HPC 4 MATERIALS

National Laboratories Partner with U.S. Industry: HPC4Materials

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U.S. DEPARTMENT OF ENERGY Energy Efficiency & Renewable Energy

U.S. DEPARTMENT OF ENERGY Office of Fossil Energy

U.S. DEPARTMENT OF ENERGY Office of Science

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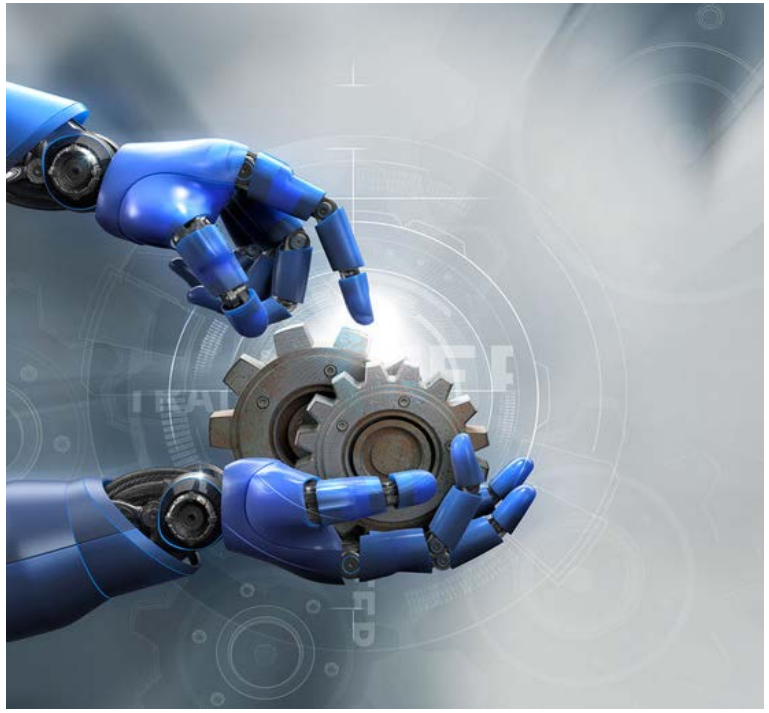
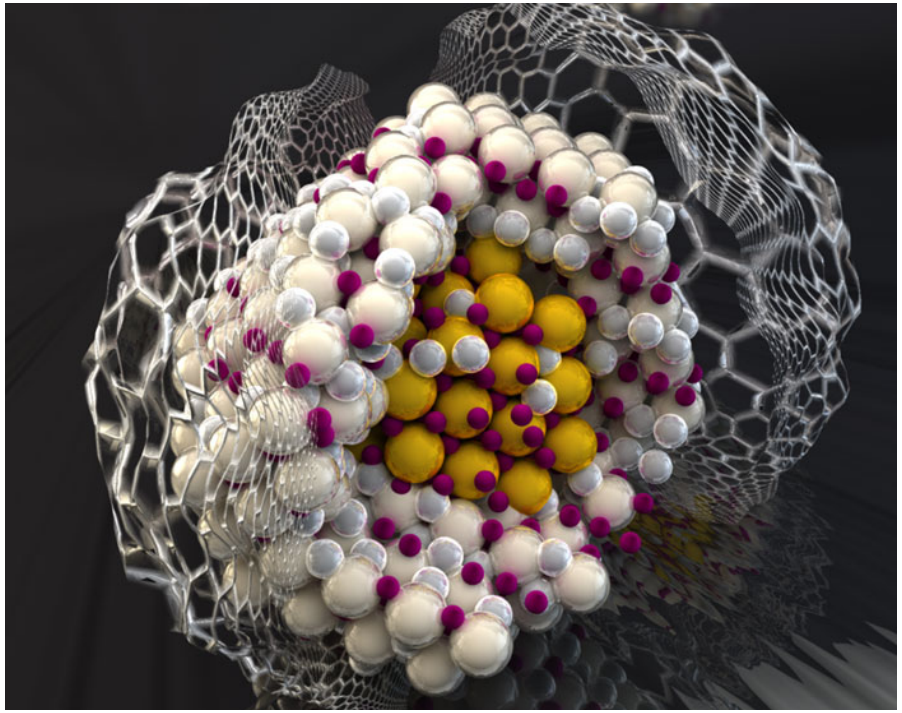
U.S. industry is undergoing a technological revolution



