SAND2022-15578C

Dan^2 Robot Party aka AMRAD…

Automation and System Integration

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Sandia National Laboratories

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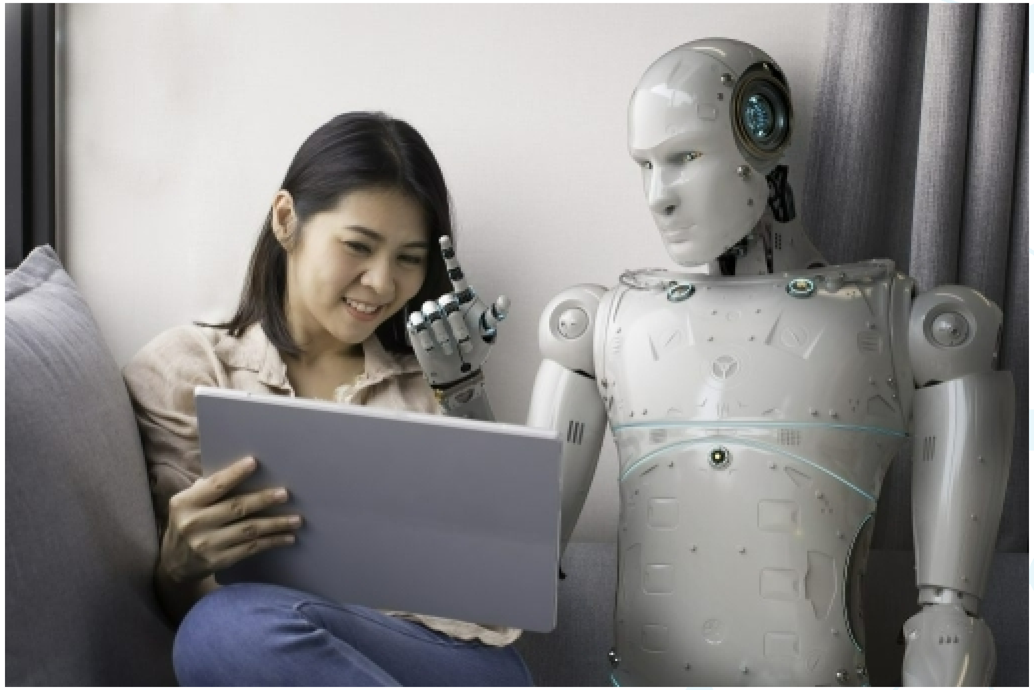
Dan² guidance:

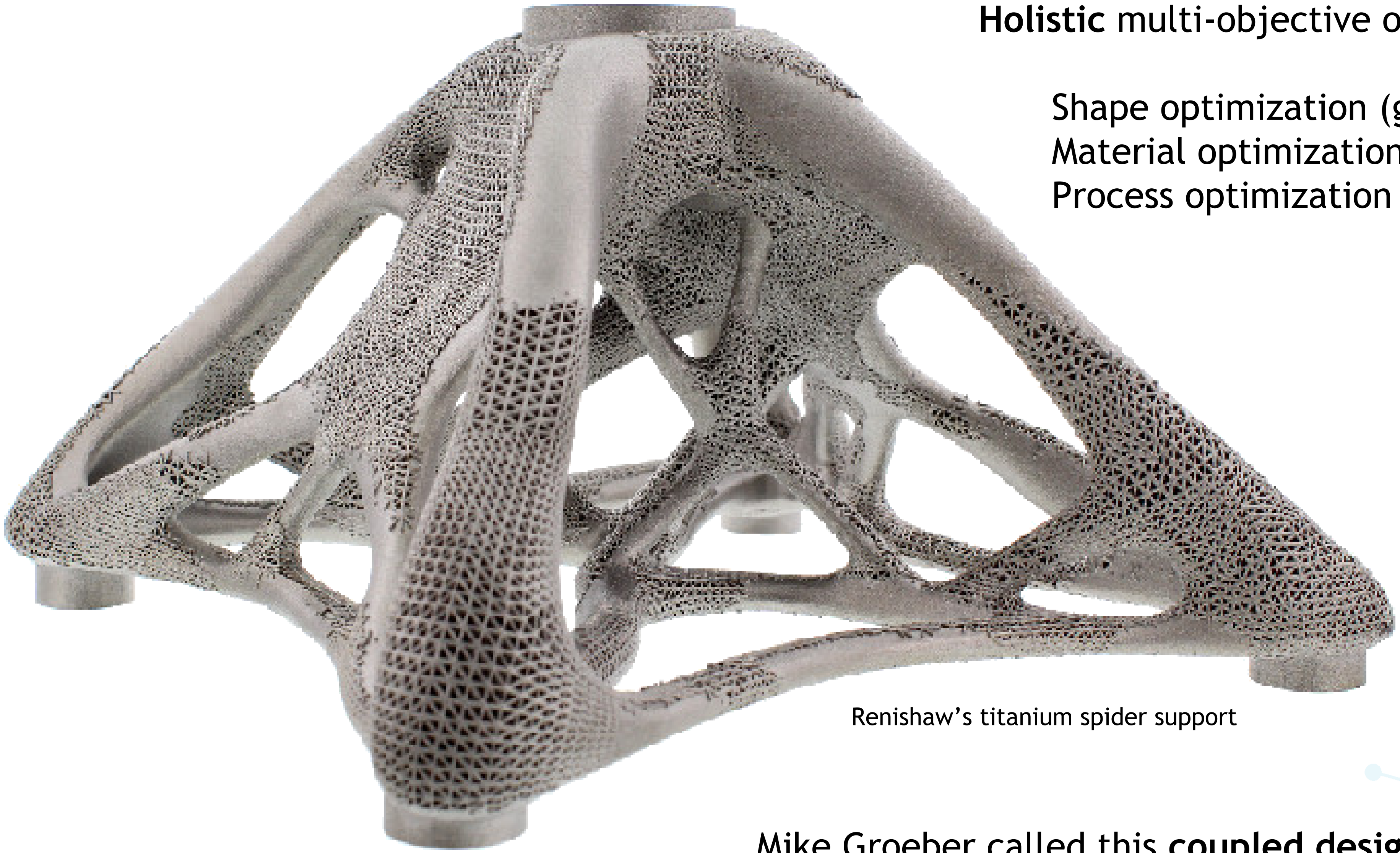
“summarize the biggest challenges to future progress”

Is autonomy the best goal?… More urgently, we need acceleration and beyond-human cognition to inform us in a *collaborative* manner.

“AI will not replace scientists, but scientist who use AI will replace those who don’t”



The essential challenge from a product development perspective



Renishaw's titanium spider support

Holistic multi-objective optimization…

Shape optimization (gradient topologies)
Material optimization (gradient materials)
Process optimization (gradient processes)

BH Jared et al., *Scripta Mater*, 2017

Mike Groeber called this **coupled design**, others call it **co-design**

Lets be honest about the Process-Structure-Property paradigm

Comprehensive PSP relations suffer from the ***Curse of Dimensionality***

Process parameters

Powder composition
Compositional range
Powder size distribution
Powder shape
Powder porosity
Powder reuse
Powder contaminants
Laser power & stability
Scan velocity
Laser focus / beam size
Delivered energy density
Scan strategy
Contouring scans
Gas purity
Gas flow rate
Wiper quality
Part layout
Sacrificial supports
Part orientation
Powder removal
Post machining
Surface remediation
Heat treatment
Joining
etc.

Physical Phenomena

Powder packing
Laser/plume interactions
Plasma fluid mechanics
Radiation heat transfer
Laser energy adsorption, radiation
Thermal expansion
Non-equilibrium vapor pressure
Evaporation with latent heat
Pressure-temperature relations
T-dependent heat capacity
Incompressible fluid dynamics
Convect./conduct. heat transfer
Capillary forces
Marangoni forces
Hydrodynamic mixing
Multicomponent liq-sol diffusion
Solidification macrosegregation
Solidification shrinkage
CTE thermal contraction
Thermomechanical deformation
Residual Stress
Solid-state diffusion
Anisotropic crystallization
Solid-state phase transformations
etc…

Structure&Chemistry

Crystal structure(s)
Phase fractions / precipitates
Phase morphology
Grain size
Grain morphology
Crystallographic texture
Microtextures
Inclusion types
Inclusion morphology
Composition
Macrosegregation
Microsegregation
Dislocation density
Dislocation arrangements
Residual stress
Inhomogeneous stresses
Interface structure
Grain boundary types
Surface roughness
Surface films
Vacancy concentration
Microporosity
Macroporosity
Density
etc…..

