Oak Ridge National Laboratory

Artificial Intelligence and Machine Learning: Issues and Opportunities

International Conference on Neuromorphic Systems

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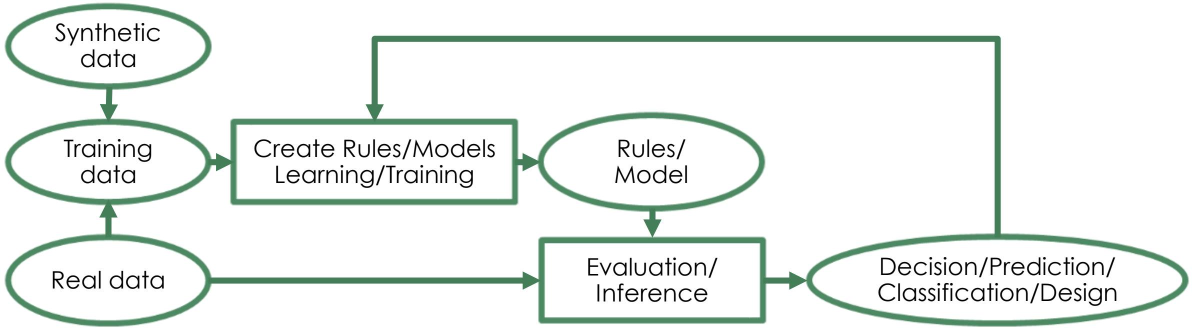
Oak Ridge National Laboratories

What are Artificial Intelligence (AI) and Machine Learning (ML)

- A class of data analytics algorithms in which the rules and/or models are not known a priori and are learned as part of the process
  - Process data to identify correlations
  - Complexity of the model is a potential problem

- Computers trained to perform tasks that if performed by a human would be said to require intelligence
  - Knowledge-based tasks
  - Computers are good at working with data, not “meaning”

Are we trying to reduce “knowledge” to an equation?



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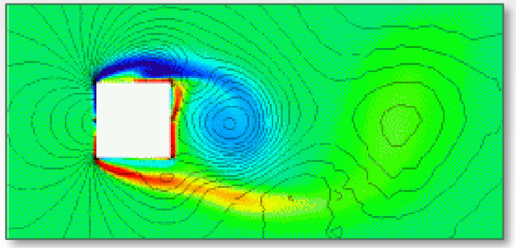
An AI Taxonomy

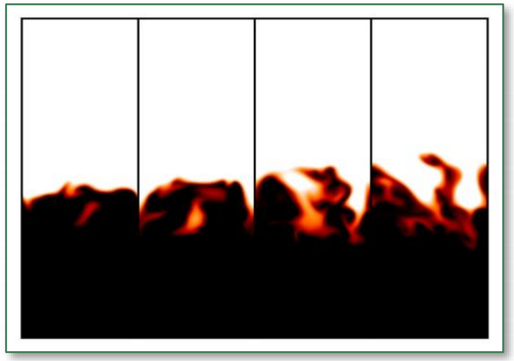
Classification and regression

Near Infrared (single band) WorldView-3 image

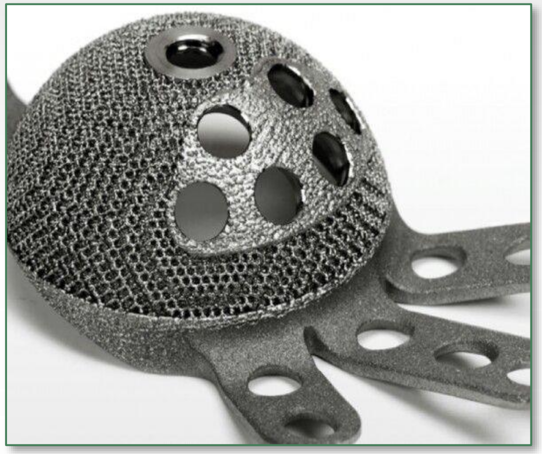
CODA cloud detection saliency map for image above