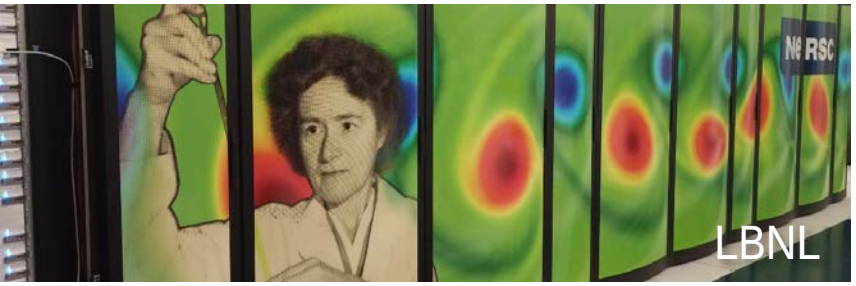
Computer Simulation — Data Analytics/AI — Material Discovery

Advance energy agenda through advanced simulation

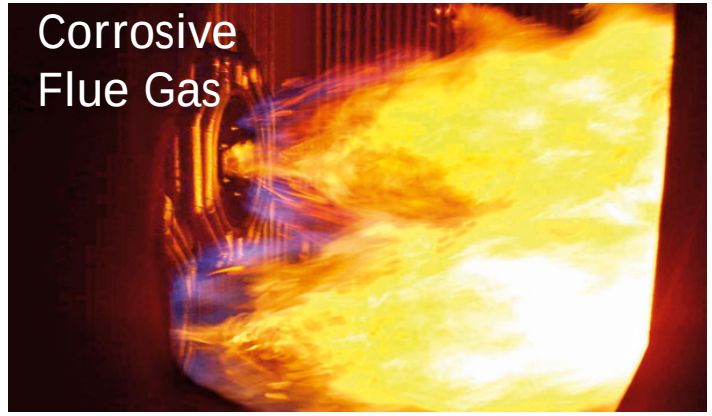


Computer Simulation — Data Analytics/AI — Material Discovery

Labs partner with industry to lower risk of High Performance Computing (HPC) adoption



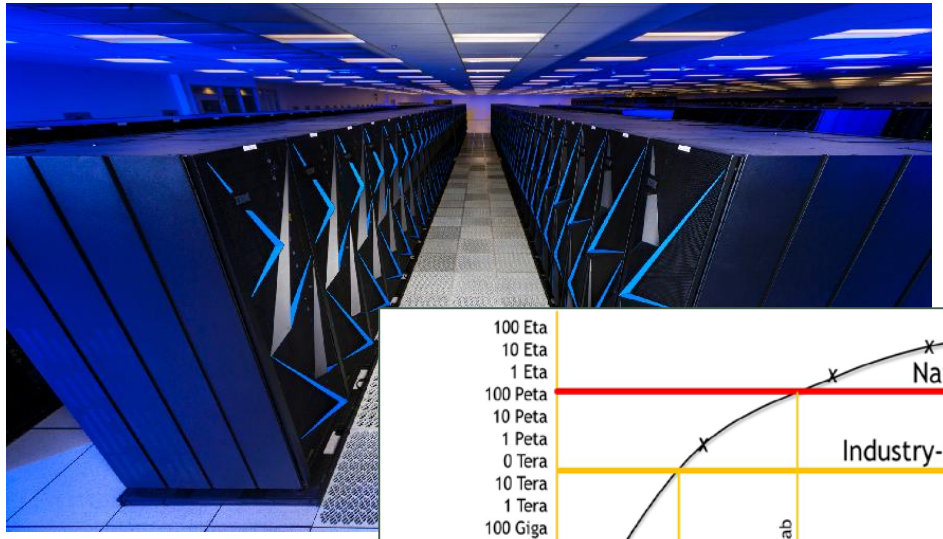
- Data analytics
- Larger, Faster Simulation
- Algorithm Development
- Computational Material Design