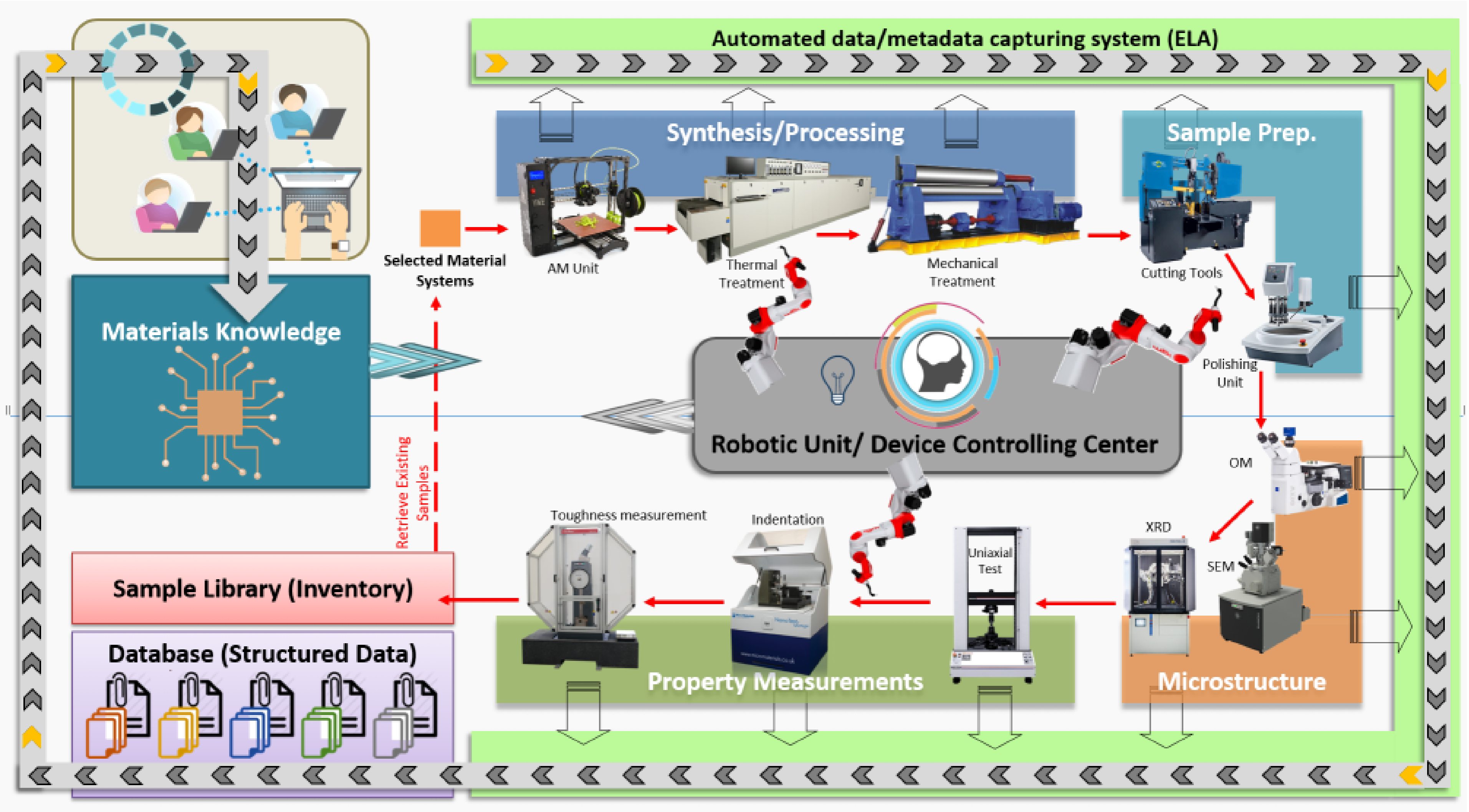
Governing Eqns

Elasticity theory
Yield surface
Strain-rate sensitivity
Hall-Petch scaling
Taylor-Quinney relation
T-dependent plasticity
Archard scaling
Solute strengthening
Precip. strengthening
Anisotropic elasticity
Anistropic plasticity
Polycyrstal plasticity
Dislocation dynamics
Twinning behavior
Grain bndry migration
Phase coarsening
Phonon transport
Electronic transport
Reaction kinetics
Nucleation processes
Crack shielding
Ion-matter interactions
etc…

Properties & Performance

Cost
Density
Modulus
Yield strength
Fracture toughness
Impact tolerance
Hardness
Wear resistance
Friction coefficient
Radiation tolerance
Max Service Temperature
Thermal expansion
Thermal conductivity
Reactivity/corrosion
Electrical conductivity
Resonance
Functional performance
Shape
Volume
Mass
Integration / joining
Inspection / acceptance
Longevity / failure modes
Reuse / recycle path
etc.

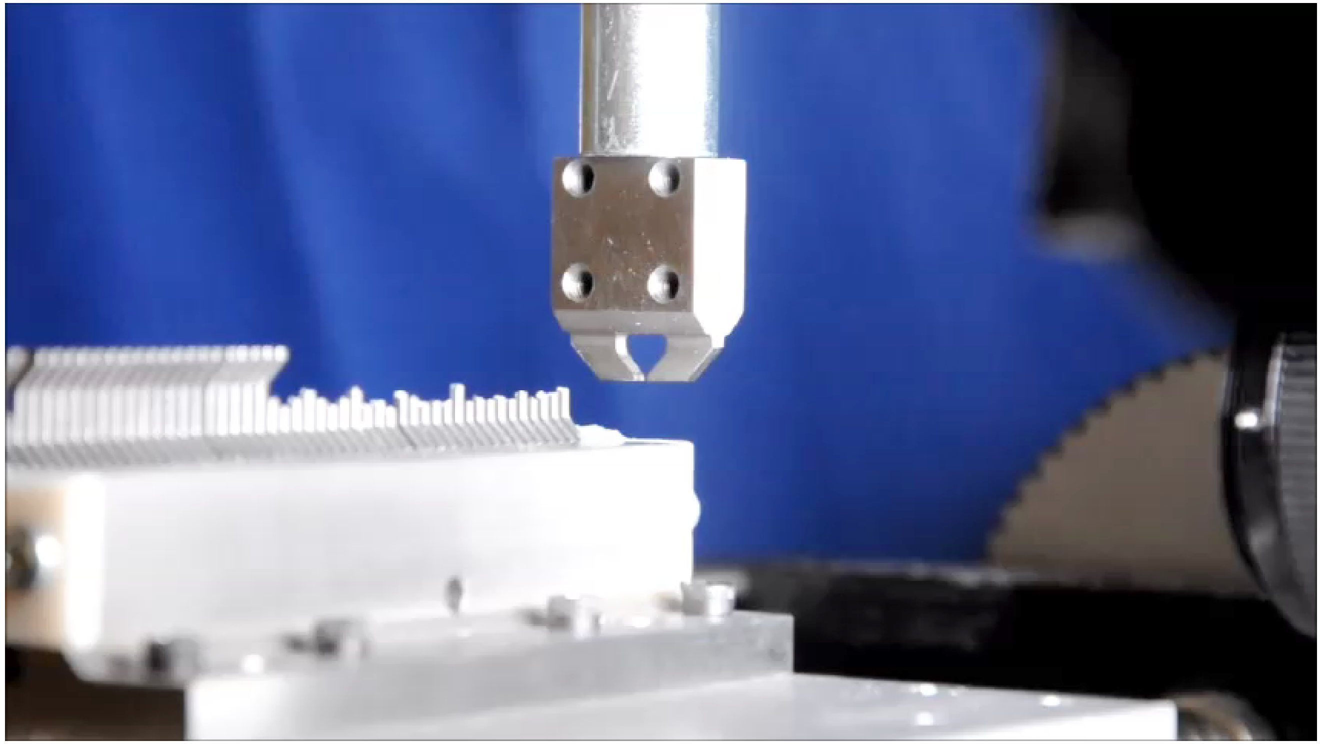
Acceleration through automation? *Surya Kalidindi's visionary graphic

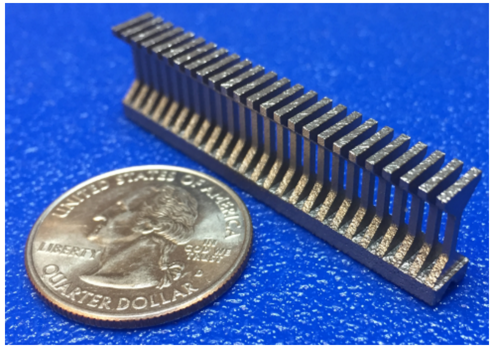


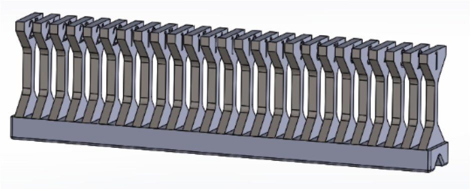
- Standardized high-throughput test methods
- Standardized witness coupons
- Adoption of parametric monitoring
- Modification of test methods for high-throughput
- Automated assimilation of experimental data into models
- New ways of handling and mixing complex, heterogeneous data

https://matin.gatech.edu/groups/mined_sg9_automation_autonomy_experiments

Non-standard and unconventional, but fast!





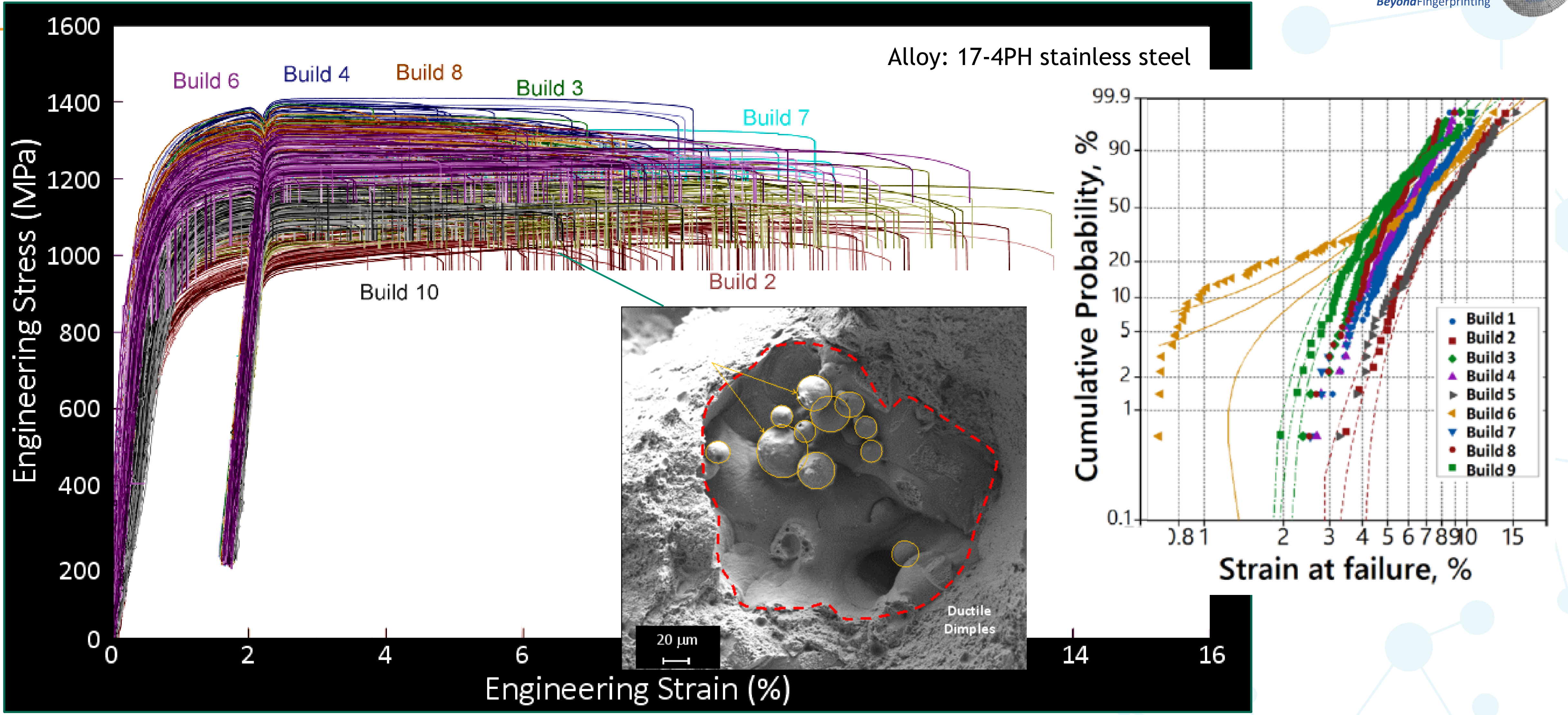


Patent: B. Boyce, B. Salzbrenner, “Apparatus for High-Throughput Sequential Tensile Testing and Methods Thereof,” U.S. Patent 11,002,649, issued May 11, 2021.

