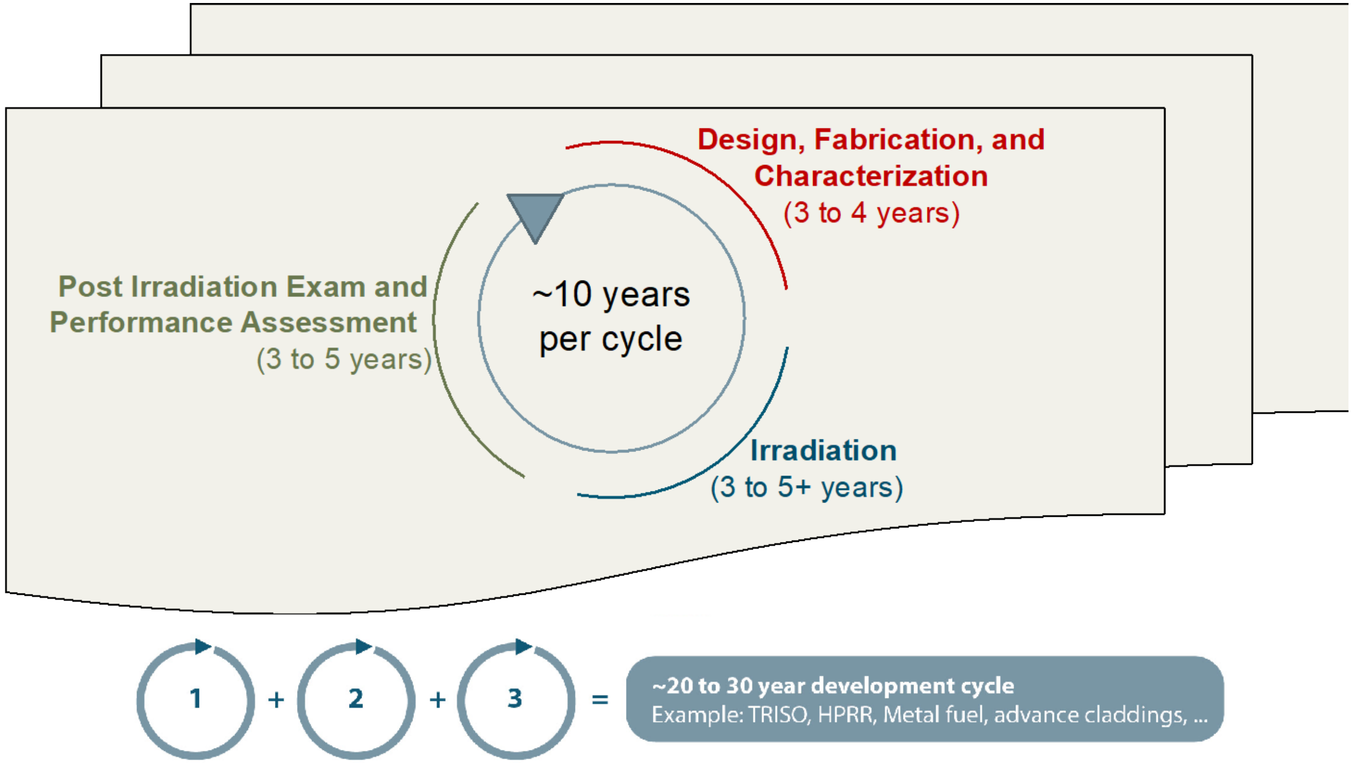
- NMDQi is
  - An Idaho National Lab (INL) Grand Challenge initiated in FY20 that is led out of the INL Nuclear Science & Technology division
  - A program under the DOE NE-5 portfolio with funding initiated in March 2020
- Distinct advantages of being both a program under NE-5 and being an INL Grand Challenge:
  - NE-5 funding allows us to develop new capabilities supporting new materials and rapid qualification
  - As an INL Grand Challenge our goal is identification of technology gaps where proposals can be submitted to the INL LDRD program and other DOE programs