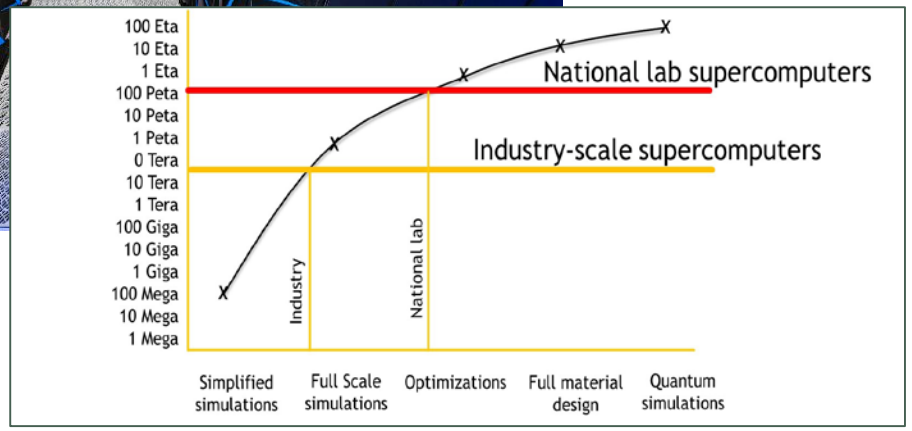


National laboratories impact industry in materials for fossil fuel

Value proposition to industry and government

HPC Computers





Multiscale Multiphysics Modeling and Simulation

ENABLE

- Optimization
- Accurate physics
- AI data analytics
- New material discovery

Industry lags national laboratories in HPC capability

Value proposition to industry and government

ENABLE

Advanced products

- Shorter time to market
- Better quality

Improved process

- Higher yield
- Less material/energy

ENABLE

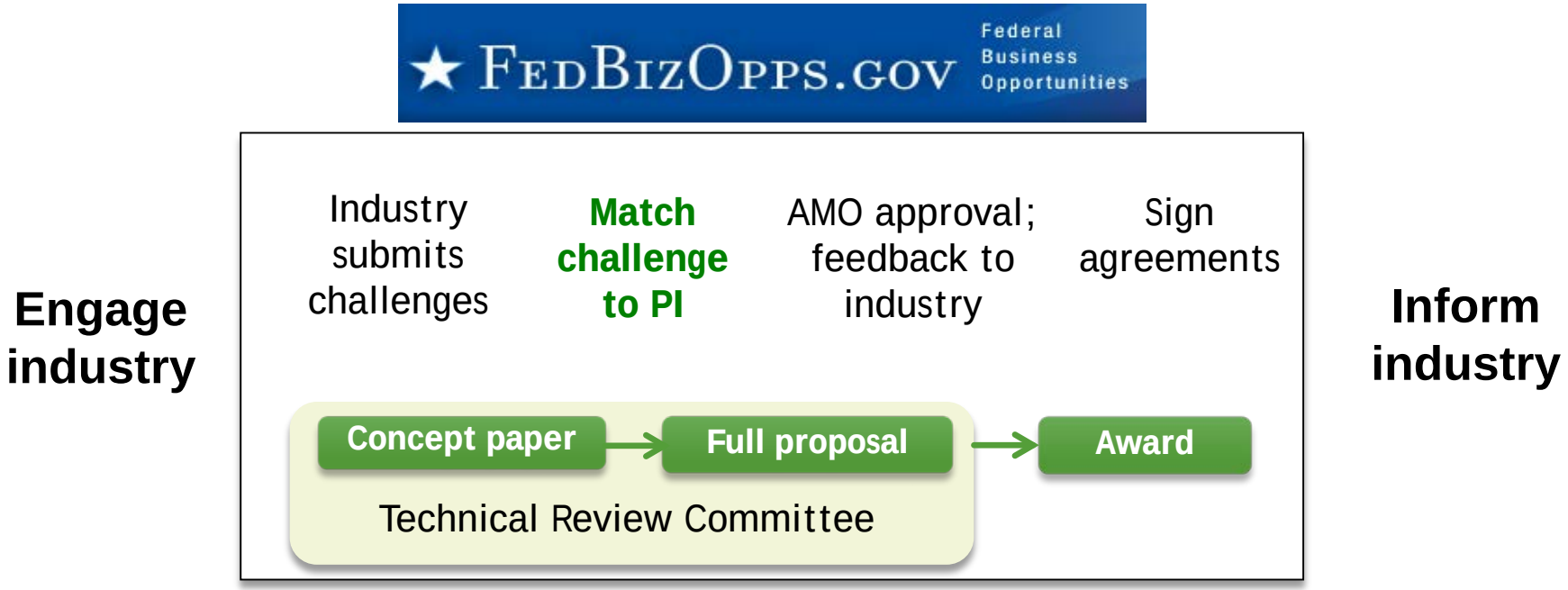
Benefits

- Energy reduction
- Higher profits
- Better jobs

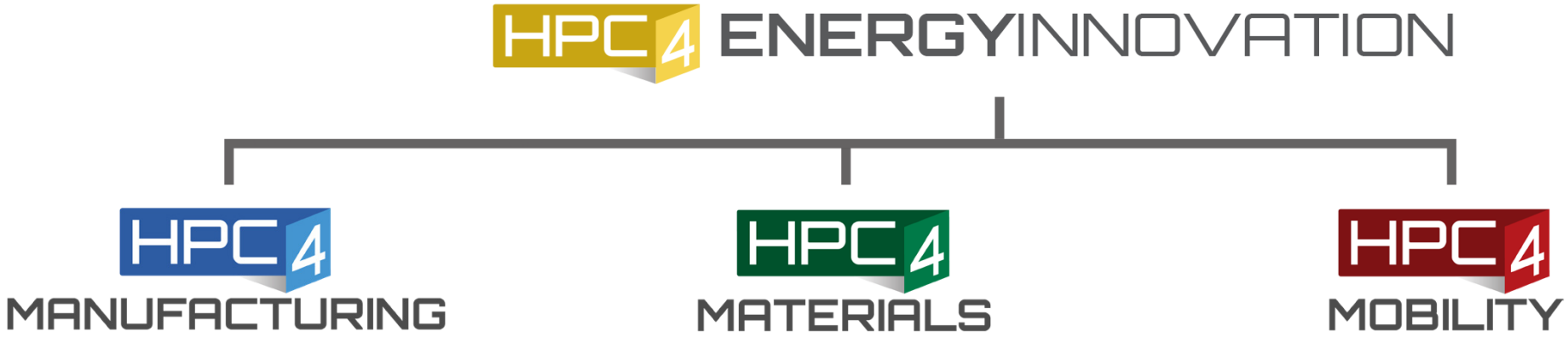
In a 2015 study, IDC estimated >$500 return on investment for each dollar spent on HPC

Program Approach

Companies apply to program through a solicitation process



HPC4MtIs is part of a growing HPC4EnergyInnovation umbrella



