INL/MIS-20-59663-Revision-0

Finite Element Method Simulation Portion of eXtremeMAT:Modeling and Simulation Thrust-2: Surrogate Modeling Approach and Finite Element Simulations

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Changing the World's Energy Future

Idaho National Laboratory

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Finite Element Method Simulations

Develop and prototype implementations of component level FEM element simulations:

1. Successfully integrated the surrogate model into to FEM solvers
2. Demonstrated capture of transient loading response of a component part enabled through the preserved connection to microstructure, where driving physics occur
3. Rapidly responded to stakeholder interest in specific simulation capabilities with prototype demonstrations

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Verifies FEM Infrastructure

- Develop and verify the FEM implementation and infrastructure with a staggered approach
- Microstructure connection from surrogate model results in component level sensitivity

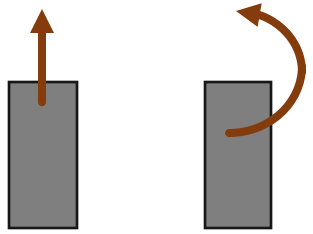
Evaluate FEM for physical response

Increasing problem complexity

Sensitivity to variations in applied **pressure**

Temperature variation effect in simulations

Response to **multiaxial** mechanical loads



Microstructure variations and gradients impact

Capture of **cyclic loading** history influence

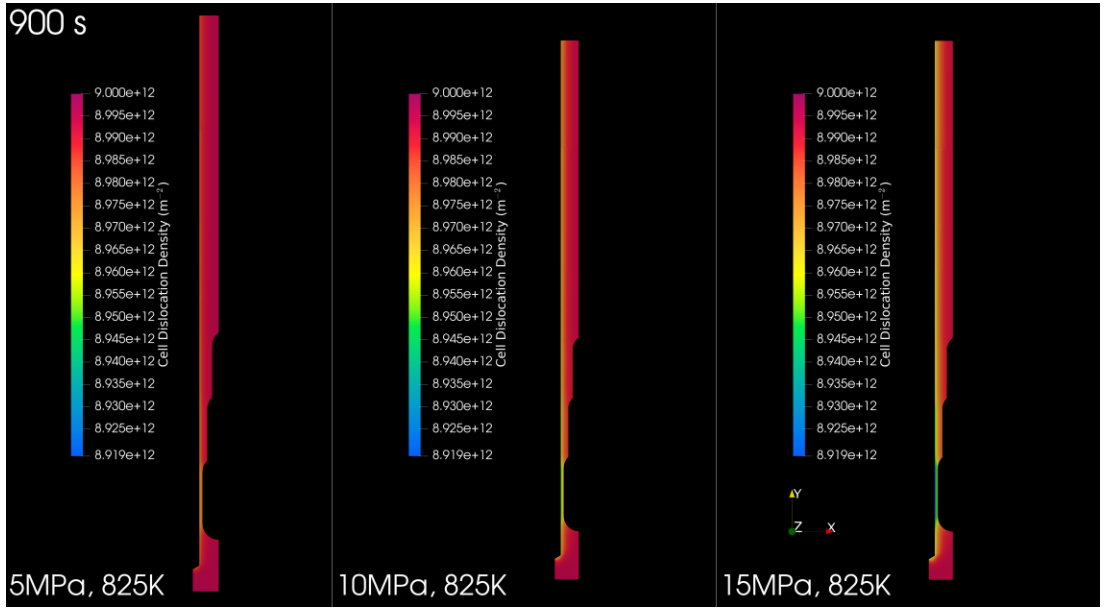
Engage industry with advancement over traditional engineering scale FEM models

Performs with Multiaxial Loads

Demonstrate initial implementation of the 316H surrogate model into an FEM solver with a series of simulations of the stepped pressurized tube geometry designed by ORNL