⇒ A 50X reduction in operator time

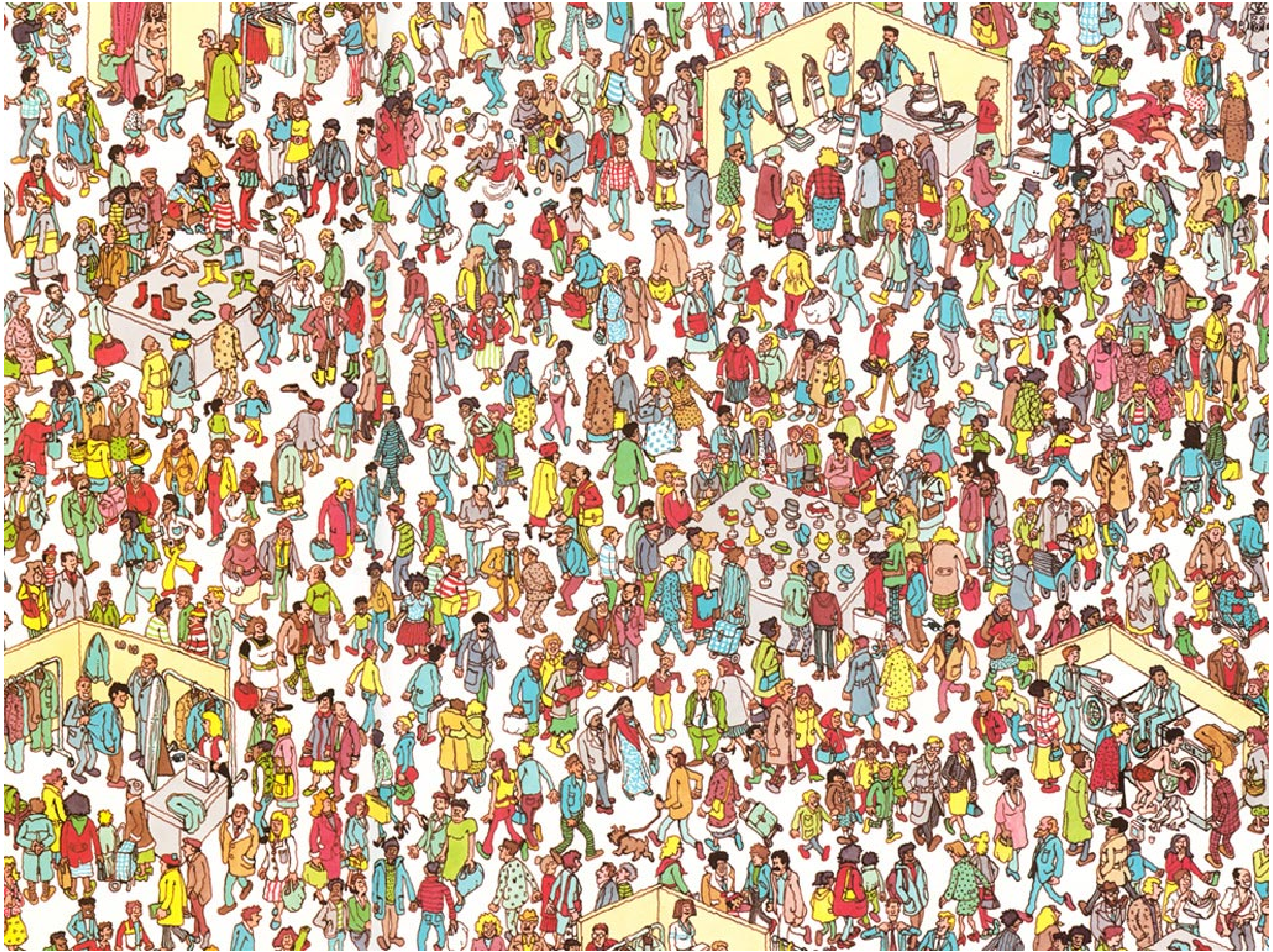
Heckman…Boyce, *Mater. Sci. Eng. A*, 2020

Do we learn anything new when we have more data?



Boyce, Salzbrenner, Rodelas, Swiler, Madison, Jared, Shen, *Advanced Engineering Materials*, 2017

Anomaly detection is so important in materials & manufacturing



“Crystals are like people, it is the defects in them which tend to make them interesting!” - Colin Humphreys.

Accelerated fractography

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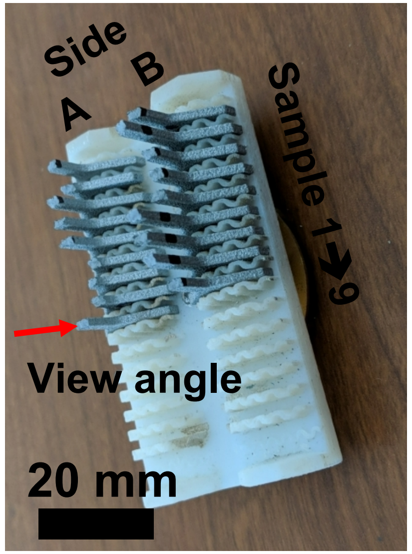
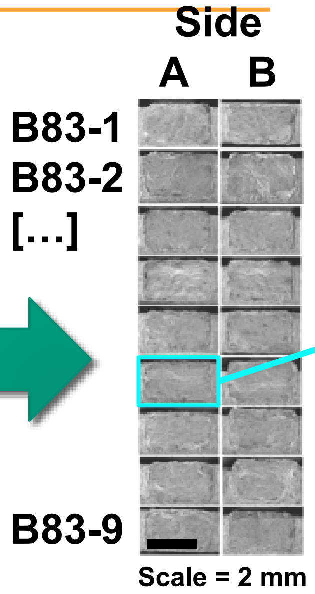
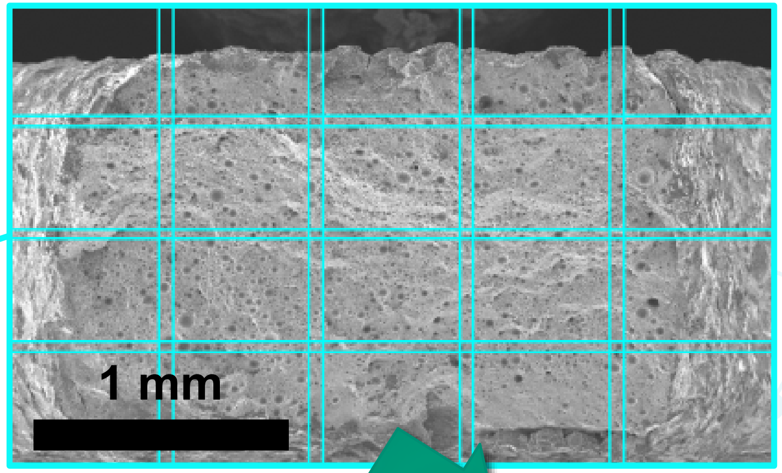
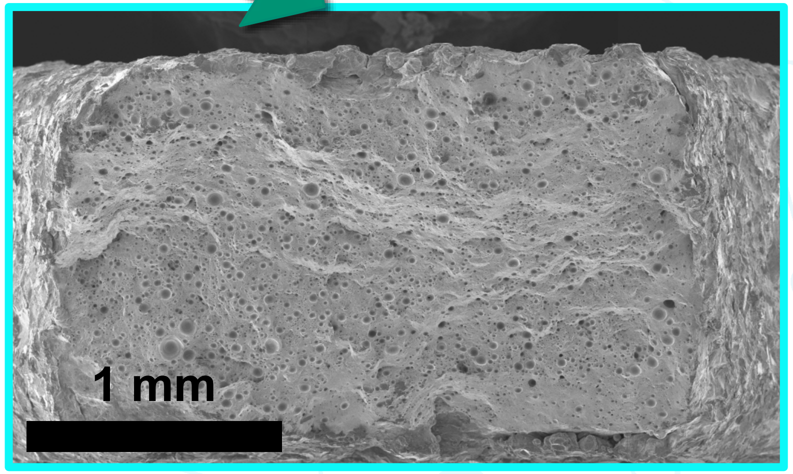
JEOL IT500HR
(python scripting!)