Over 70 projects have been funded in the overall program

Seven projects have been funded by FE in the HPC4Mtls portfolio

- First-principle material evolution (kinetics; microstructure)
  - **Arconic** : Solidification kinetics in additively manufactured materials
  - **UTRC** : Hot corrosion kinetics
  - **Siemens** : Crack growth from forging flaws
  - **Pratt and Whitney** : microstructure of abradable coatings on rotor tips
- Understanding of operational environment effects on materials
  - **Vacuum process** : Fatigue in cyclical, high temperature heat exchangers
  - **SPS** : Apply machine learning to plant operations to predict component lifetimes
  - **SPS** : Analyze plant data to identify components and conditions of failure and model fatigue failure

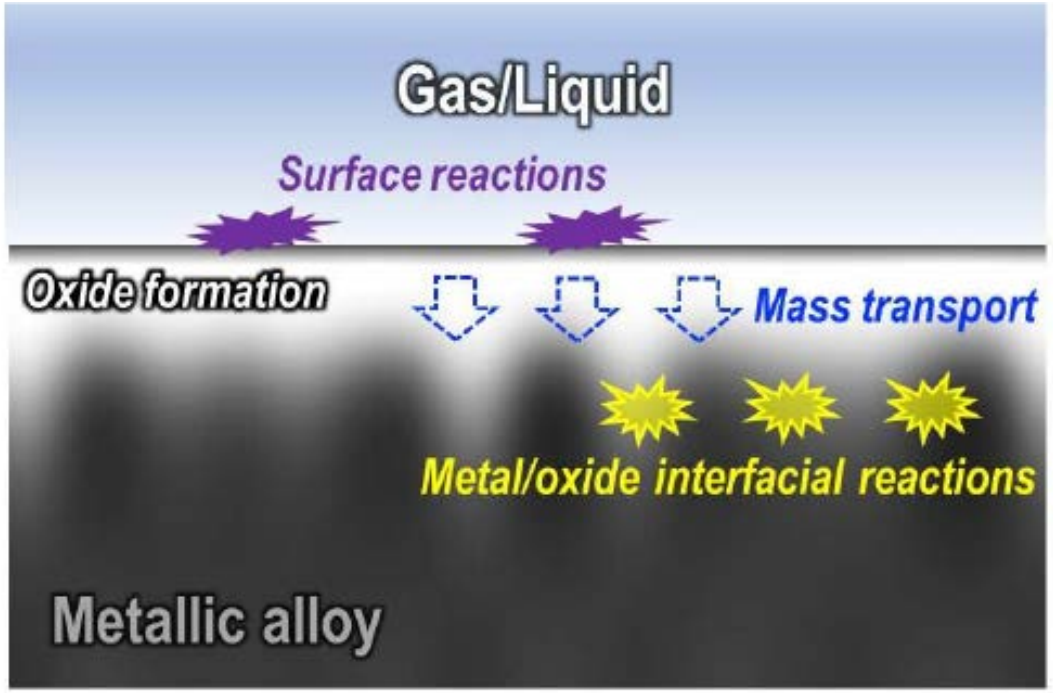
Corrosion-resistant materials for cyclical, high temperature environments