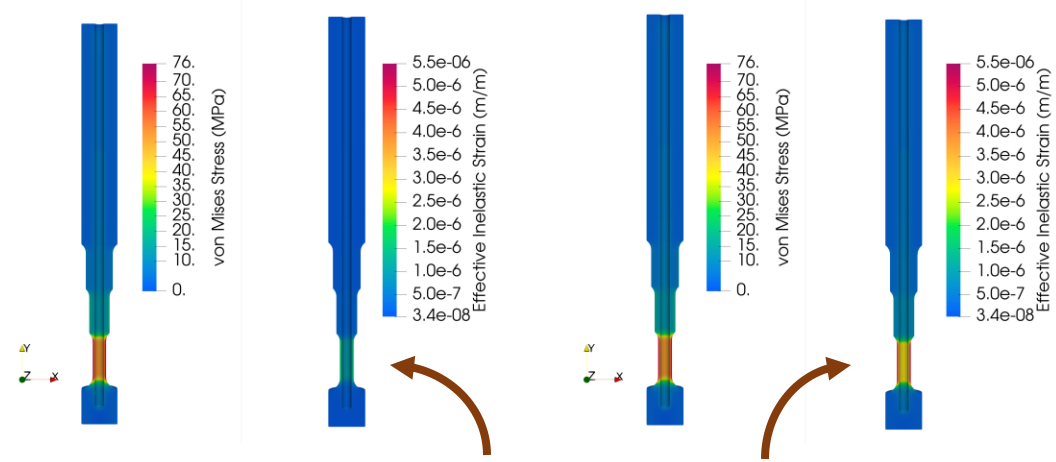
- Identify and correct initial robustness issues with integration, in cooperation with LANL
- Verification will be performed with the complex geometry and loading, and will freeze parameters

