Materials Informatics at GRC

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Materials Informatics

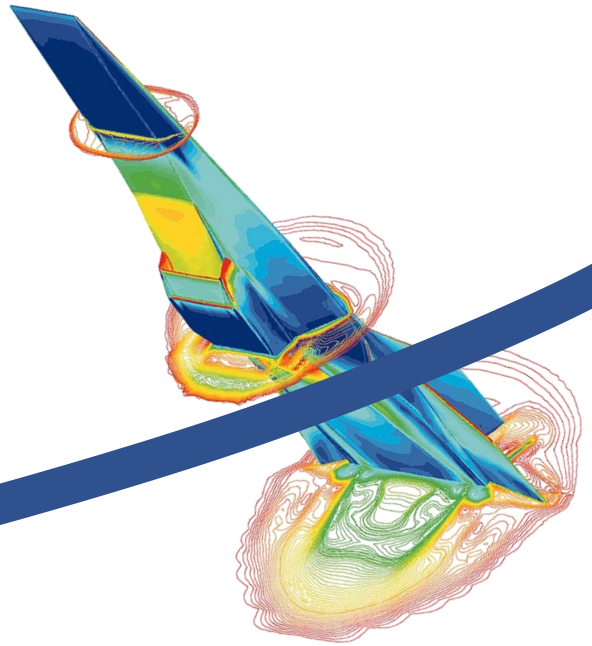
LM Division
Machine Learning

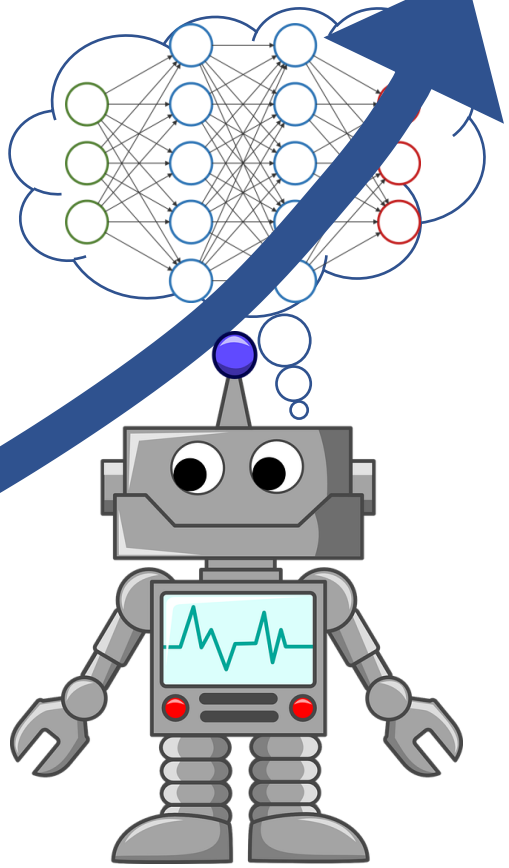
Prehistory
Materials 1.0
Empirical Science