⇒ A 33X reduction in operator time



Multiscale Fractographic montage:
25,600 x 15,360 pixels

Boyce & Uchic, *MRS Bulletin*, 2019

Unconventional low-cost surrogate *fingerprints*

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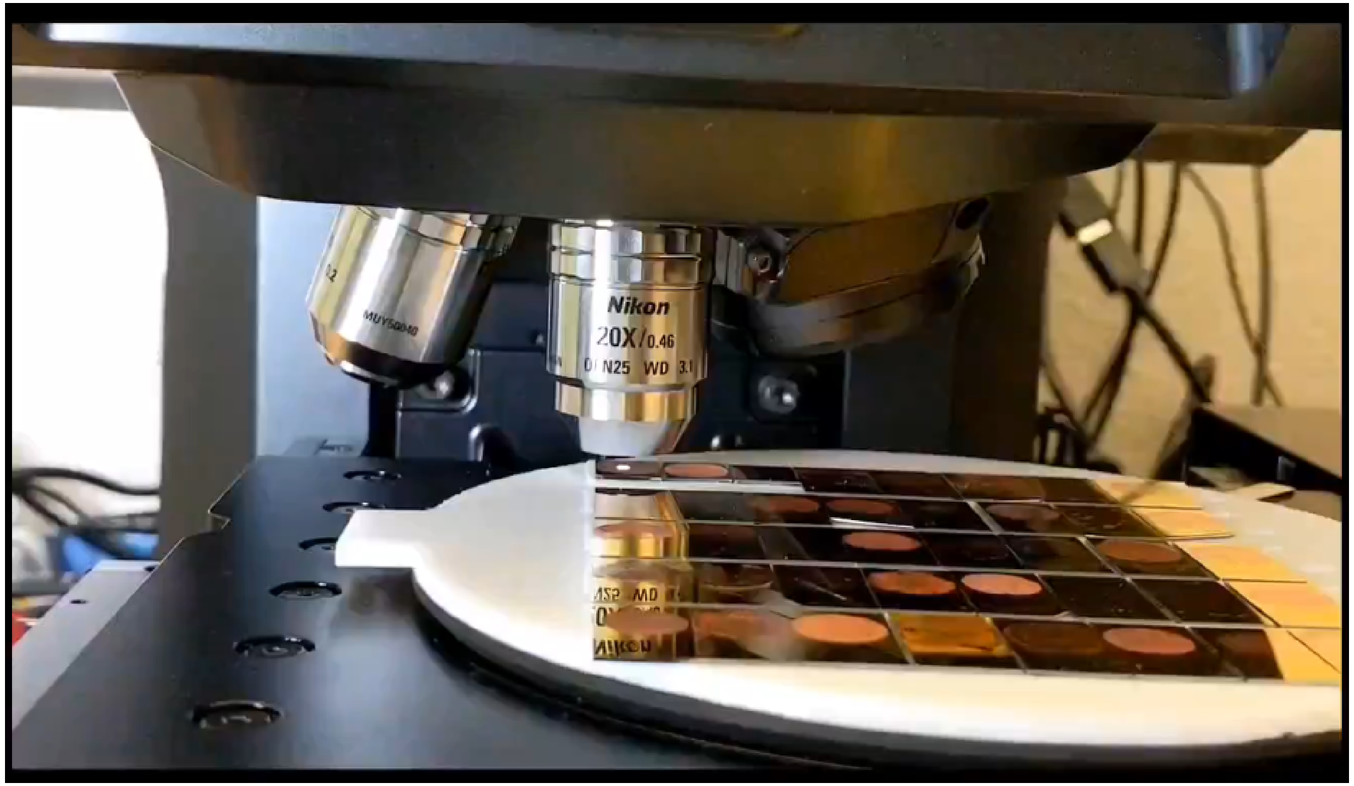
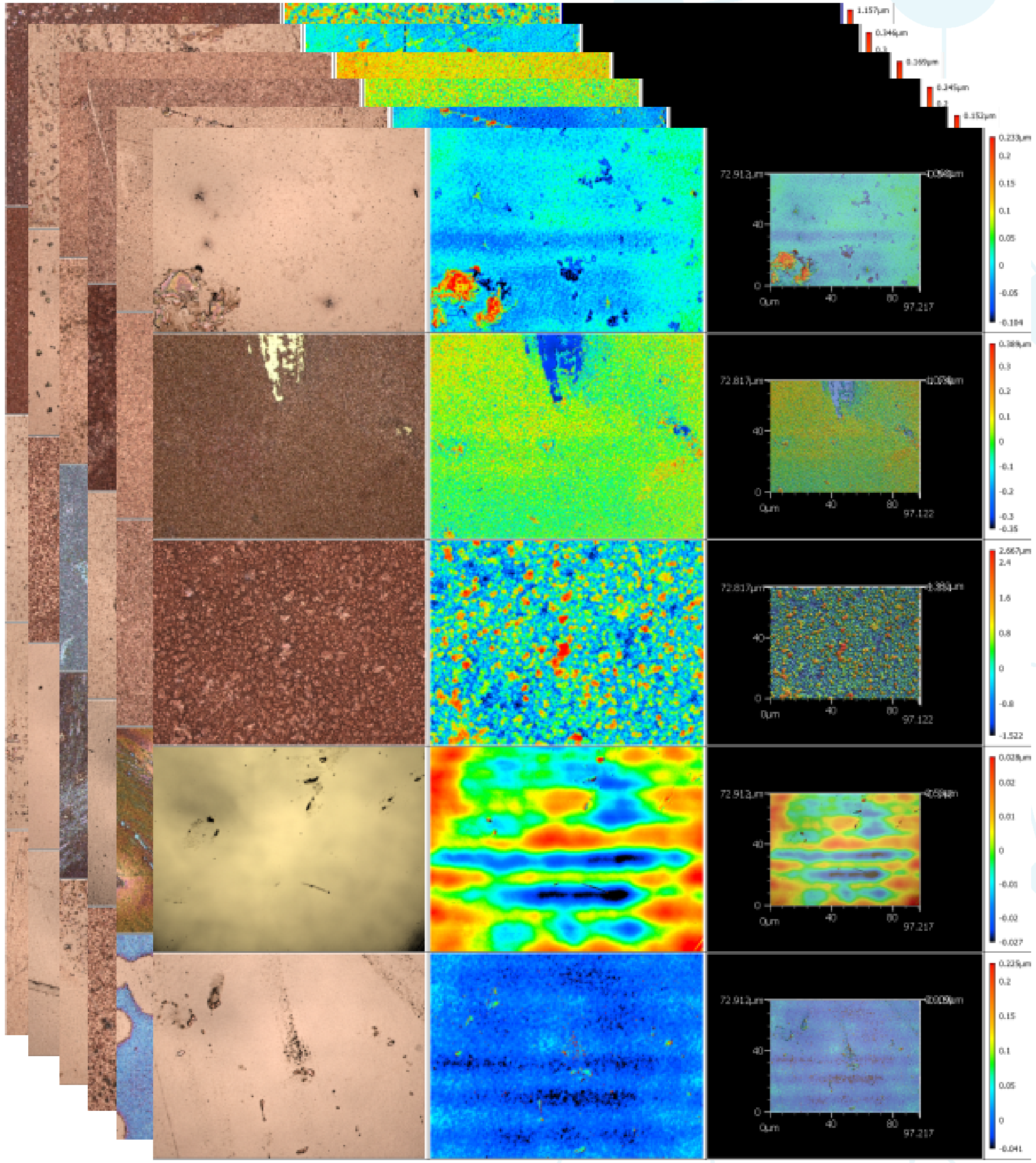


Mapping Profilometer with programmable stage



Dan^2 guidance:

"…describe the integrating issues…"

Part II: Integration of hardware & multimodal data

Properties 'Alinstante'

An Aspirational Goal:

Can we reduce materials science evaluation from months to hours?

Geometric metrology probe

Surface roughness probe

Mechanical properties probe

Compositional probe

Phase probe

Thermal probe

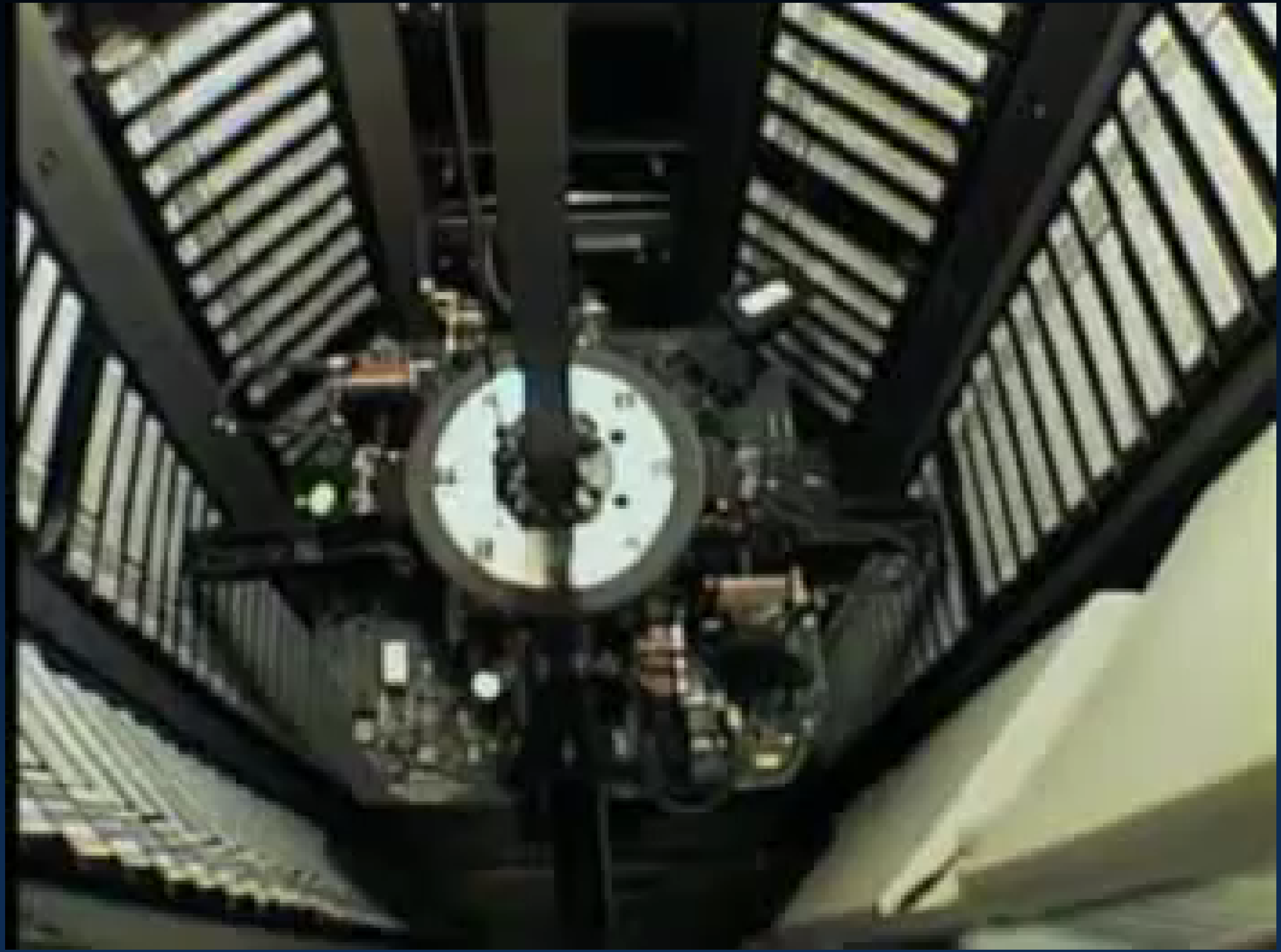
Electrical probe

Tribology probe

Resonance probe

...

