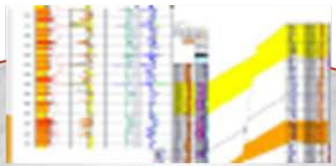


# Predicting Materials Performance in Extreme Environments

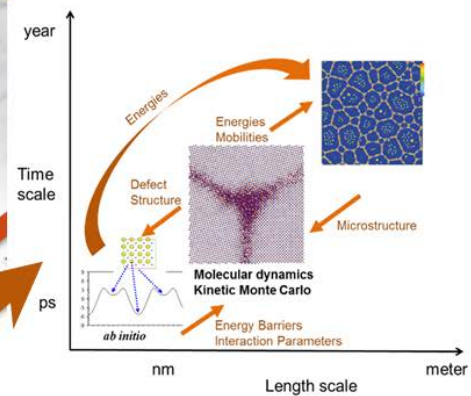
Data mining, open framework, machine learning

Alloy name	Cr	Ni	Nb	Si	C	10 <sup>5</sup> h rupture strength (MPa) at 700 °C
316H	16-18	10-14	0.0	0.7	0.10	39 (at 675 °C)
347HFG	17-20	9-13	0.8	0.7	0.10	58
Tempaloy A-3	21-23	14.5-16.5	0.5-0.8	1.0	0.03-0.1	63
Tempaloy AA1	17.5-19.5	9-12	0.1-0.4	1.0	0.07-0.14	77
Super 304H	18	9	0.4	0.2	0.1	70
HR3C	24-26	19-22	0.2-0.6	1.0	0.04-0.1	67
SAVE 25	23	18.5	0.4	0.1	0.1	89

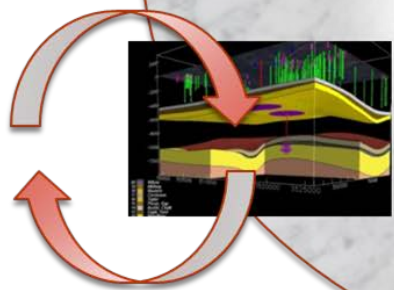
Input Data



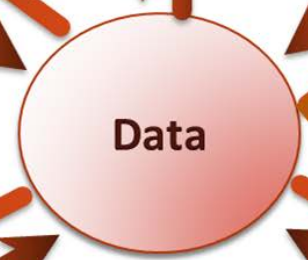
Multiscale Modeling From DFT to Finite Elements



Uncertainty Quantification



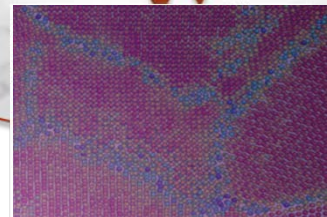
Validation, Diagnostics, & Monitoring



HPC resources  
Cascade: 3.4 PetaFLOPS



Visualization & Analytics



We integrate physics-based multi-scale materials modeling with machine learning and an open data framework to predict materials performance and design new alloys.

POC: Ram Devanathan, [ram.devanathan@pnl.gov](mailto:ram.devanathan@pnl.gov), 509-371-6487