1600s
Materials 2.0
Theoretical science

1960s
Materials 3.0
Computational Science

2010s
Materials 4.0
Data-driven Science





and error,
experiments

Physics, chemistry,
thermodynamics

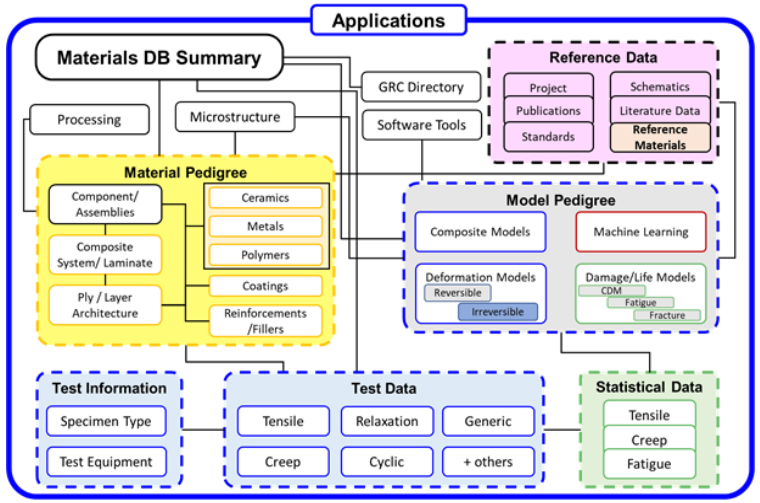
Molecular dynamics,
DFT, modeling

AI, ML, clustering,
anomaly detection

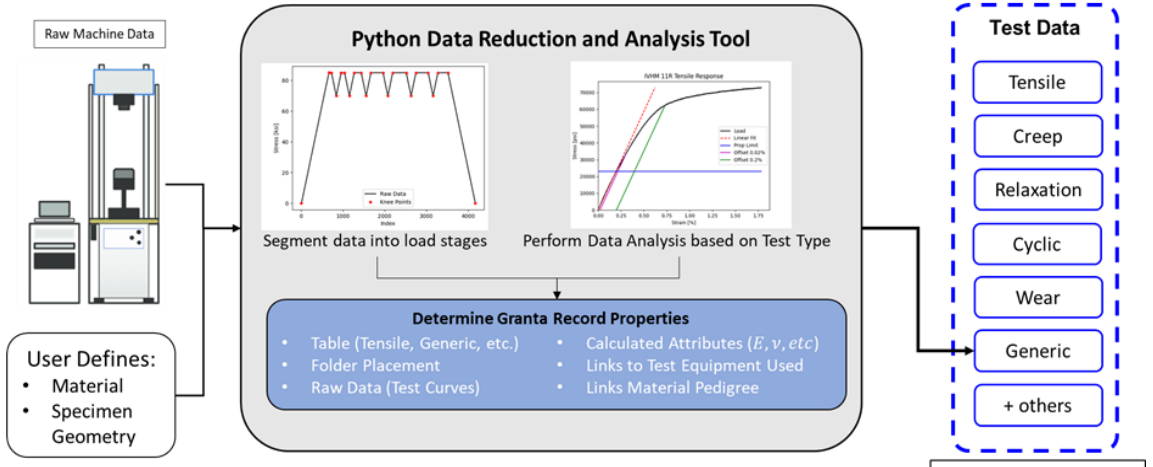
Data Management

Ingestion of GRC Test Data into Granta MI

- Granta MI is a material information management system that provides users the ability to import, store, link, and export material data
- Developed the database schema for various types of Data
- Developed Python-based import/export tools that perform consistent and reliable data analysis and reduction, upload data to the correct location in the database, and allow users to get data out the right data, at the right time, in the right format
- Effective database management of material information enables data to be maintained with its full pedigree, reducing the likelihood that data is lost, misused, or repeated.
- Easily expand current schema, import/export tools, etc. to material, test, and model data for EBC's and CMC's