Initial Cell Density 9e12, Various Constant Pressure Loads



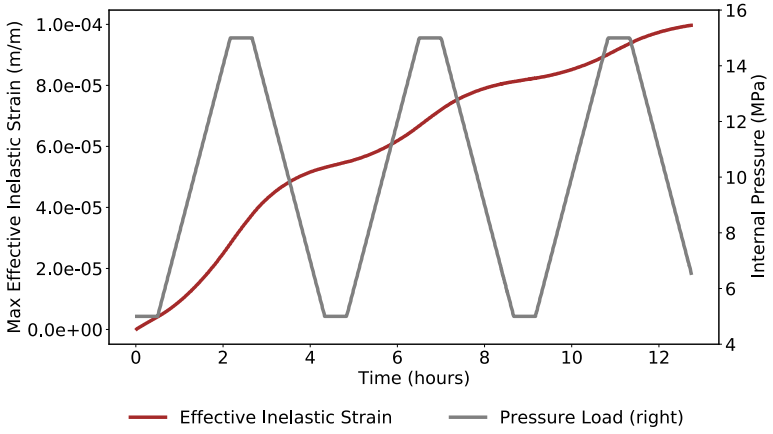
Initial Cell Density 8e12, Torsion Load

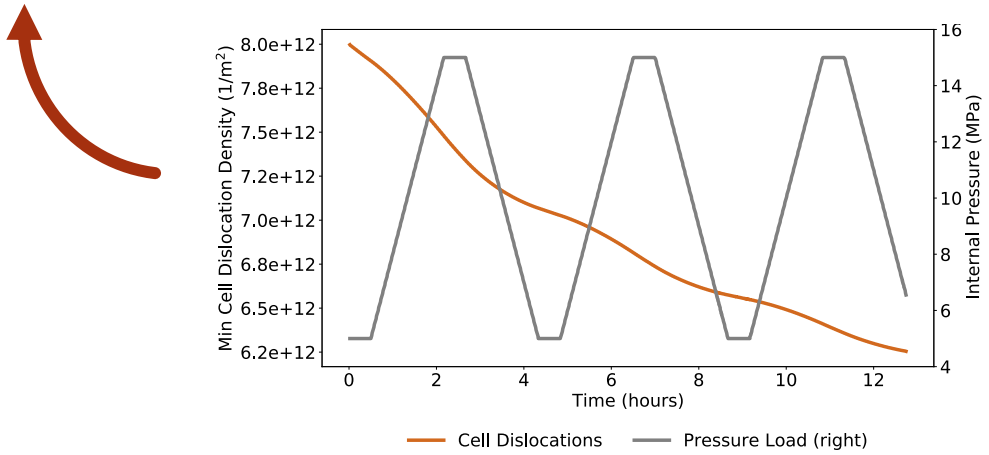
Initial Cell Density 9e12, Torsion Load

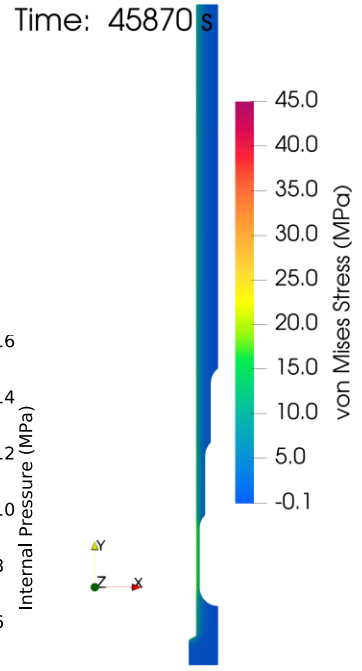


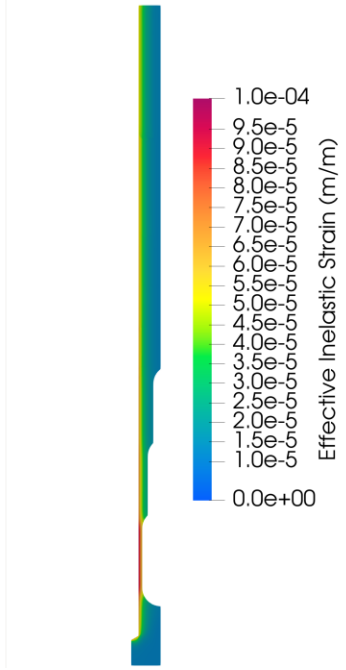
Impact of the initial microstructure is propagated to the component level simulation by the surrogate model, consistent with expected physics