Model Concept: Cylindrical Tape Storage



The *Alinstante* Modular Pedal Concept

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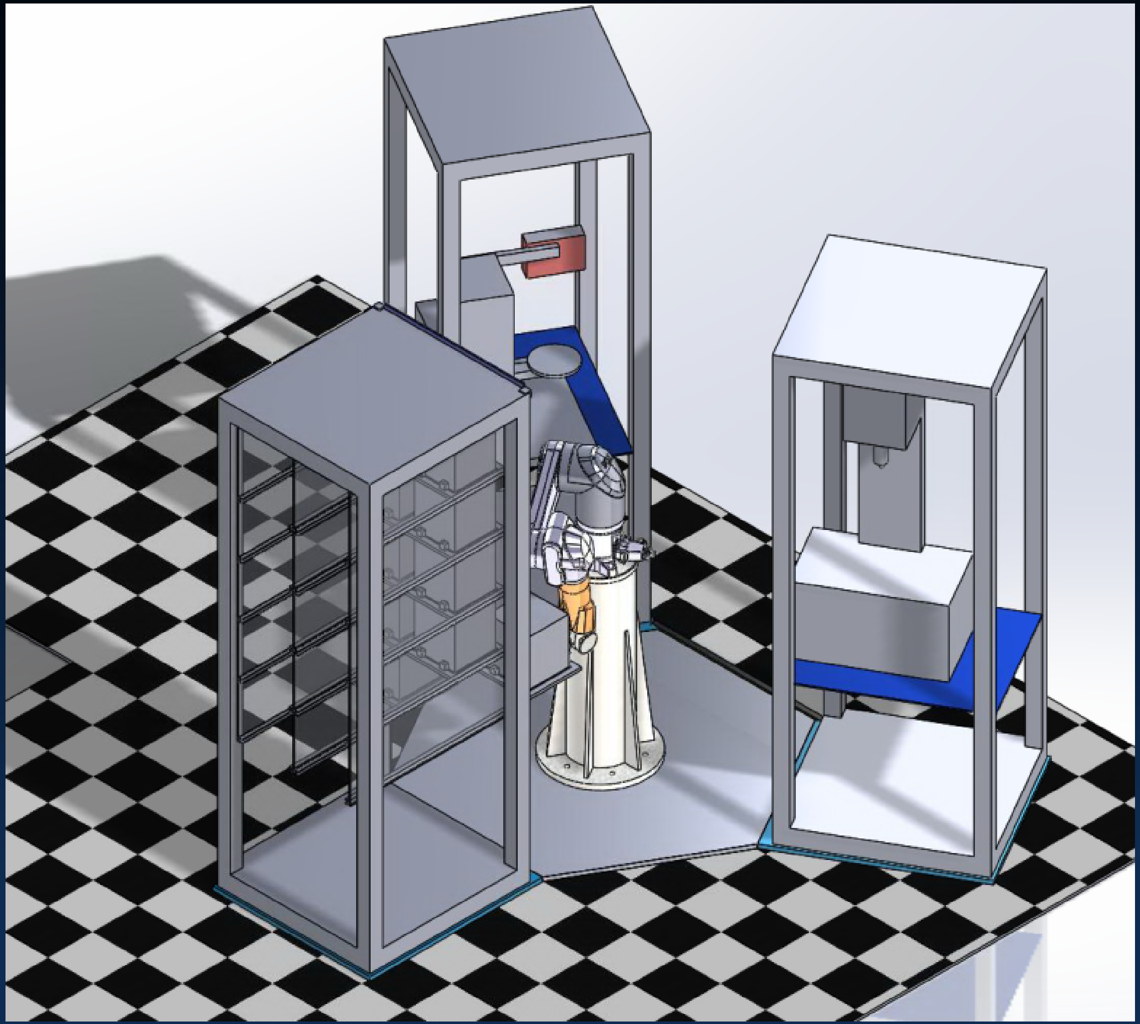
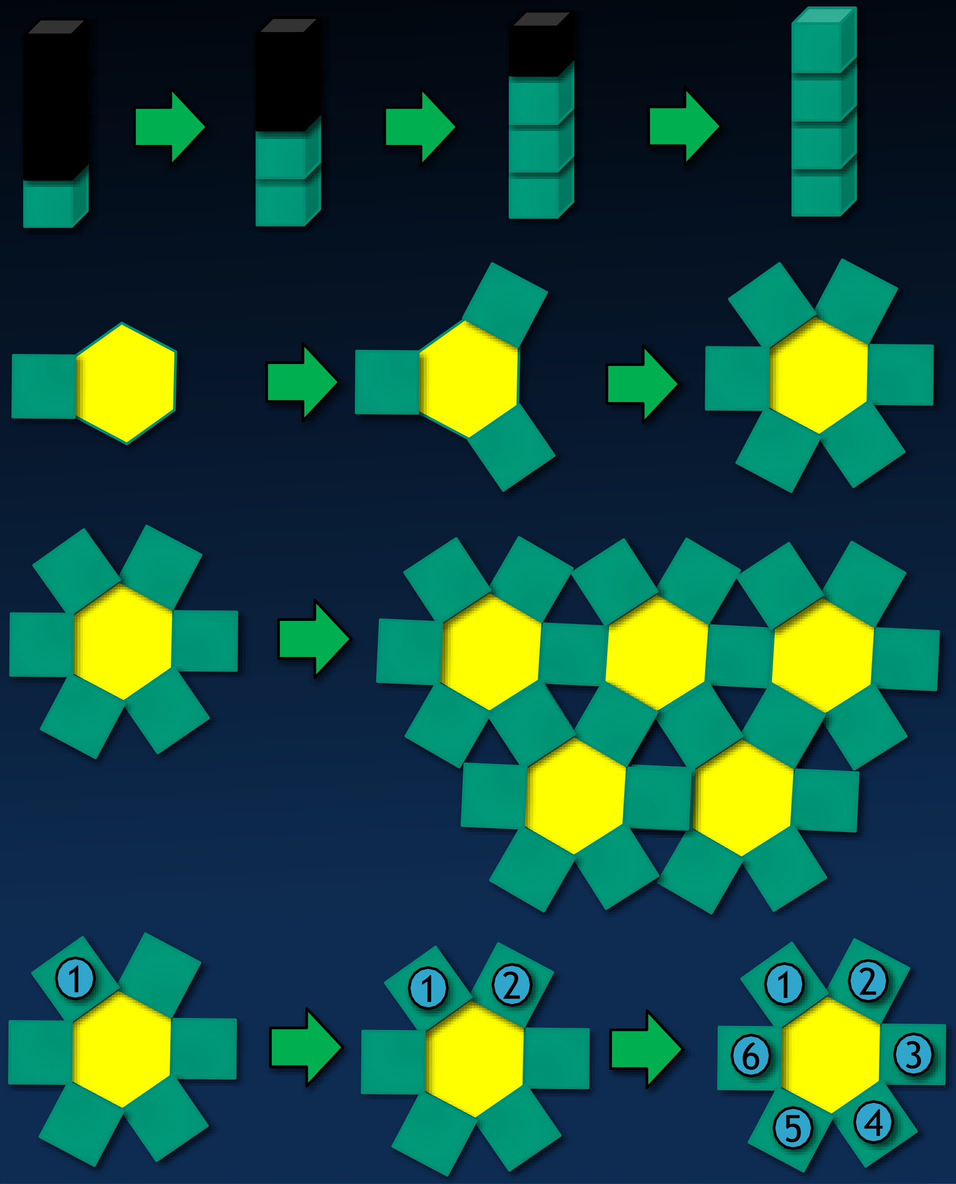


Material loading module
Processing modules
Characterization modules

Patent: R.L. Burchard, K.R. Klinger, B. Boyce, "Inspection Workcell," U.S. Patent 10,955,429, issued March 23, 2021.

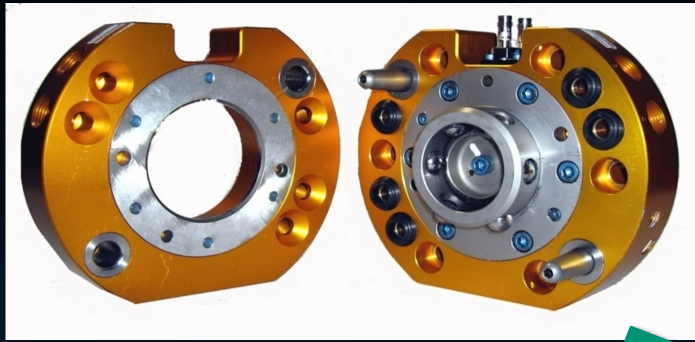
Modularity is key to *Alinstante* to enable flexibility, upgradability, etc.

- Stackable
- Extendable
- Scalable
- Parallelizable

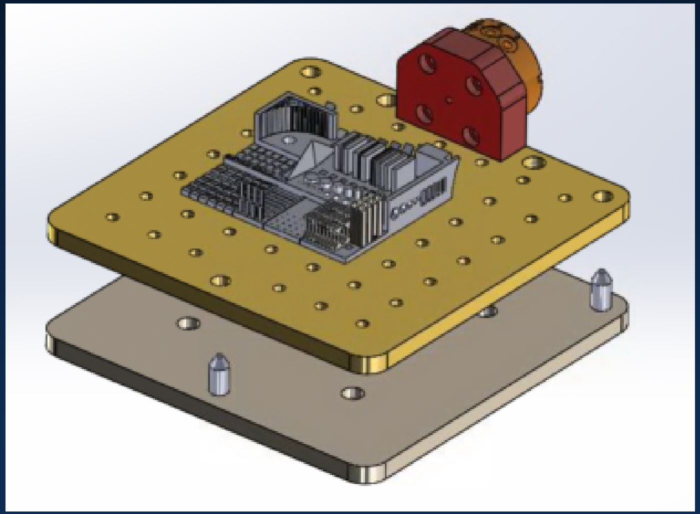


Patent: R.L. Burchard, K.R. Klinger, B. Boyce, "Inspection Workcell," U.S. Patent 10,955,429, issued March 23, 2021.