NASA GRC ICME Schema



Test Data Analysis and Upload Procedure

Shape Memory Alloy Database

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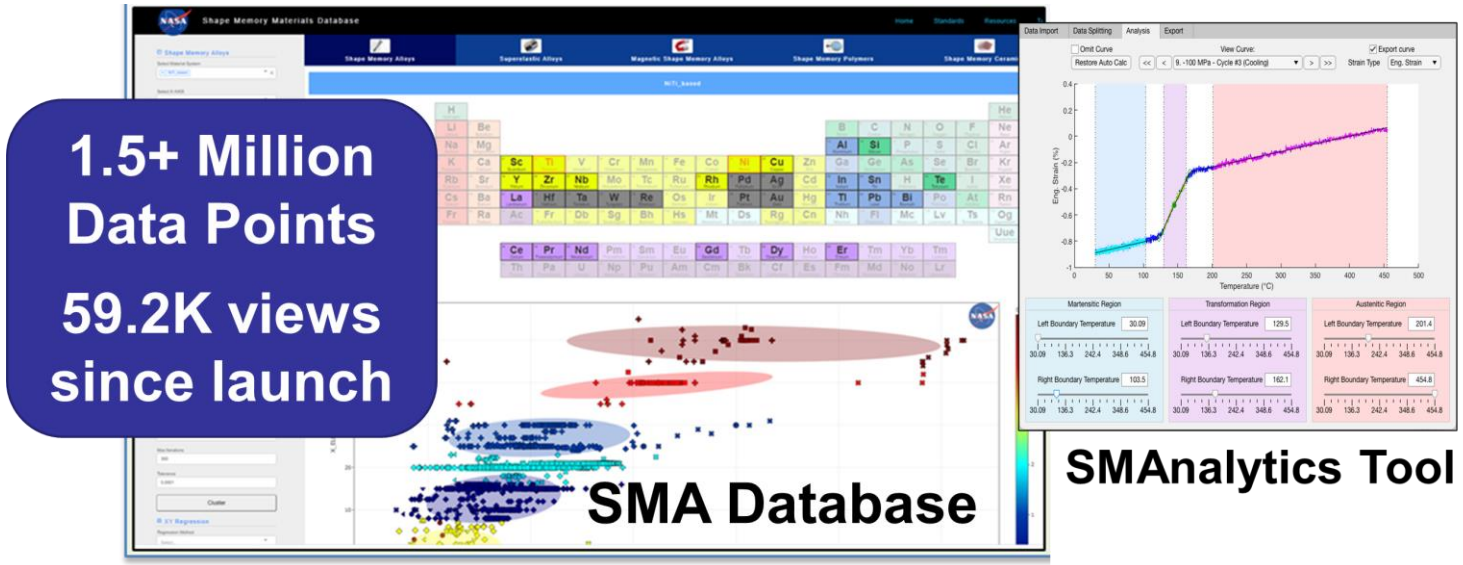
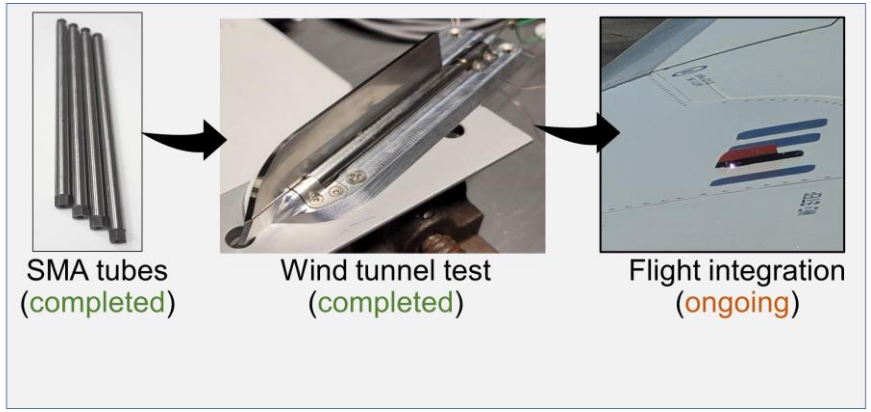
- World's Largest Shape Memory Alloy (SMA) Database Enables Development of Two New Alloys in One Year
- Tool publicly launched via a web application
- Impact: Enable faster, efficient, accurate design of SMAs
- Impact: Promote database growth and data mining via direct scientific community contributions
- Developed TWO new experimental alloys for FY22 Boeing ecoDemonstrator flight test with two key advancements