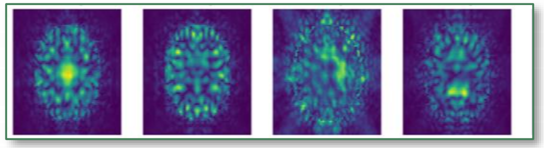
Surrogates





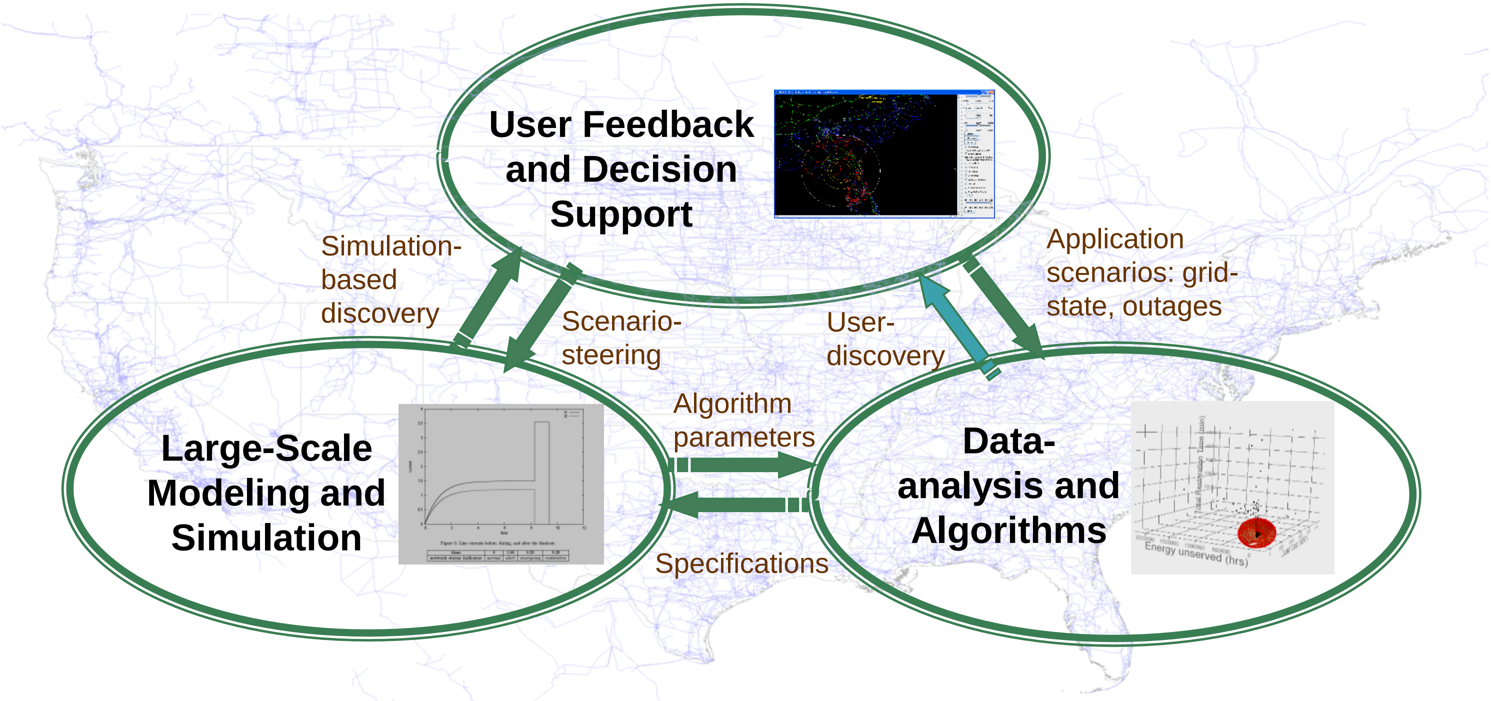
Inverse problems, including design and optimization