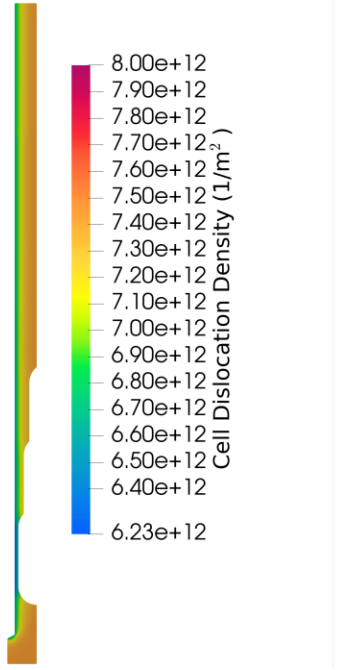
Captures Cyclic Pressure Effect

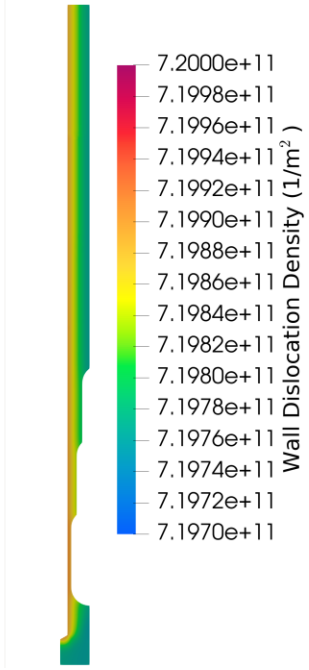








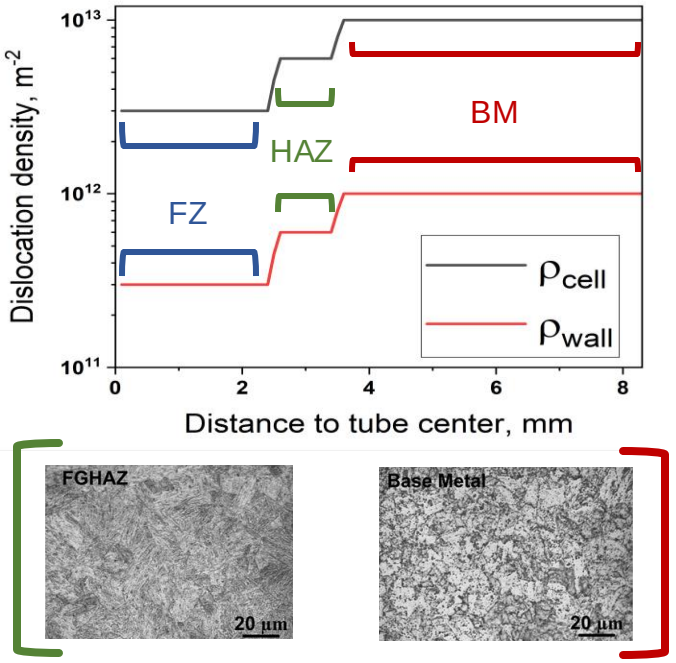




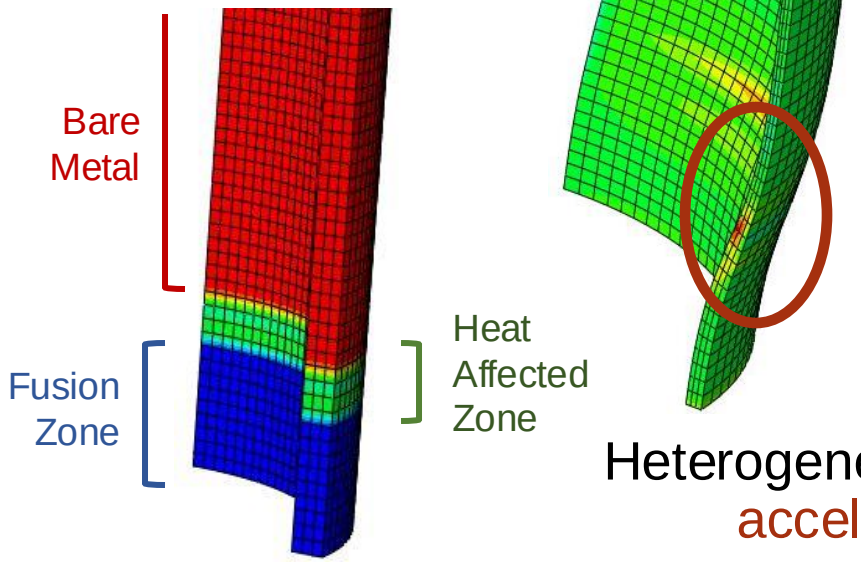
Successful capture of loading history and rate on the component part behavior is enabled by the inclusion of microstructure characteristics such as the dislocation evolution

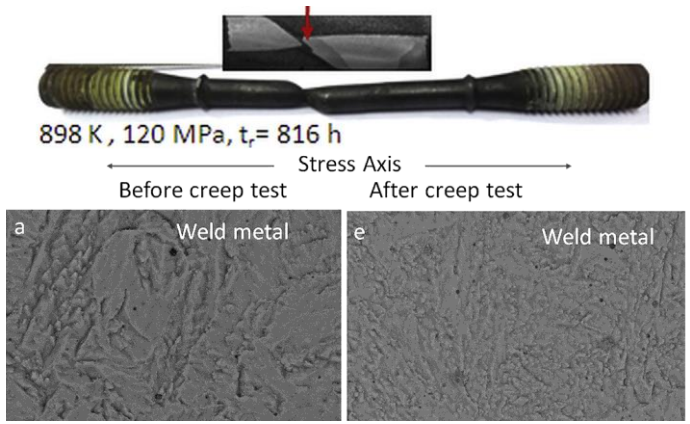
Stakeholder Interest Focused

- Idealized weld problem to demonstrate the influence of microstructure gradients on the component level strain behavior in rapid response to stakeholder inquiry
  - Lessons learned with the MOOSE development efforts aid integration into additional FEM solvers
- Two cases: a) constant internal pressure and temperature, b) cyclic loads (1day cycles), for a year
  - Simulations performed with two different surrogate models: 316H (austenitic steel) and P91 (ferritic steel)