Multiscale Modeling of Microstructure Evolution During Rapid Solidification for Additive Manufacturing, Arconic/LLNL,ORNL

- Molecular dynamics (MD) simulations of kinetics at grain interfaces to better determine grain size, morphology, composition during rapid solidification
- HPC needed for MD to microstructure multi-scale models

More accurate microstructure prediction during rapid solidification

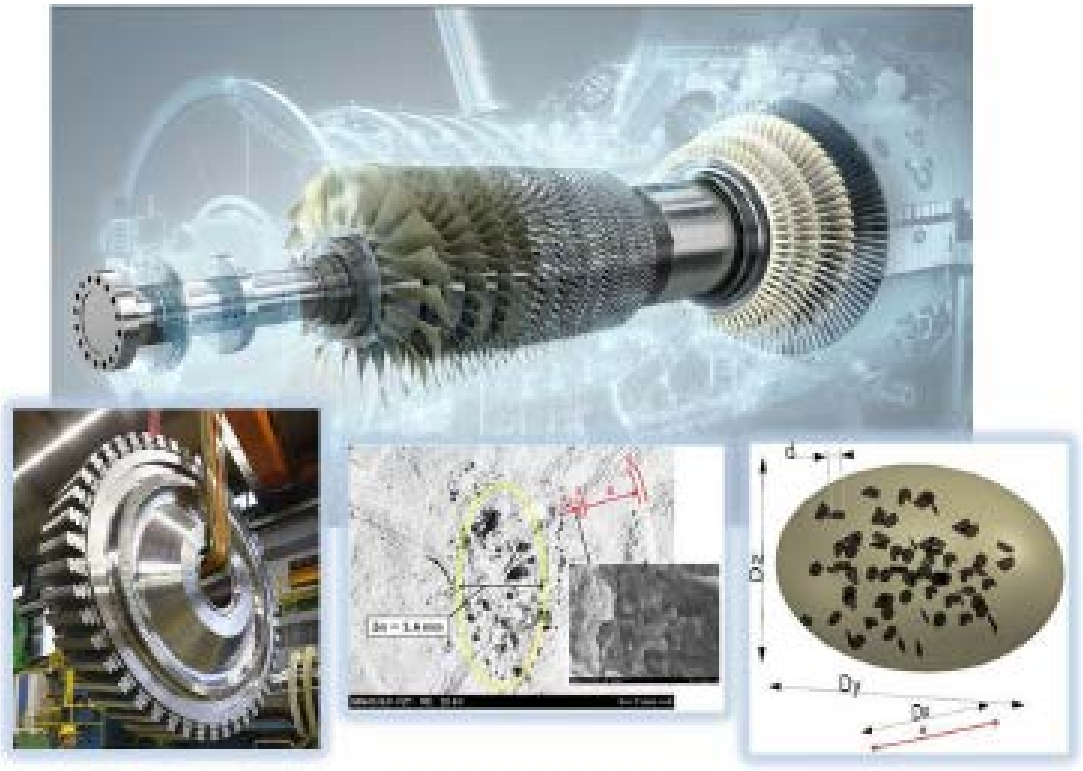
Understanding Complex, Coupled Mechanisms of Oxidation and Hot Corrosion Degradation with Computational Models, **UTRC/LLNL**



- Study oxide stability in Ni-Cr-Al alloys for turbines in hot corrosion environments (SOx, H_2O)
- HPC for *ab initio* density functional theory (DFT) and phase-field models