ML Surrogate Modeling

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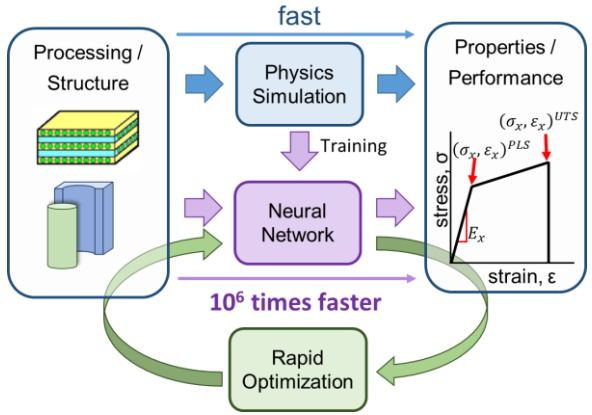
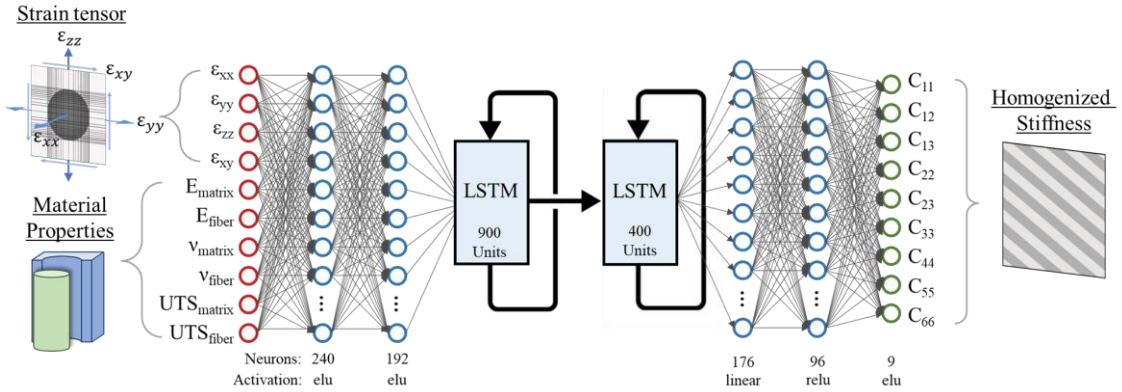
Machine Learning Model For Fast and Accurate Multiscale Modeling

- ML surrogate models **bypass the speed/accuracy trade-off** enabling much larger simulations, optimization over the model, and rapid design tools that don't rely on simplifying assumptions.
- Currently integrating ML models with physics models built in FORTRAN.
- Using Graph Neural Networks to capture microstructure.

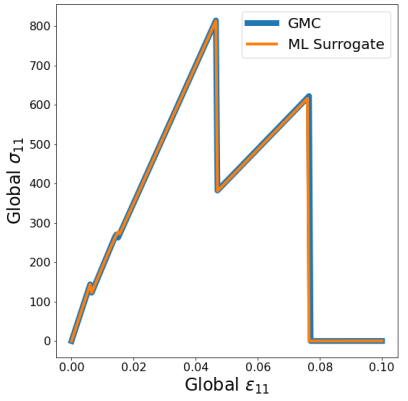
Optimal Experimental Design with a fast surrogate