NMDQi Nuclear Materials Discovery and Qualification Initiative

U.S. DEPARTMENT OF ENERGY | Office of NUCLEAR ENERGY

# Background

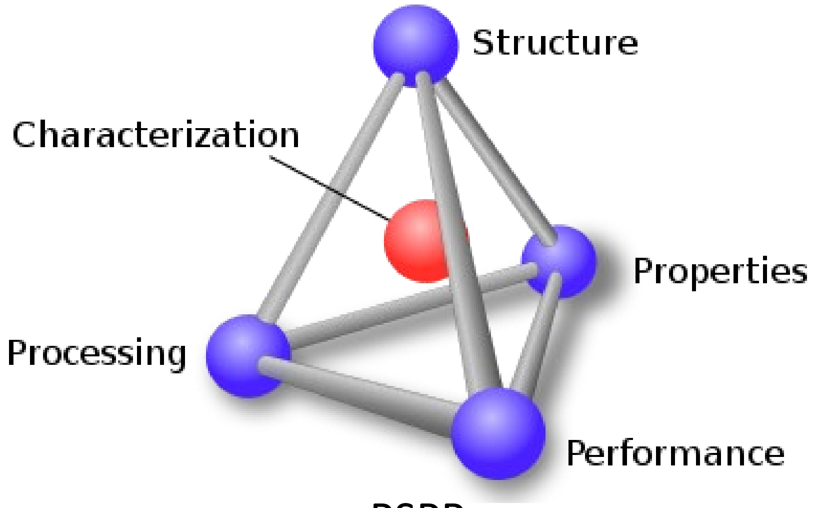
- Time horizons for nuclear materials development and qualification must be shortened dramatically to realize future concepts - Congress mandated demonstrations of advanced reactor technology by 2030
- Nuclear material innovations are needed
  - In-reactor applications for reactor life extension/long-term operation
  - Materials for high temperature advanced reactor applications
  - Increased need for materials qualification and assessment programs
- Advanced materials, such as HEAs or MPEAs, can provide material performance previously unavailable to reactor designers




***Can we qualify materials designed for use in advanced reactors in a single development cycle?***

# Begin with Materials

- Traditional material qualification is an iterative process during the fabrication of a material to create a material that gives desired properties and performance required for qualification
- Materials Genome Initiative (MGI) (https://www.mgi.gov)
  - "discover, manufacture, and deploy advanced materials twice as fast, at a fraction of the cost"
  - MGI does not include nuclear materials or irradiation effects
  - MGI Focus for capability development: tightly integrating computation, experiment, and data management to accelerate materials discovery and design
- Can we reverse-solve material design to determine the structure required to meet performance requirements = ***materials-structure-based qualification of new, designed materials?***