Understanding corrosion at high temperature will result in better materials

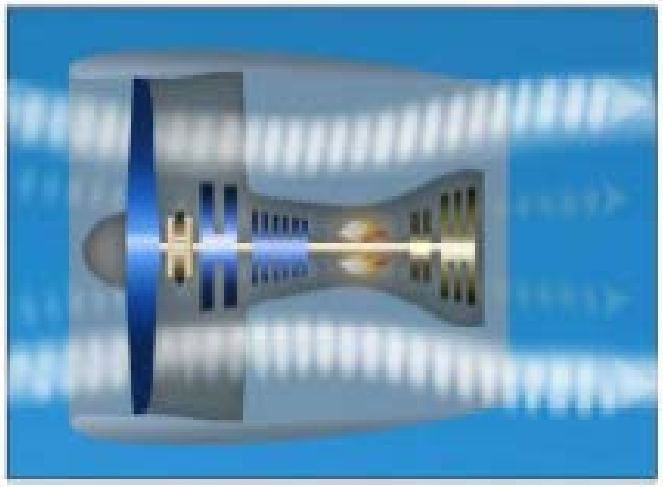
High-Performance Particle-Based Modeling of Damage Nucleation from Forging Flaws in Fossil Power Generation Rotor Components, Siemens/LANL

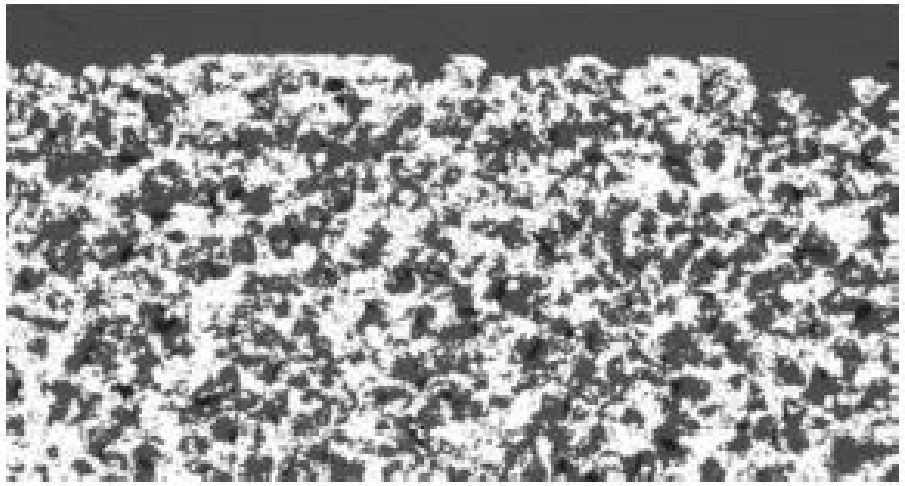


- Understand crack nucleation and growth from forging flaws to enable higher temperature, higher load operation
- Particle-based methods for capturing continuum and interface features

Higher temperature operation on turbines increases plant efficiency to over 65%

Predicting Limit Rub Response in Advanced Gas Turbine Engines, Pratt and Whitney/ORNL