LSTM captures load history and damage



145X speed with 98% accuracy



MicroNet

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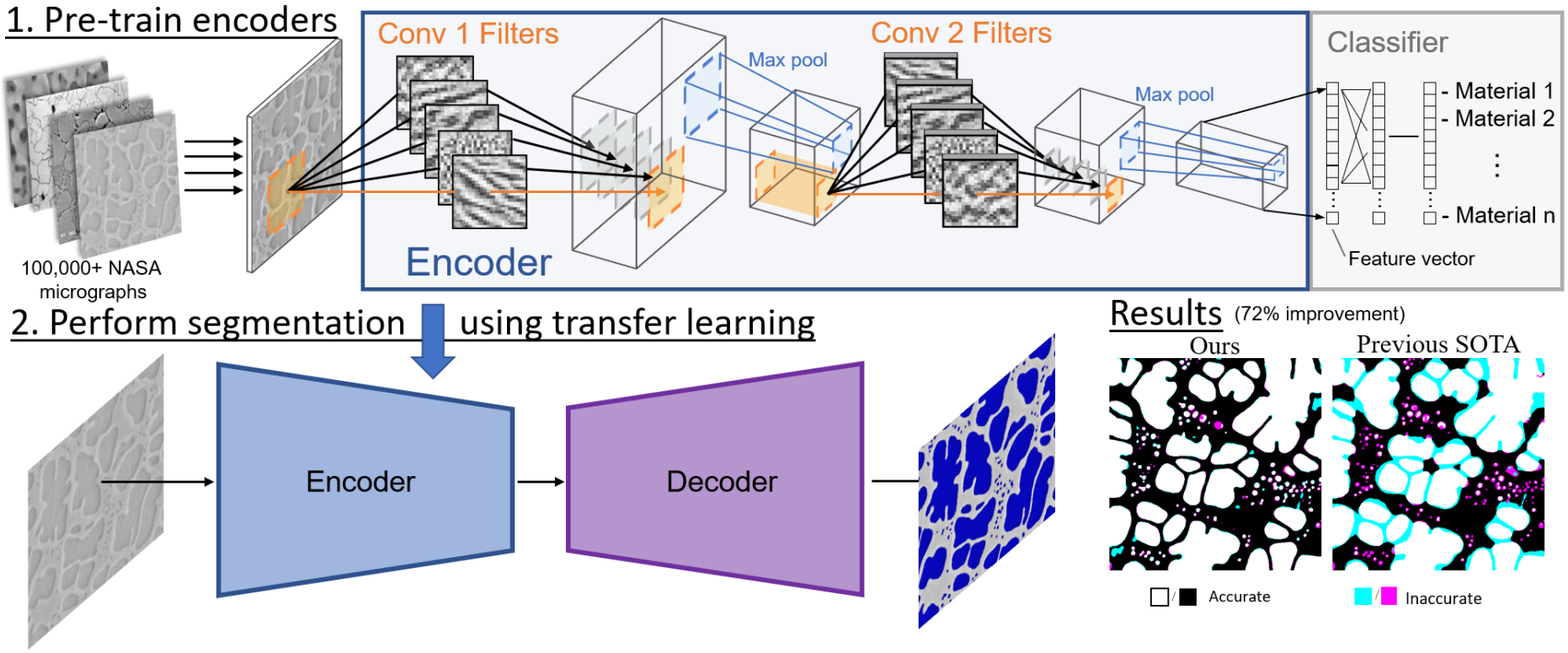
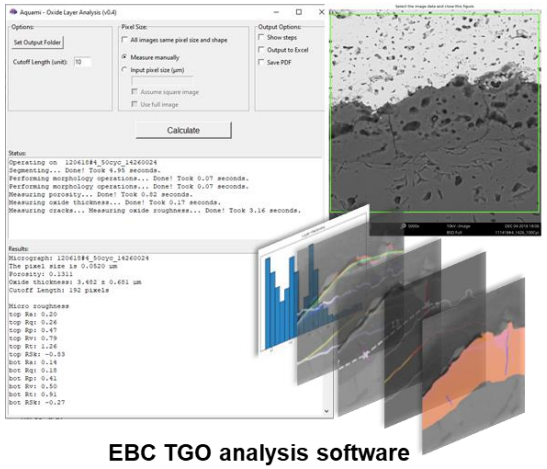
Neural network encoders trained on 100,000+ microscopy images from NASA

- Provides superior performance on downstream microscopy tasks – more accuracy with less training data.
- Opensource code and models. Swap ImageNet encoders with just a couple lines of code.
- Applied to numerous materials inside and outside of NASA to extract microscopy features to establish PSP relationships.