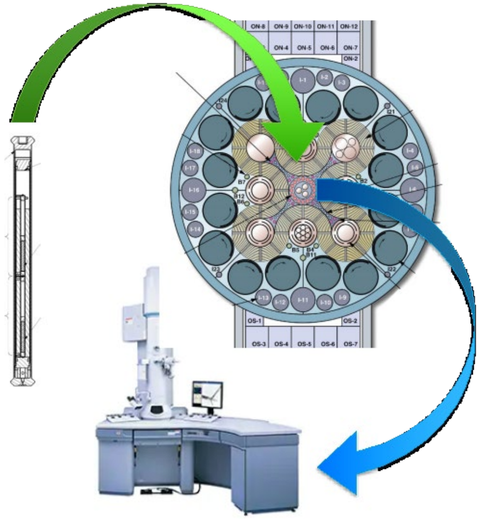


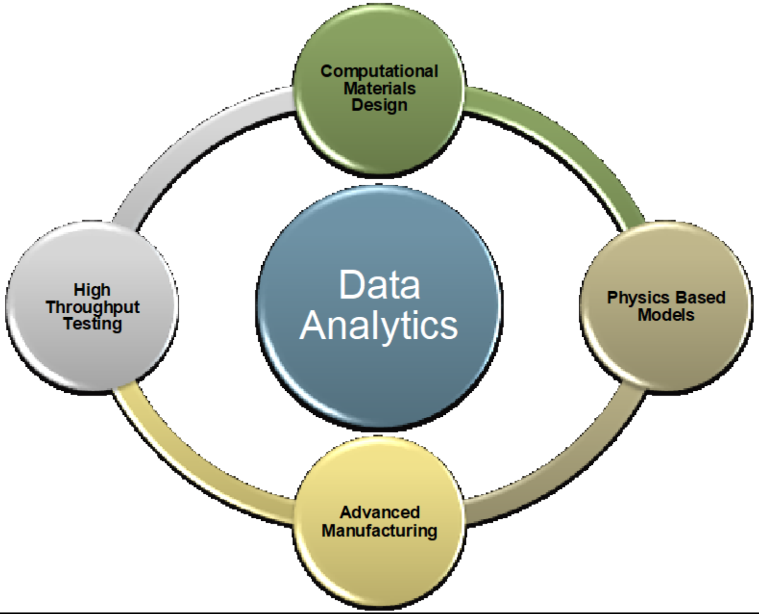

PSPP
(Process-Structure-Properties-Performance)

NMDQi Nuclear Materials Discovery and Qualification Initiative

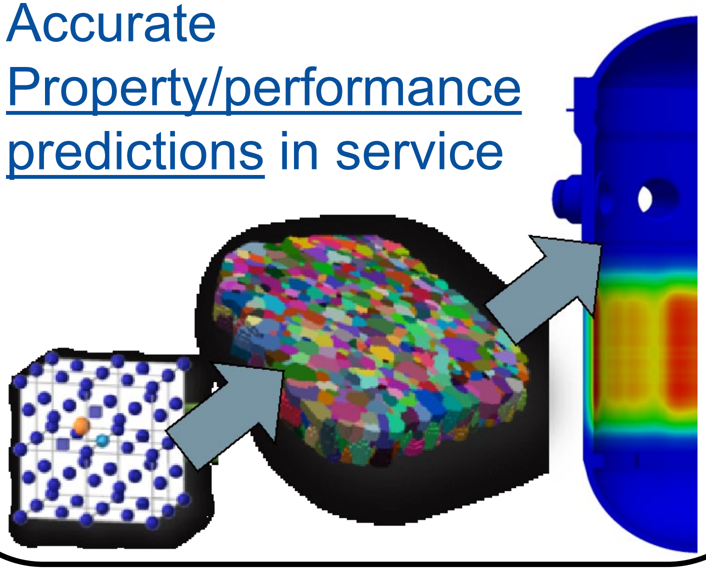
For nuclear energy applications, environmental conditions must be correlated to materials’ evolution and degradation in service

Physics-based modeling and rapid testing & characterization links microstructures & service conditions to properties