Control systems

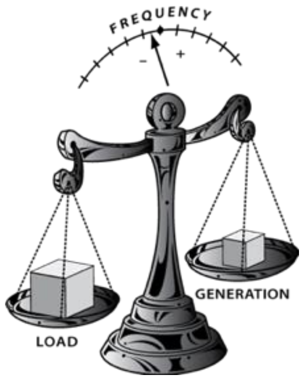
Applications at ORNL: Smart Grid



- Learning algorithms for wide-area, hierarchical information sources
  - Distribution: Intelligent loads, SCADA devices, DERs
  - Transmission: Protection systems, power flow control
  - Generation: Planning and coordination
  - Control: Situational awareness, fine-grained control of DERs, enhanced reliability and resilience

Smart Grid: Challenges

Application challenges	• Integrating variable distributed energy resources (DERs) with intelligent interfaces • Integrating storage at multiple layers • Integrating electric vehicles (EV) • Managing demand – Residential, Commercial, Industrial – Enabling energy coordination and trading between buildings and trading between buildings and grid
Technology challenges	• Connectivity across DERs • Scalable control and diagnostics algorithms that are driven by data • Actionable, real-time situational awareness • Data and physical system security, including privacy



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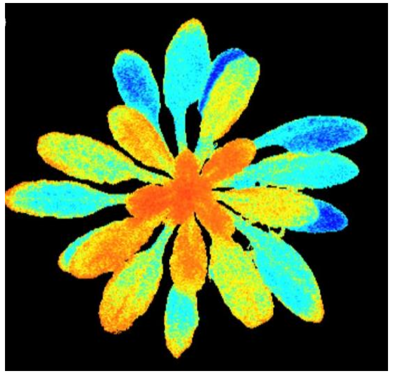
Applications at ORNL: Biosciences

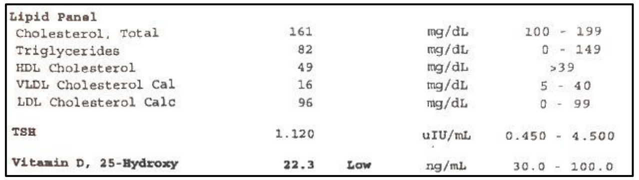
Image analysis

The Cancer Imaging Archive

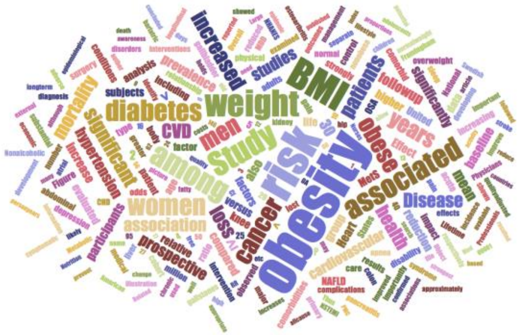


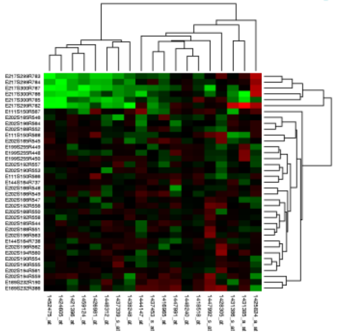
Phil Trans R Soc London B **363** (1491), 639-658

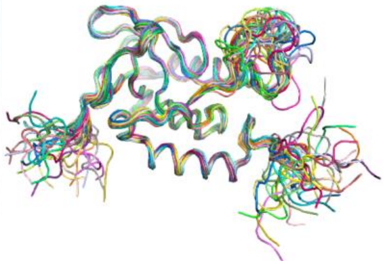
Multimodal data

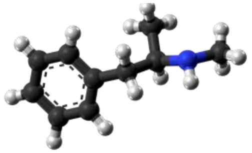


Lipid Panel				
Cholesterol, Total	161		mg/dL	100 - 199
Triglycerides	82		mg/dL	0 - 149
HDL Cholesterol	49		mg/dL	>39
VLDL Cholesterol Cal	16		mg/dL	5 - 40
LDL Cholesterol Calc	96		mg/dL	0 - 99
TSH	1.120		uIU/mL	0.450 - 4.500
Vitamin D, 25-Hydroxy	22.3	Low	ng/mL	30.0 - 100.0