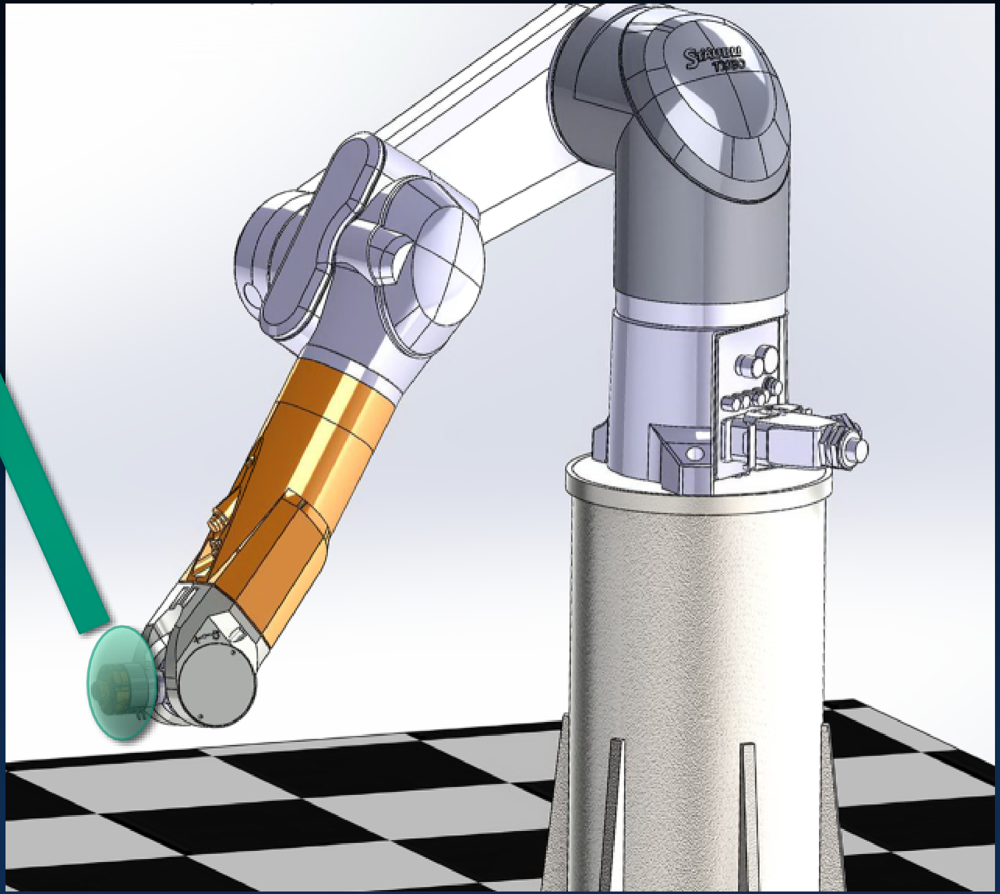
A multitude of system integration design compromises



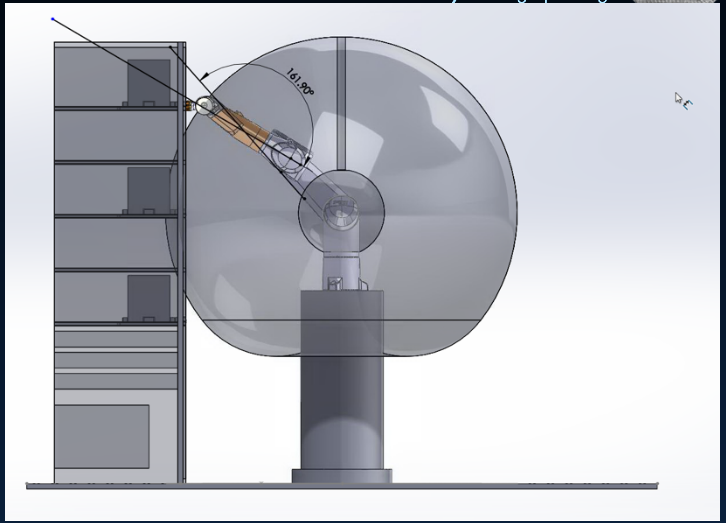
Pneumatic interface



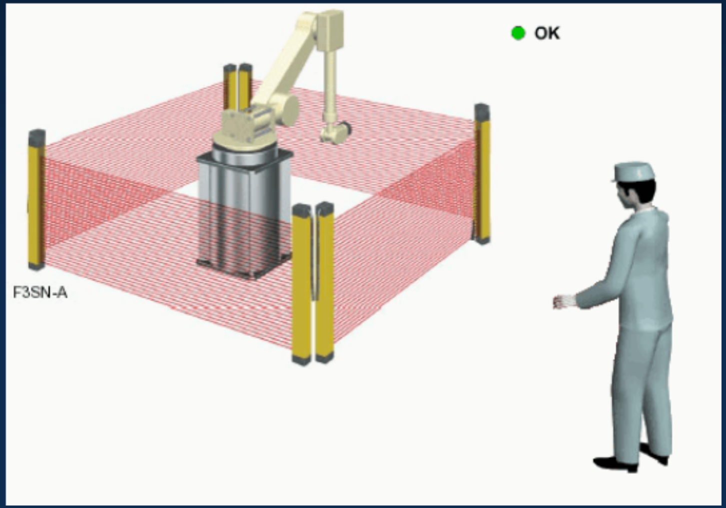
Part tray design



Arm range, position resolution, payload capacity



Reachability Analysis



Access Interlocks (Safety)

To accelerate materials science, we also need unconventional "samples"

Material Properties

Mechanical Properties
Arrays of tensile bars used to investigate stochastic tensile properties. Arrays of two different-sized tensile bars allow exploration of size-dependent mechanical properties

Structural Dynamics
Several cantilever beams of two heights can be used to test the resonance frequency of the material.

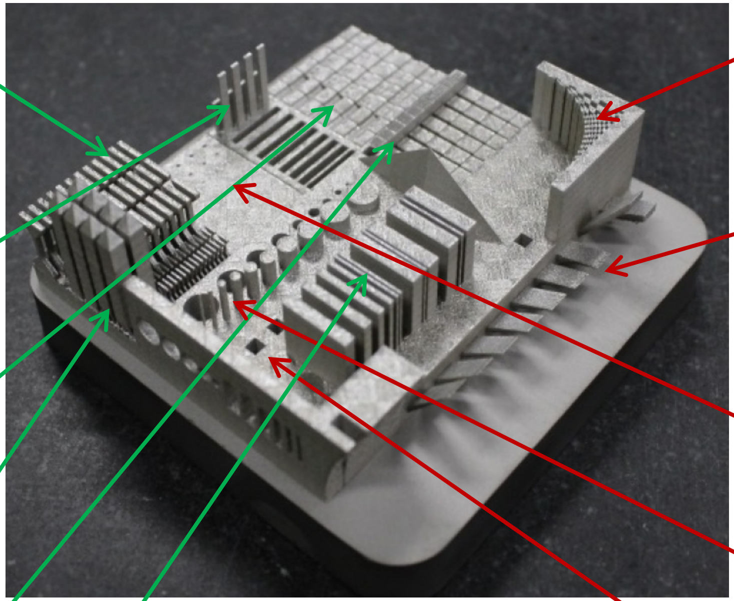
Notched Features
Arrays of notched features intended to explore stress-concentration effects on reliability and develop break-away coupons

Material Chemistry
Coupons to readily verify the composition and monitor contaminant levels.

Surface Roughness
Several features explore the interplay between geometry and the resulting surface roughness

Residual Stresses
Several features may be used to quantify the stress-induced warpage. Also, regions of the part exacerbate internal residual stresses to be measured by x-ray/ neutron diffraction or hole drilling.

Sandia Artifact printed in stainless steel alloy 17-4PH using a commercial vendor (Fineline) with a ConceptLaser Mlab Printer



Printability Limits & Metrology

Minimum Feature Dimensions
Evaluate printability and dimensional accuracy for a wide range of feature types including theoretical sharp corners

Overhangs & Bridges
Incrementally sized features intended to determine the maximum dimension that will maintain structural integrity of the part. Features push printer to failure point.

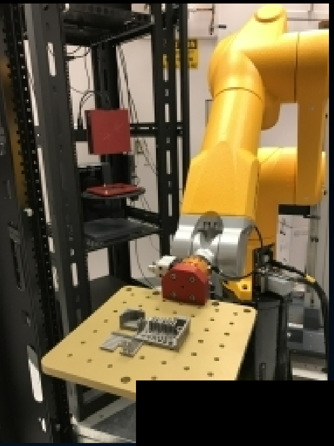
Internal voids
Intentional internal void arrays of varying dimension allow inspectability assessment

Aspect Ratios
A wide range of aspect ratios explores the printability limits of positive and negative features

Consistency features
Arrays of nominally identical features allow evaluation of repeatability

Most existing artifacts (e.g. NIST AM artifact) emphasize dimensional metrology and ignore material/structural properties. This compact array employs many dual-purpose features and many arrays of features for statistical repeatability analysis.

*Beyond*Fingerprinting



Putting it all together…

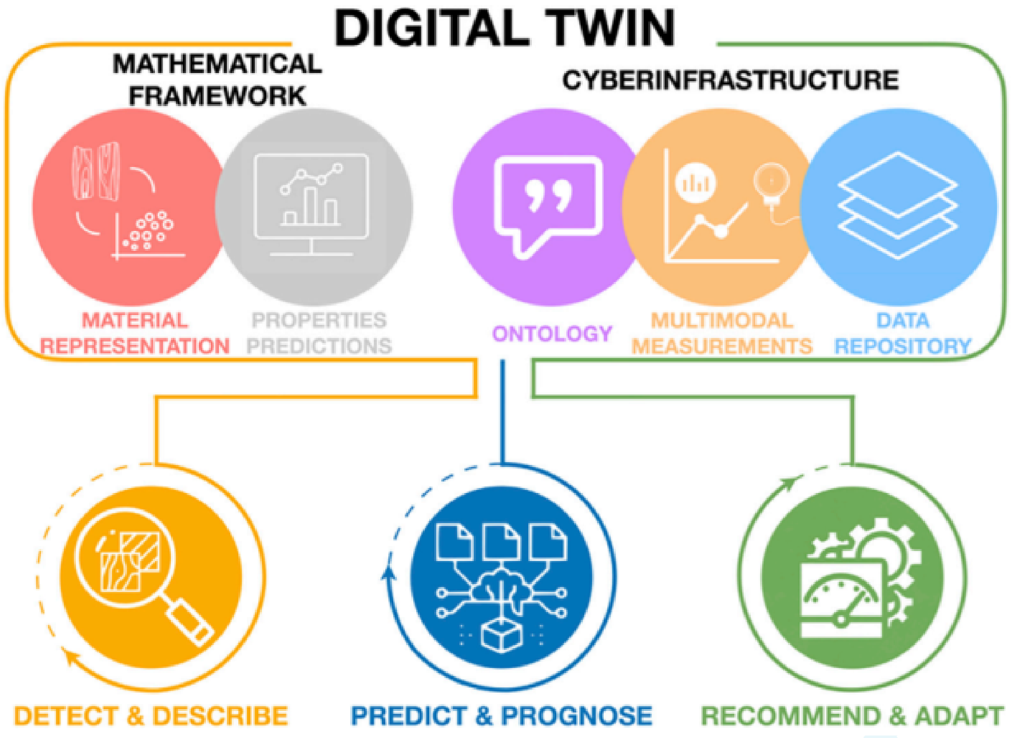
Enablers:
+ custom 6DOF robot arm w/ standard knuckle
+ custom light-curtain safety interlock system
+ custom (patented) end-station layout
+ a flexible, modular, expandable platform
+ workflow scheduling software
+ modular architecture allows incremental development and expansion.