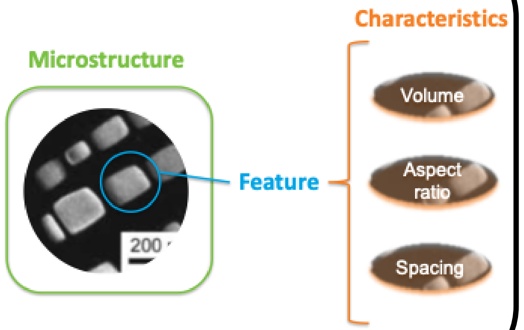





Accurate Property/performance predictions in service

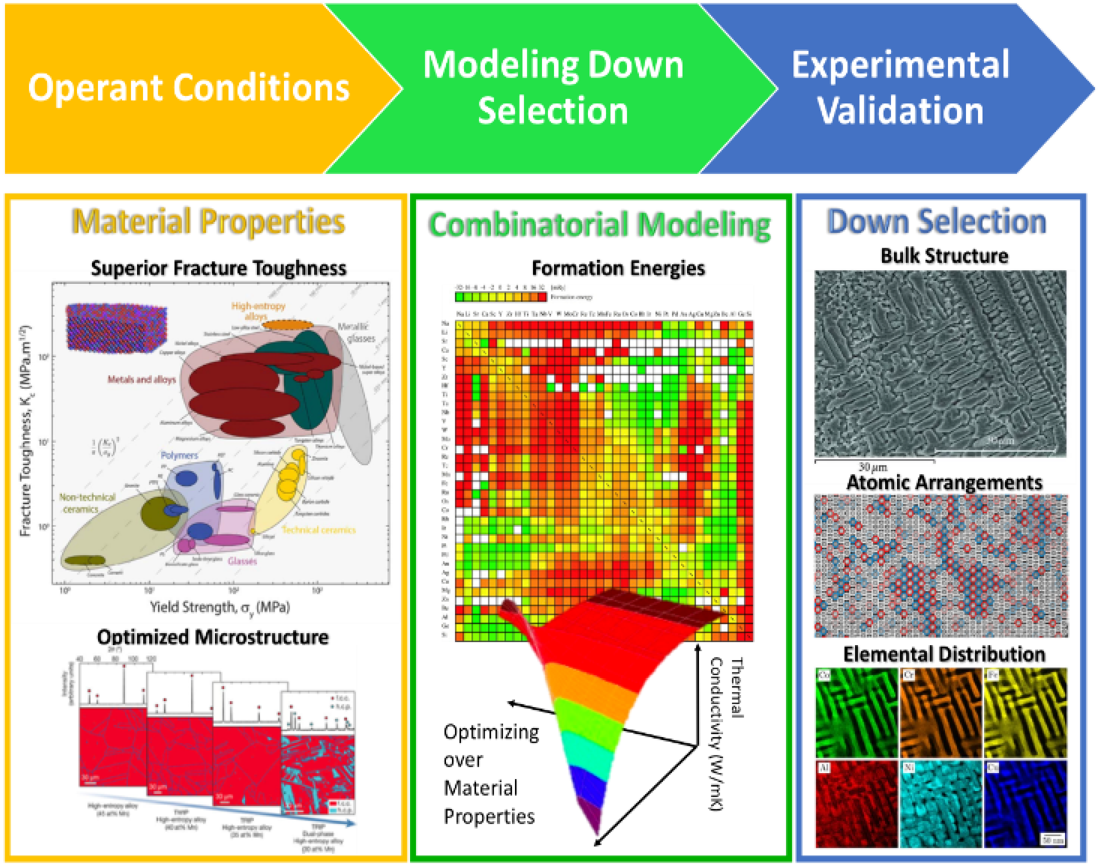


Machine learning to harness data in new ways for improved physics-based predictions



# Materials Design

## *Supports new materials and pipeline development for high-throughput methods*




1. Huang, Jen-Ching. *Scanning*, 2012, **34**, 325-31.
2. Z. Li,K. Pradeep, Y. Deng, D. Raabe, and C.C., *Nature*, 2016, **534**, 227–230.

Comput. Sci. Discov, 2009, **2**, 015006

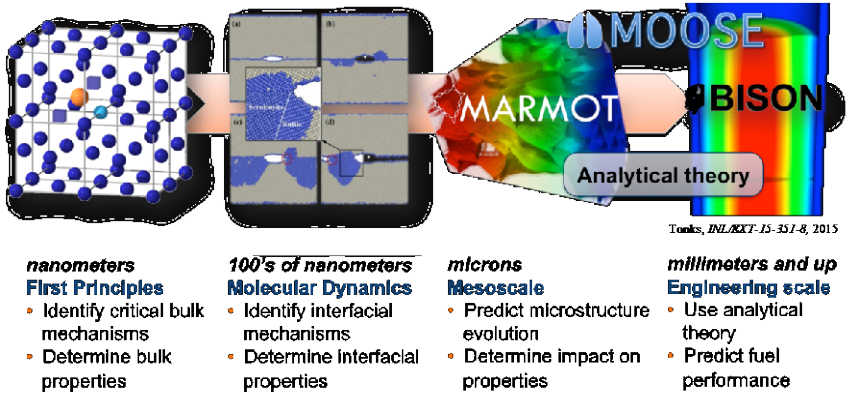
https://www.rrutc.msm.cam.ac.uk/research-themes/high-entropy-alloys

- **Targeting** discovery of new alloy classes that are high strength, chemically compatible, and radiation resistant above 400 °C
- **Incorporating** modeling and experimental results in the same workflows to enable training, evaluation, and deployment
- **Establishing** frameworks to shorten the nuclear materials development and research cycle