Complex traits

Human health

- Cancer
- Heart disease
- Suicide
- Addiction
- Interventions

Plant science

- Drought tolerance
- Disease resistance
- Biomass yield
- Carbon fixation

Applications at ORNL: Biosciences

Massive multi-modal data sets

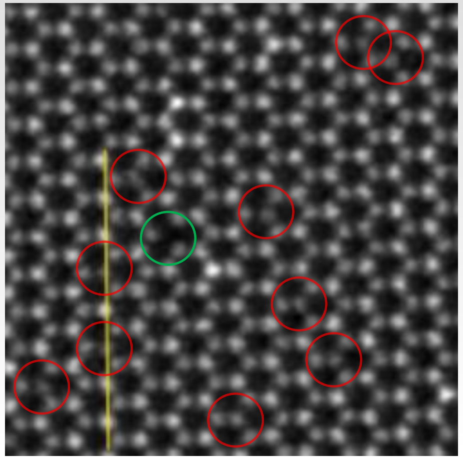
- Million Veterans Program health records
  - Clinical records, genomic data
- Plant phenotyping
  - Imaging data, genomic data
- Genes to cells model
  - ExaLearn, physicochemical data

Data to mechanism

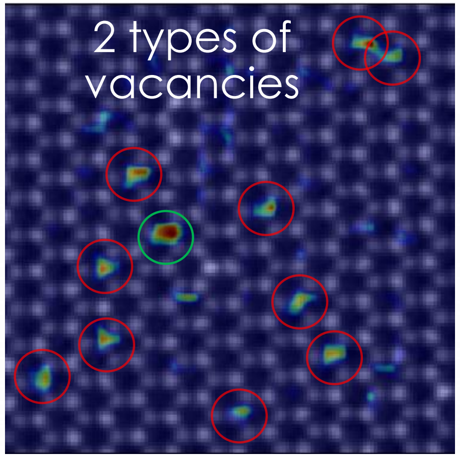
- Experimental/computational feedback loops
  - Hypothesis testing
  - Uncertainty quantification
  - Experimental design
- Explainable AI
  - Mechanistic understanding
  - Hypothesis generation