Pandey et al., Arch Civil Mech Eng, 19 (2019) 297-310

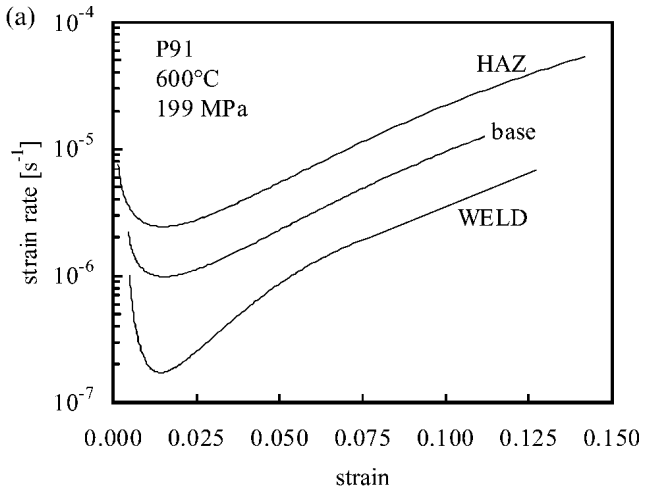




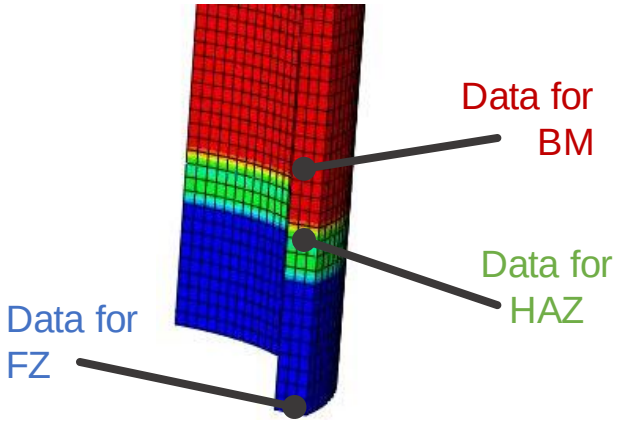
Baral et al., J Nuclear Mater, 490 (2017) 333-343

Heterogeneous microstructure demonstrates accelerated deformation near the weld, consistent with experiments