***Physics-informed combinatorial approach for accelerated materials development***

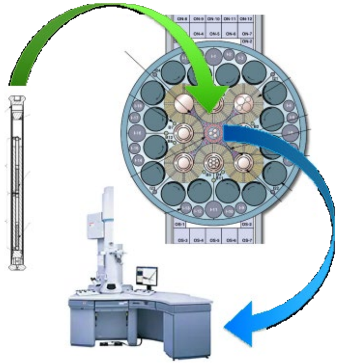
# FY21 Plans for Physics Models and Data Analytics

- Focus: Incorporate physics-based models and machine learning capability for a new paradigm of PSPP predictions to predict material performance in advanced reactors
- Demonstrate stochastic tool module within MOOSE supporting integration of high-throughput data from experiments to reliably represent important material features

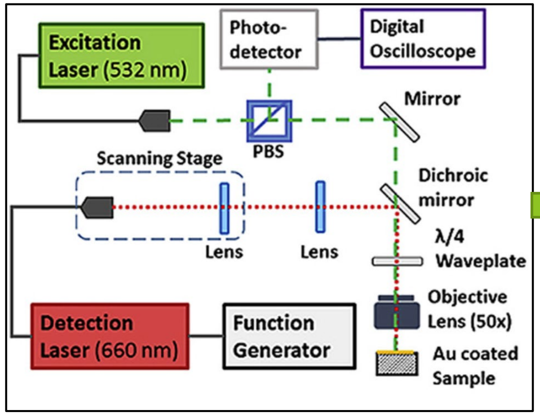


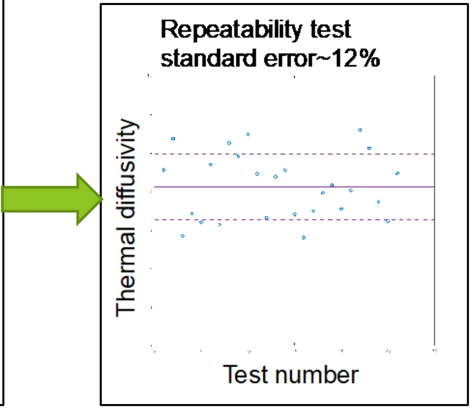

- Develop capability to solve "inverse problem": optimizing properties in computational domain to obtain given boundary conditions - for example, back-calculate thermal properties from temperature data
- Enhance MOOSE crystal plasticity capability to support high fidelity models of dislocation-driven and creep-driven deformation
- Develop modern machine-learning tool for use with database of high-throughput DFT simulations to target energetics of different defect structures for property prediction of irradiated materials
- Demonstrate Magpie + phase field for a real materials system with focus on recombination from the initial radiation damage event

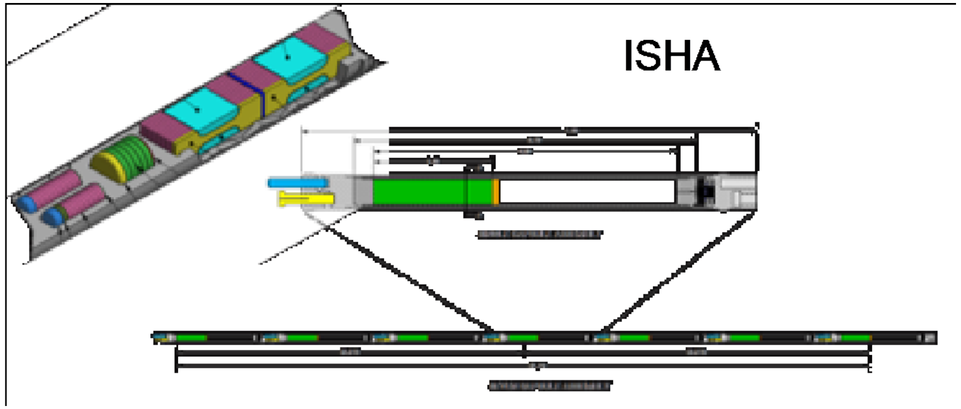
# FY21 Plans for Rapid Testing and Characterization