Challenges:
- Software interface with each instrument requires custom solutions (not standardized).
- Weight and volume limits on sample.
- Environmental exposure limits on sample carrier.
- Limits on size of end-stations due to reachability limit of robot arm.
- Samples are manually loaded onto individual carriers.
- Expensive and time-consuming to create.
- **Need dedicated permanent space!**

Youtube: Sandia Alinstante

Multiple **Integration** Challenges

1. Scripting/Calling Individual Instruments/Modules
2. **Instrument APIs** and cross-hardware interfaces
3. Workflow management & scheduling
4. Harvesting data from proprietary formats
5. Automated data upload
6. Automated **metadata tagging**
7. Pedigree & **ontology** relationships tracking
8. Spatial registration of multiple datasets
9. Database/repository management (**SQL**?), curation/search
10. Integrated data access & **visualization** across platforms
11. Data down sampling / **compression** / augmentation
12. Stochastic reduced order data representation
13. Integration of modeling & simulation data
14. Bayesian experiment planning
15. Integrated **multimodal** analysis



Kalidindi, Buzzy, Boyce & Dingreville, “Digital twins for materials”, *Frontiers of Materials*, 2022

Are we prepared for a multimodal data avalanche?

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Pre-process | In-process | Post-process

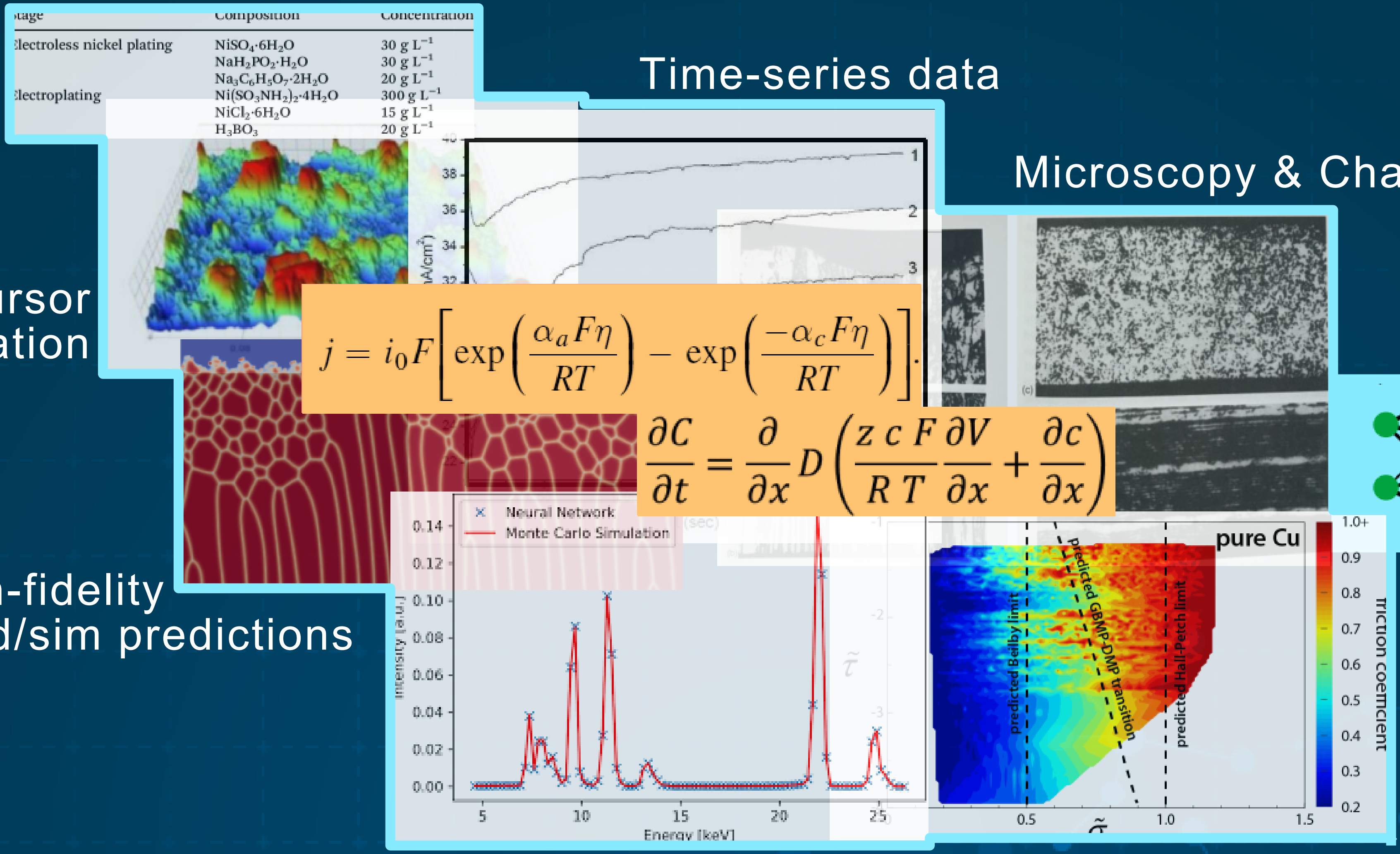
Process settings

Precursor characterization

High-fidelity mod/sim predictions

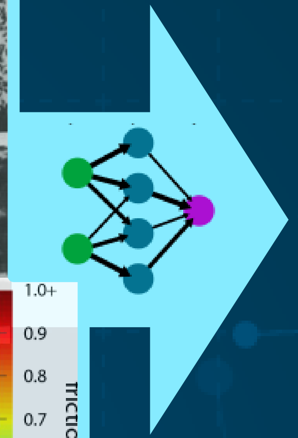
Time-series data

Microscopy & Characterization



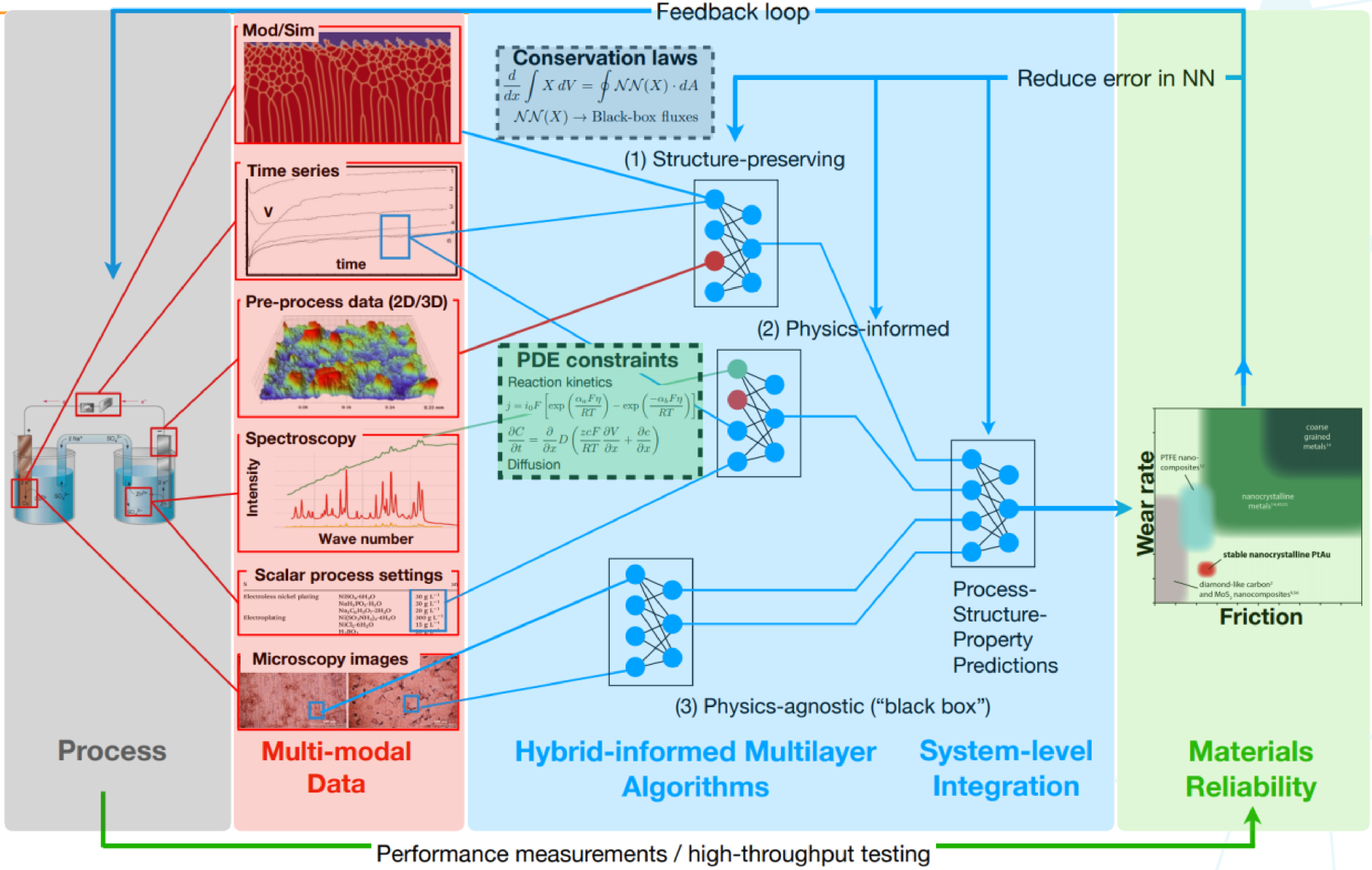
In-situ characterization

Property/Performance/Aging Measurements

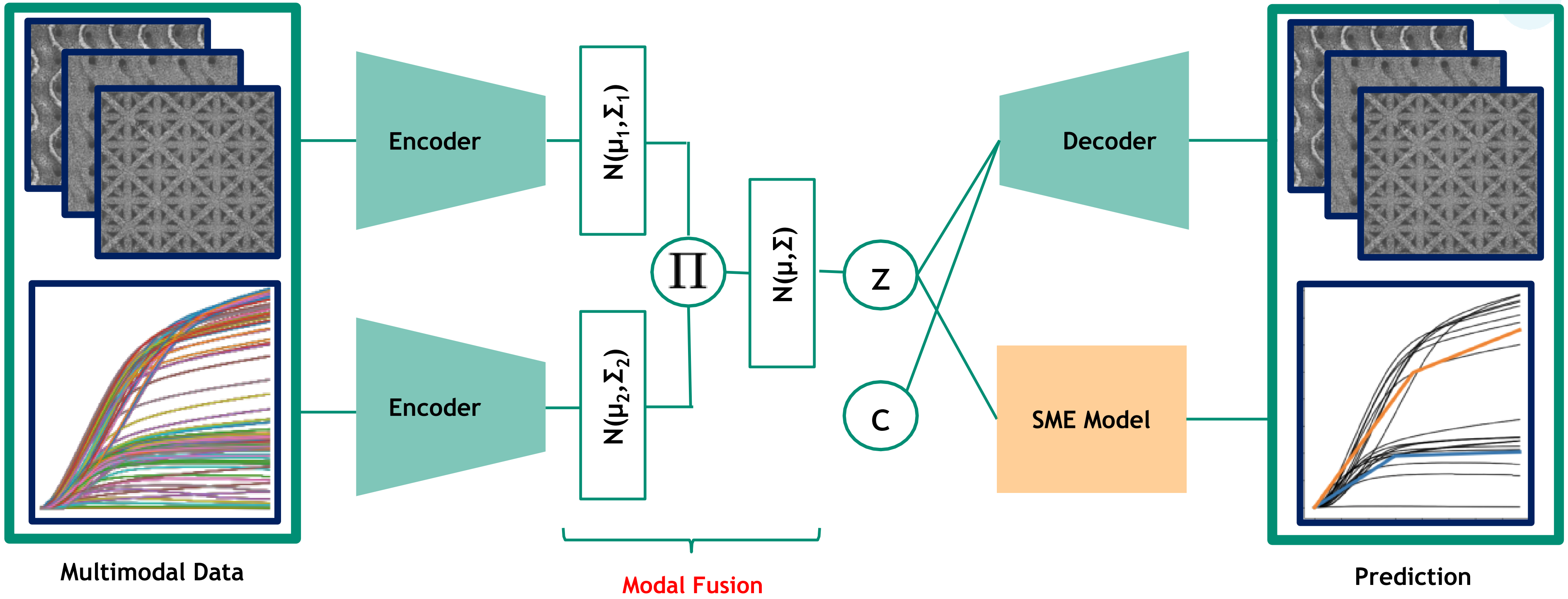


Discover Reliable Materials/ Processes

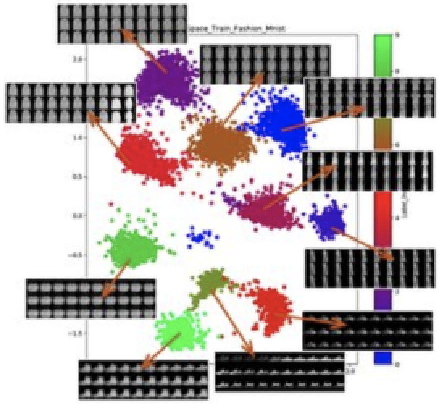
Himulaya: Hybrid-Informed Multilayer Algorithms



Physics-Informed Multimodal Autoencoder



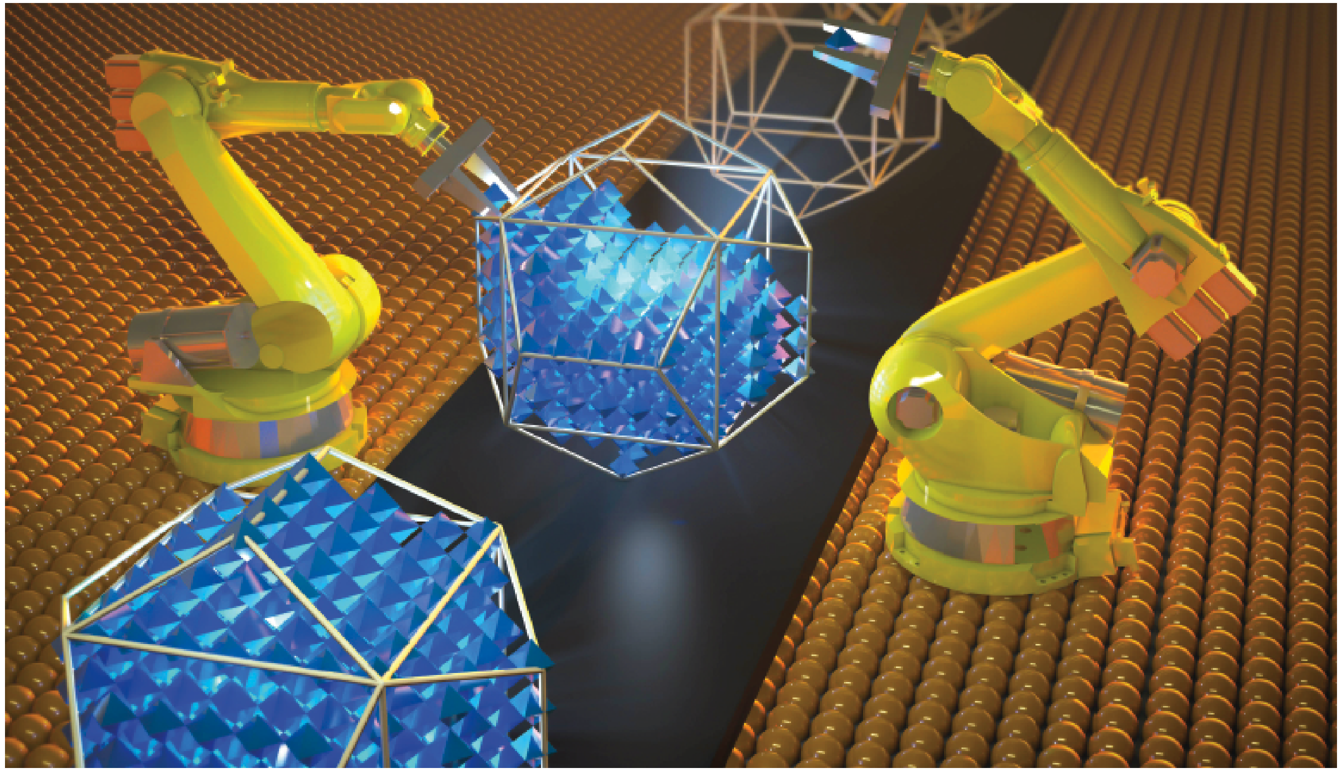
Informal Idea:
We discover a shared latent representation of data providing a Rosetta stone for across modalities
w/ uncertainty estimation

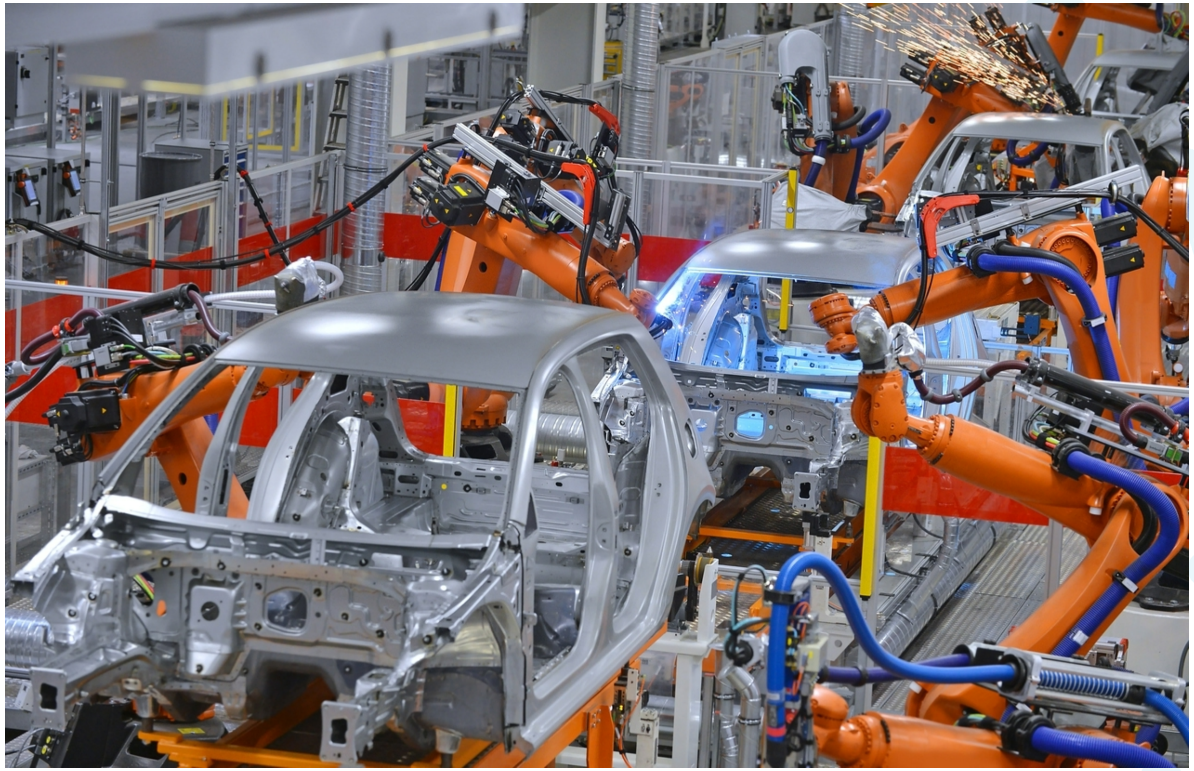


Formal Idea:

- Gaussian product distribution gives deep posterior embedding for each modality
- Gauss mixture prior in latent space identifies populations in data across modalities
- *Closed form expressions* for loss - no Monte Carlo
- Supports Bayesian inference across modalities

Parting words: the bridge between materials discovery and manufacturing





Beyond material discovery, acceleration (and autonomy) will enable materials scientists to develop <u>robust</u> materials and processes, often in a way that's compatible with digital manufacturing (**Industry 4.0**).