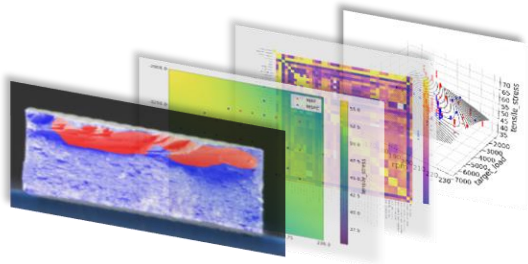
MicroNet

LM Division
Machine Learning



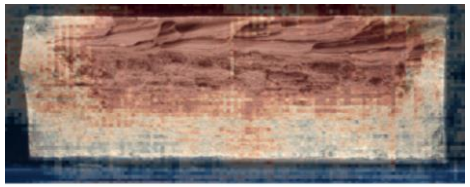
EBC TGO analysis software

SLS Core Stage Welds

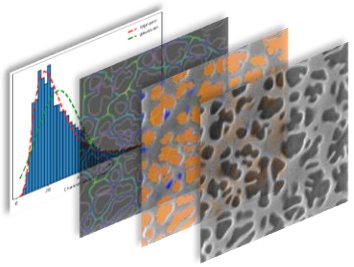


MicroNet

Direct regression and interpretability



Ni-Superalloys



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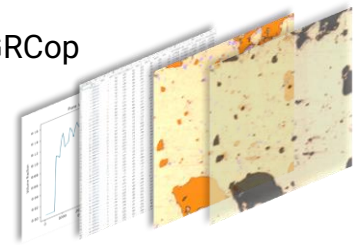
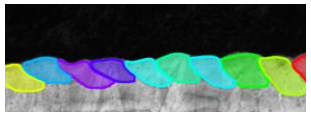
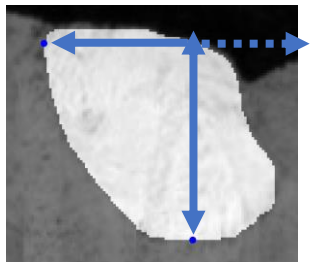
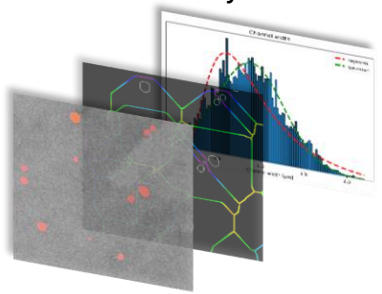




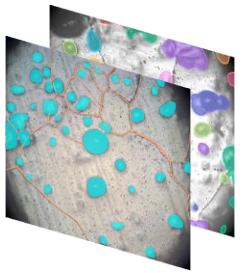


Automatic image analysis of melt pool geometry

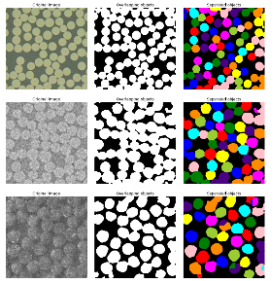
ODS Alloys



Wind tunnel Icing



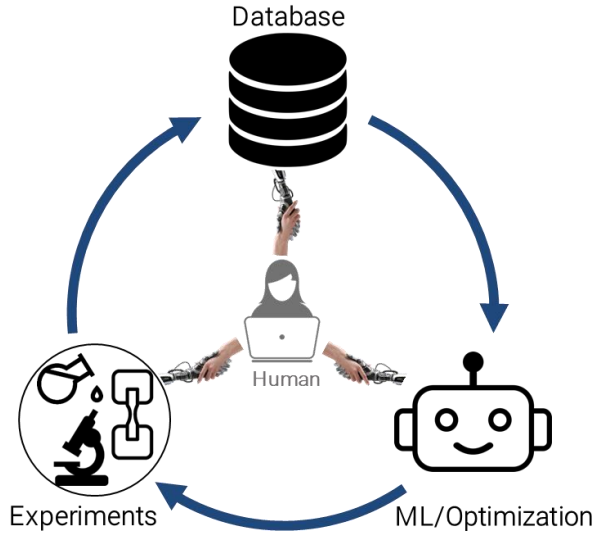
Composite Fibers



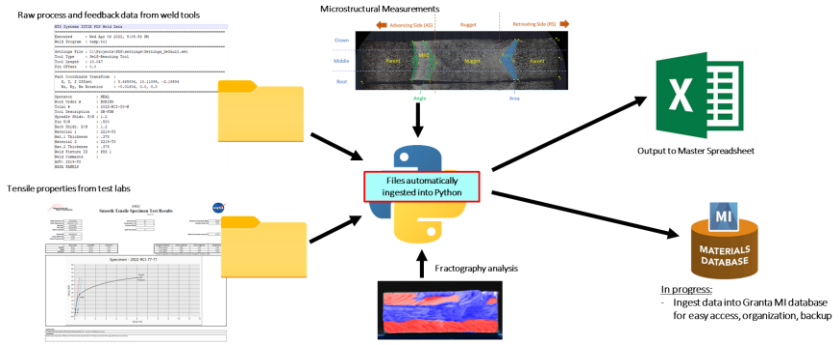
JARIMIS

"Just A Rather Intelligent Materials Interrogation System"

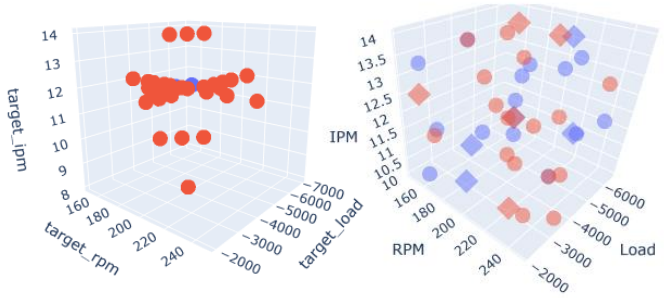
- A methodology and software framework that combines tools to efficiently apply materials informatics to more projects.
- Tools being applied to improve SLS weld quality.