- Focus: High throughput testing and irradiated materials characterization capabilities to support our data analytics and machine learning efforts
- Capability for using continuous wave laser spectroscopy methods within microscopy tools to couple microstructure and chemical analysis with thermal-mechanical properties
- Develop ISHA capsule as a drop-in capsule with bounding safety design to accommodate multiple materials systems (both fissile and non-fissile materials) with goal to make future irradiation planning faster, cheaper, and with less administrative burdens



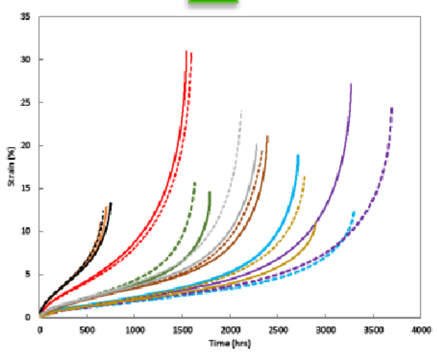



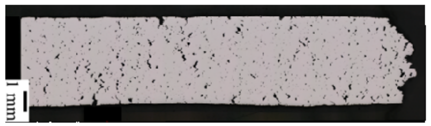



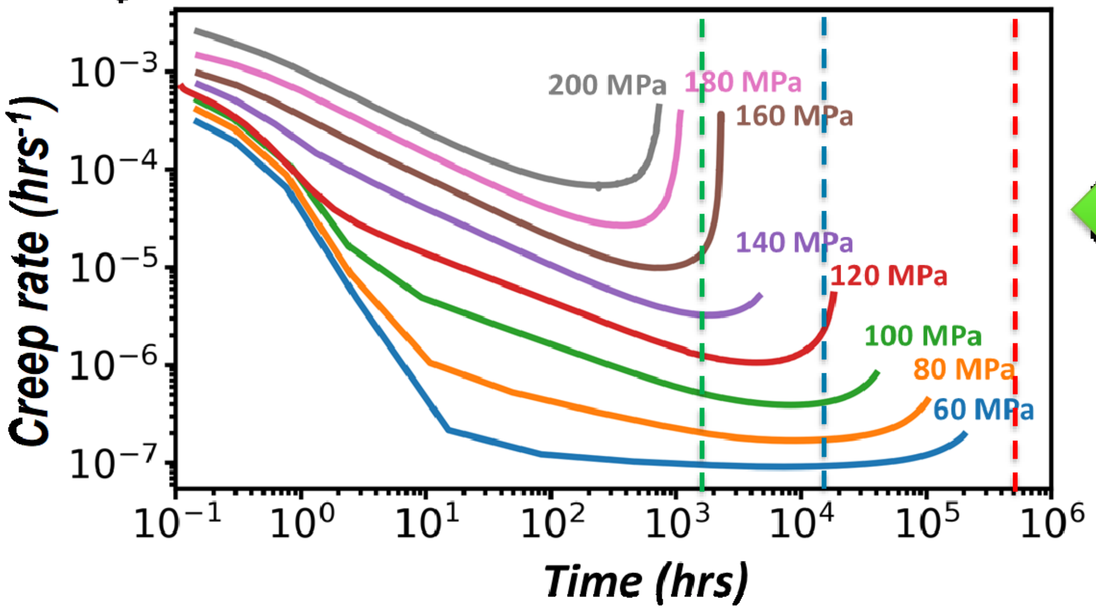
# FY21 Plans for Rapid Qualification

Focus: Strategy development for how to approach and scope a new qualification paradigm for materials in advanced reactors using enabling physics-based modeling, data analytics, high-throughput testing and characterization