Qualitatively Response Aligns

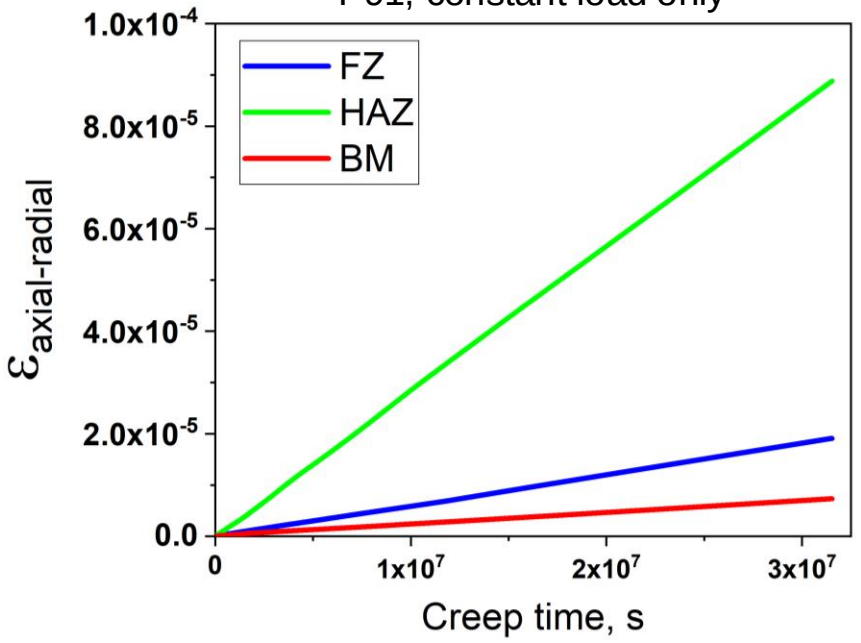


Spigarelli and Quadrini, Mater Design, 23(2002)547-552

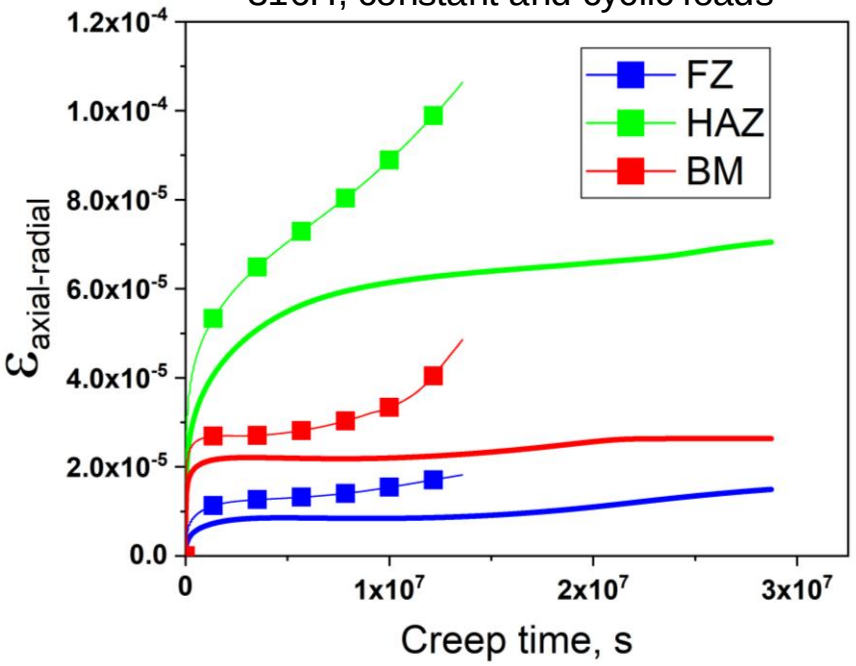


- Prediction of the HAZ as the region experiencing the highest strain is consistent with experimental data despite short timeframe

P91, constant load only



316H, constant and cyclic loads

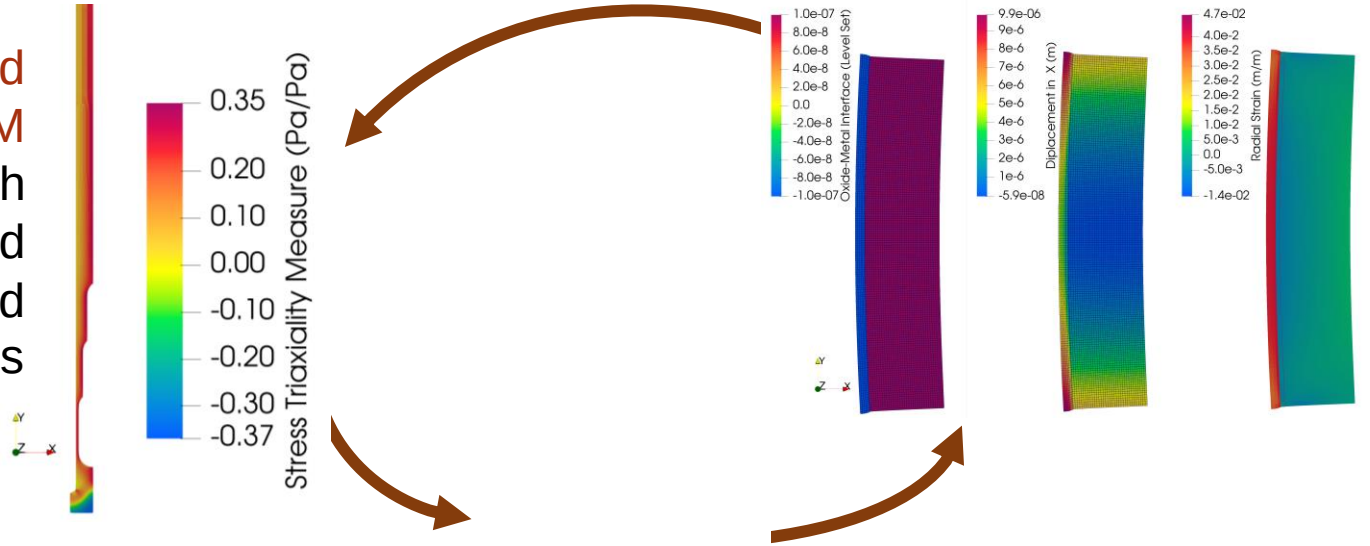


Dynamic recovery and the availability of cell dislocations, captured by the surrogate model, enable transient response simulations

Summary and Next Steps

- Demonstrated the FEM implementation through multiple problems, with rapid response to industry
- Successfully integrated surrogate model-FEM framework results for transient loading conditions qualitatively agree with physical observations

Validate the integrated surrogate model-FEM against experiments with set parameters, and apply identified corrections



Extend framework to model the mechanical aspects of oxide spallation and creep damage

Engage industry with a vision of tailor-made lifetime predictions for components and structures, validated with carefully designed experiments