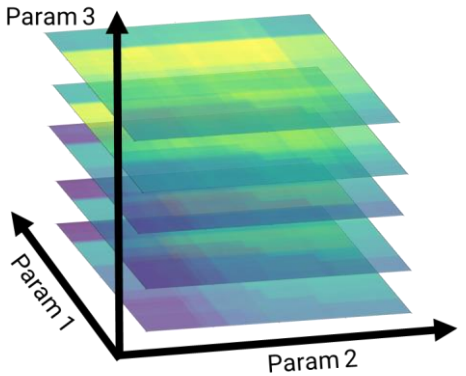
JARIMIS Framework



Automatic Data Ingestion



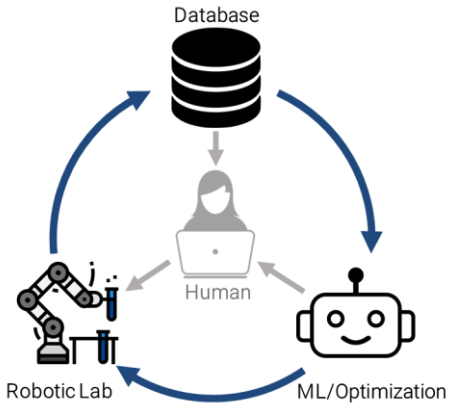
Space-filling DOE to capture non-linear effects

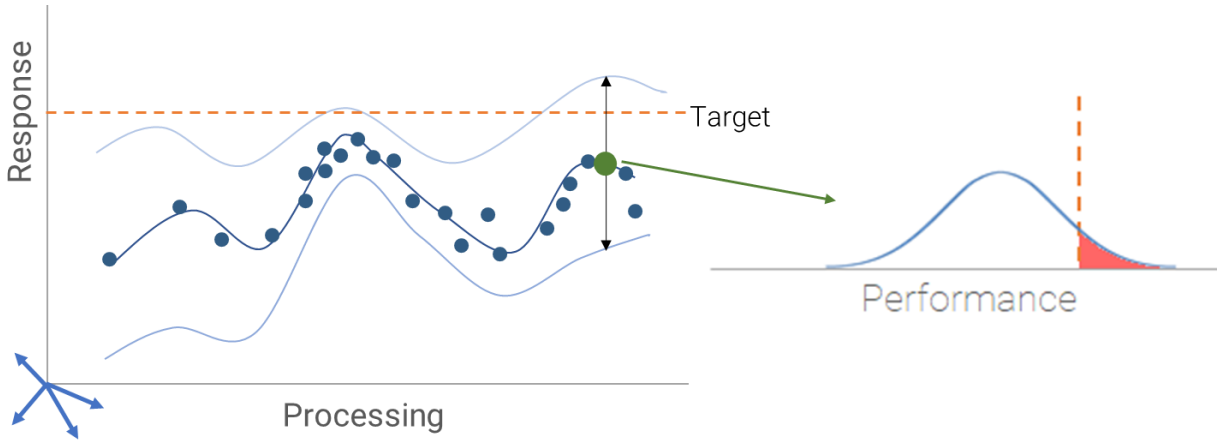


PSP Models

Automated Lab

- Inverse design uses ML models and Active Learning to iteratively suggest optimal experiments to achieve target properties with fewer experiments.
- Self-driving laboratory that iteratively designs, executes, and learns from materials science experiments in a fully autonomous loop
- Increases the speed of materials experiments by orders of magnitude (hundreds of experiments in a few days) and accelerates materials discovery and optimization
- Prototyping technology on the development of high voltage materials for high energy and high-power electrified aircraft propulsion





Questions?

Thank you!