Experimental validation for 1, 10, 30 year design life

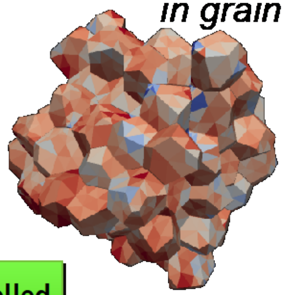


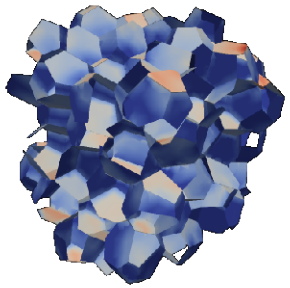





Long term modelled design properties

*Effective stress in grain bulk*



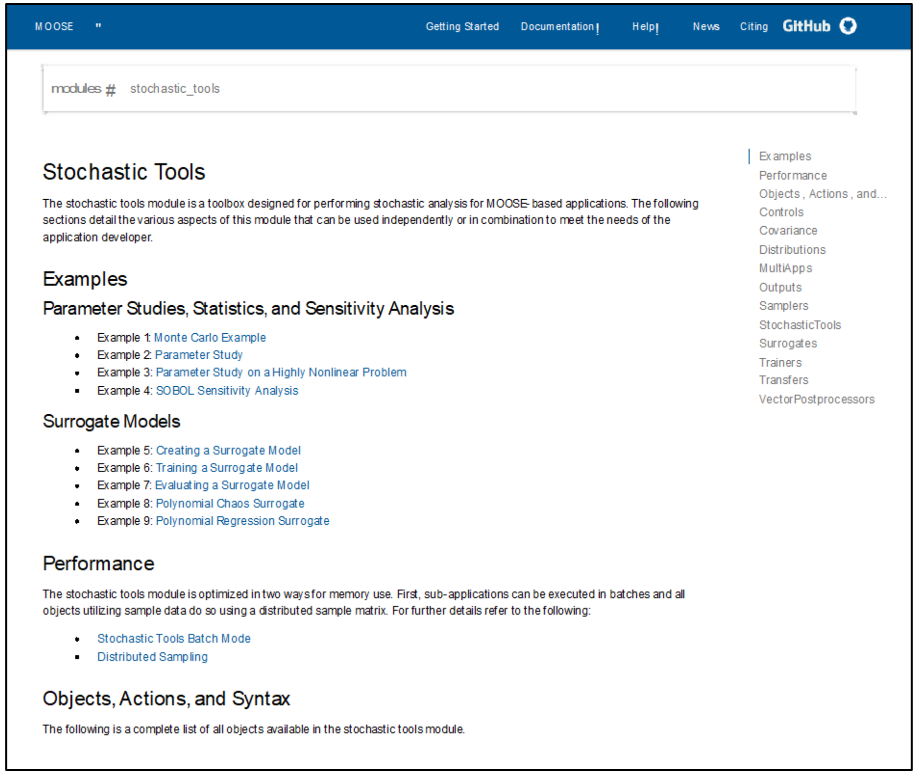


*Creep cavity density on grain boundaries*

***Staggered qualification for structural materials: begin with materials outside the reactor first then apply to irradiated materials***

# FY20/21 Highlights

- First-generation data analysis framework (MOOSE compatible Data Analytics Framework)



MOOSE Getting Started Documentation Help News Citing GitHub

modules # stochastic_tools

## Stochastic Tools

The stochastic tools module is a toolbox designed for performing stochastic analysis for MOOSE-based applications. The following sections detail the various aspects of this module that can be used independently or in combination to meet the needs of the application developer.

### Examples

#### Parameter Studies, Statistics, and Sensitivity Analysis

- Example 1: Monte Carlo Example
- Example 2: Parameter Study
- Example 3: Parameter Study on a Highly Nonlinear Problem
- Example 4: SOBOL Sensitivity Analysis

#### Surrogate Models

- Example 5: Creating a Surrogate Model
- Example 6: Training a Surrogate Model
- Example 7: Evaluating a Surrogate Model
- Example 8: Polynomial Chaos Surrogate
- Example 9: Polynomial Regression Surrogate

### Performance

The stochastic tools module is optimized in two ways for memory use. First, sub-applications can be executed in batches and all objects utilizing sample data do so using a distributed sample matrix. For further details refer to the following:

- Stochastic Tools Batch Mode
- Distributed Sampling

### Objects, Actions, and Syntax

The following is a complete list of all objects available in the stochastic tools module.