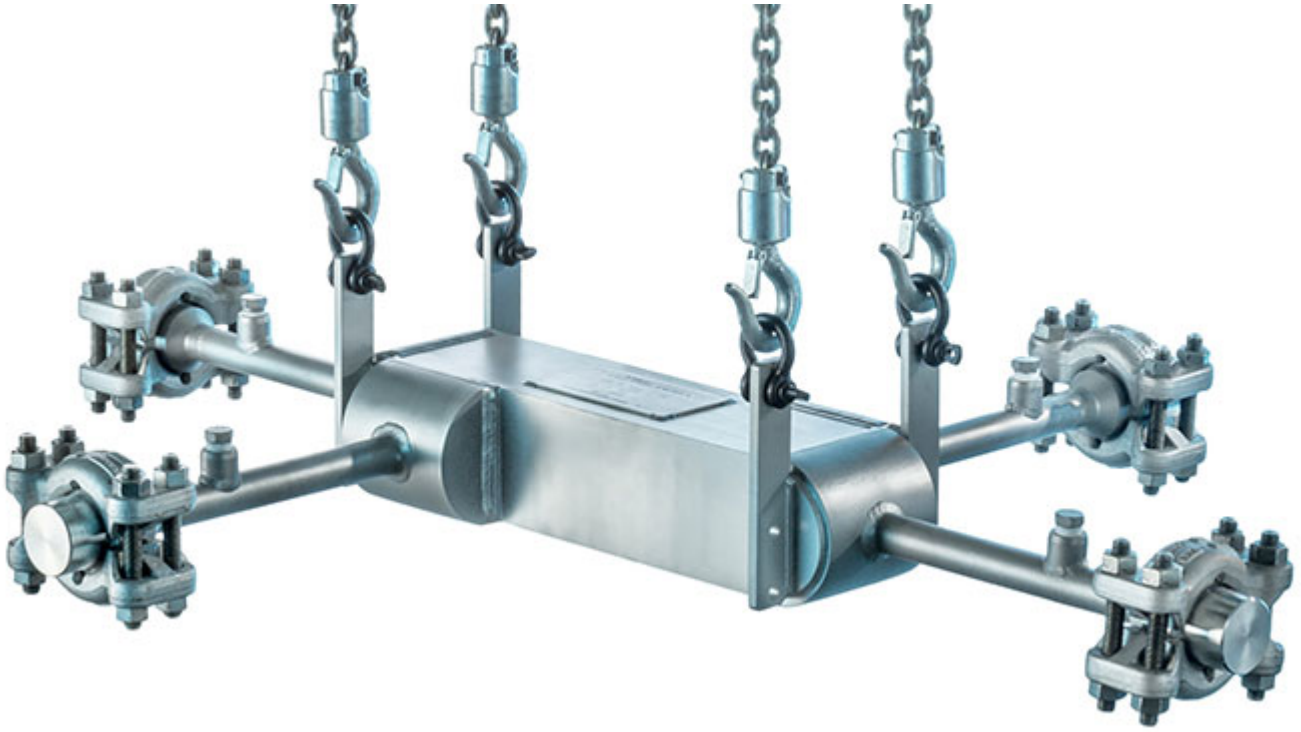




- Study microstructure evolution of abradable coatings at the tips of turbine blades
- HPC needed for high-fidelity model of grain structure under high strain-rates

Enables higher temperature operation on turbines

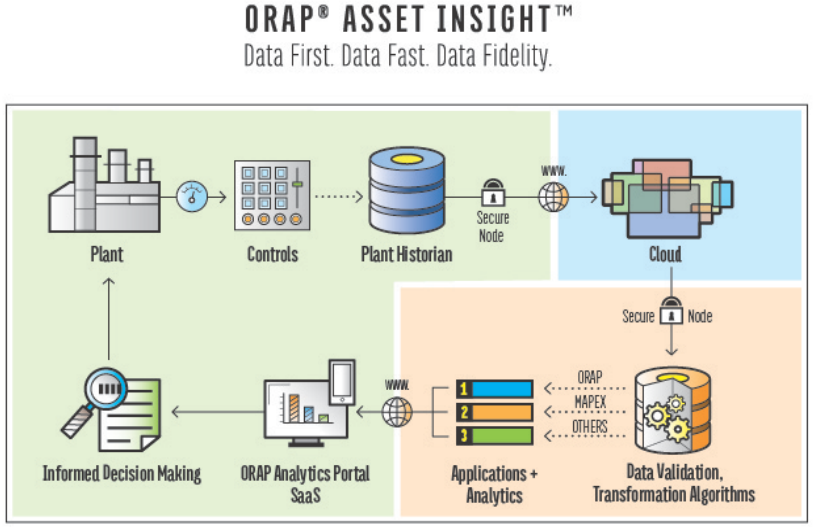
Compact Diffusion Bonded Heat Exchanger Fatigue Life Simulations, Vacuum Process Inc./SNL



- Modeling fatigue in metals for cyclical, high temperature, sCO_2 heat exchangers
- Complex geometry required HPC
- Specialized SNL Sierra codes

Enables compact heat exchangers for cyclical supercritical CO_2 operations

HPC Analytics of Thermal Plant Data to Optimize Operating Envelope



- Apply machine learning techniques to plant operational data to predict component lifetimes
- Requires AI expertise and computational capacity to analyze large amounts of data

Predict component failure under fluctuating plant conditions

Effect of Cyclic Operation on HRSG and Coal-fired Boiler Tubes – Failures Induced by High Thermal Stress and Component Fatigue, SPS/NETL

- Determine conditions in heat recovery steam generator (HRSG) using operational reliability analysis program (ORAP) data which lead to fatigue failure
- Simulate fatigue failure using CFD/structural simulations using DOE expertise to improve components

Predict component failure under fluctuating plant conditions

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