Examples
Performance
Objects, Actions, and...
Controls
Covariance
Distributions
MultiApps
Outputs
Samplers
StochasticTools
Surrogates
Trainers
Transfers
VectorPostprocessors

- Parameter Studies
  - Compute affect of perturbations on quantities of interest
  - Example- vary diffusivity, heat flux input, initial temperature then compute resulting average temperature distribution and out-going heat-flux
- Surrogate/Reduced-Order Modeling
  - Perturbations of input parameters and create a simple/fast model for quantities of interest
  - Current models so far: polynomial regression, polynomial chaos expansion, proper orthogonal decomposition (limited), Gaussian process regression

# FY20/21 Highlights

- Vision Setting

INL/EXT-20-57732
Revision 0

**Nuclear Materials Discovery and Qualification Initiative**

Idaho National Laboratory
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http://www.inl.gov
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U.S. Department of Energy
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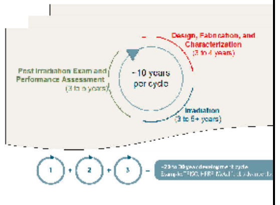
Under DOE Idaho Operations Office
Contract DE-AC07-05ID14517

Advanced Manufacturing/Fuel Special Section

## Helping to bring a new generation of reactors to life

*The goal of the DOE's Nuclear Materials Di… Qualification Initiative is to bring new materials f… nuclear reactor designs to market quicker and at …*

*By Joel Hiller*




The current development cycle for nuclear materials.



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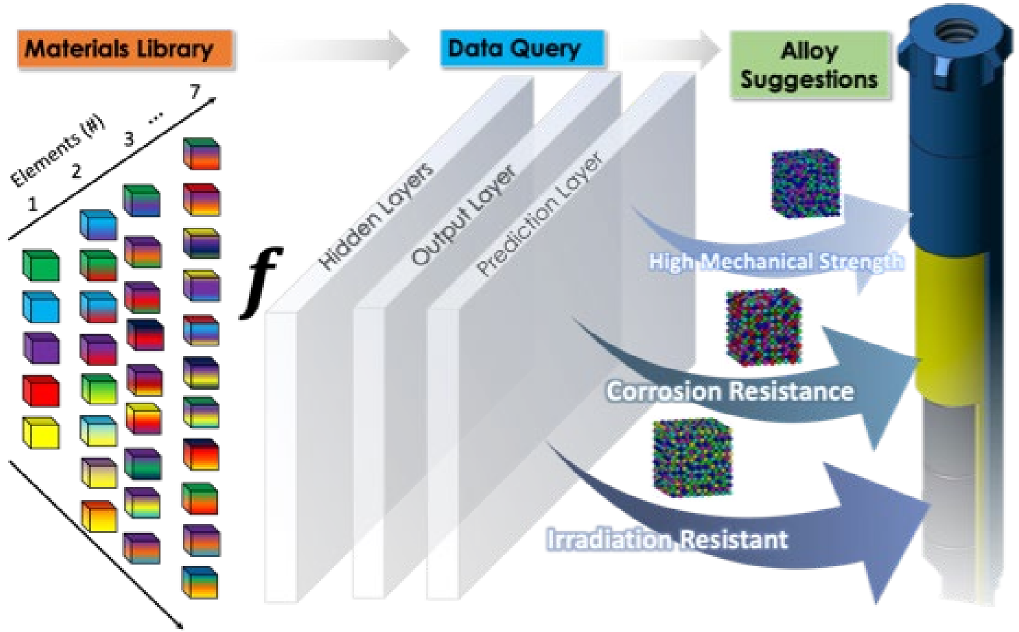
# Future Outcomes

- Development and demonstration of new methods, approaches, techniques, & tools for accelerating development and qualification of new materials
- Establishing rapid qualification capability that is materials-structure-based and grounded in science
- High throughput irradiation and characterization capabilities - refitting new capabilities into existing facilities and obtaining multimodal data from individual samples
- Establishing combinatorial approach to shorten the nuclear materials development and research cycle by integrating physics-based modeling, data analytics, and rapid experimental frameworks



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