Applications at ORNL: Materials science

Automated defect classification

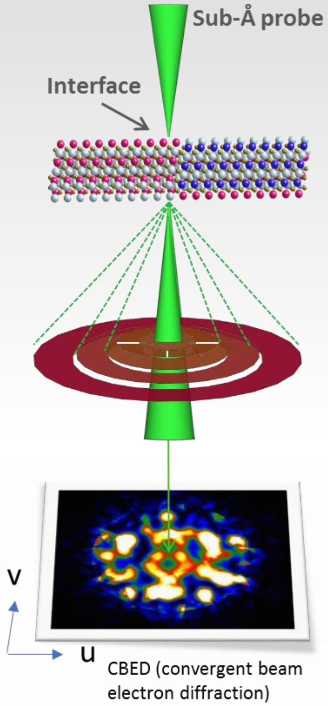


Experimental image

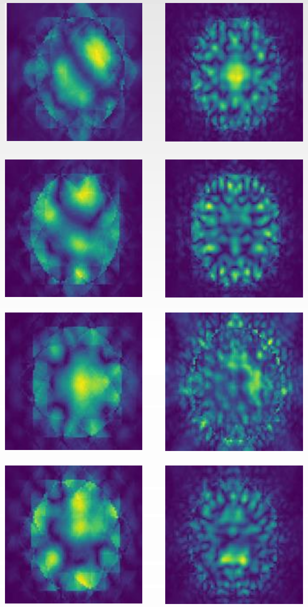


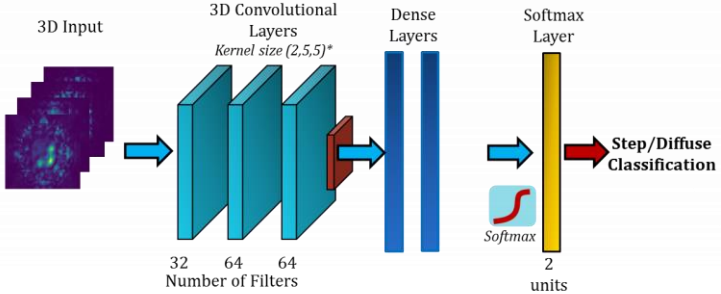
Model output

Inverse problems in imaging

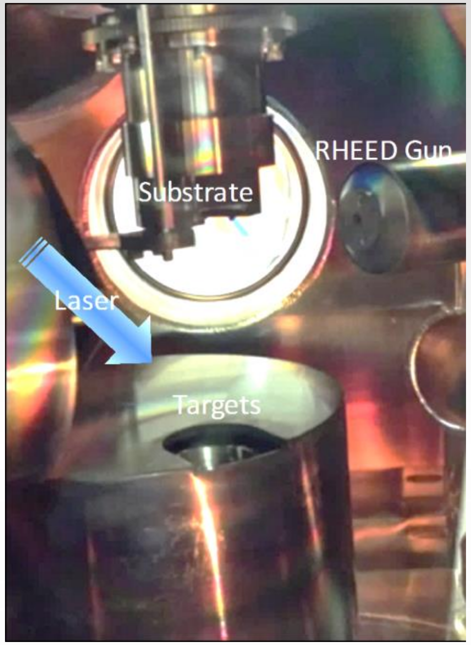


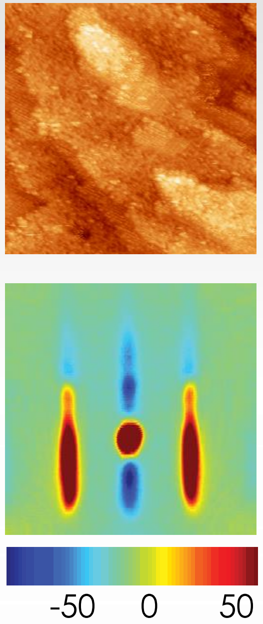
Interface structure classification





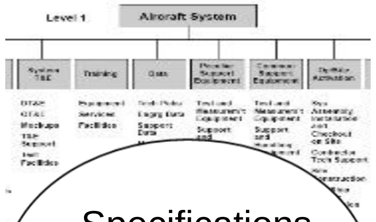
Pulsed laser deposition



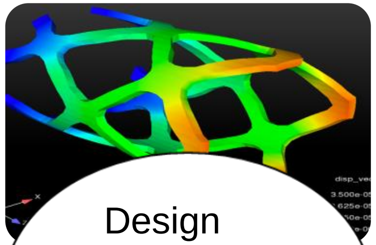


- Design and control of thin-film heterostructures
- Prediction of growth conditions and control of trajectory

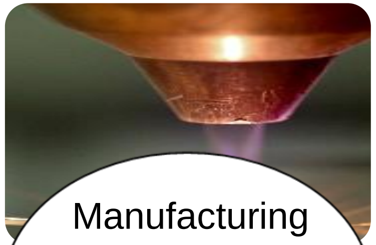
Applications at ORNL: Additive Manufacturing



Specifications
- Functional
- Environmental
- Margins



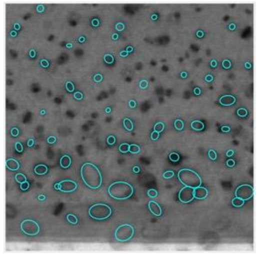
Design
- Shape
- Topology
- Material
- Process

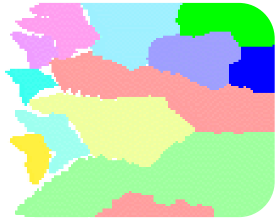


Manufacturing
- RT controls
  - Environment
  - Process
- Diagnostics

Testing
- Validated Process
- Test design

- Impact of machine learning
  - Surrogate models
  - Steering high-fidelity simulation
  - Design, particularly materials and processes
  - Real time diagnostics and control during manufacturing
    - Defect detection and mitigation
    - Control of local structures
  - Predicted performance based on manufacturing data
  - Test design and control



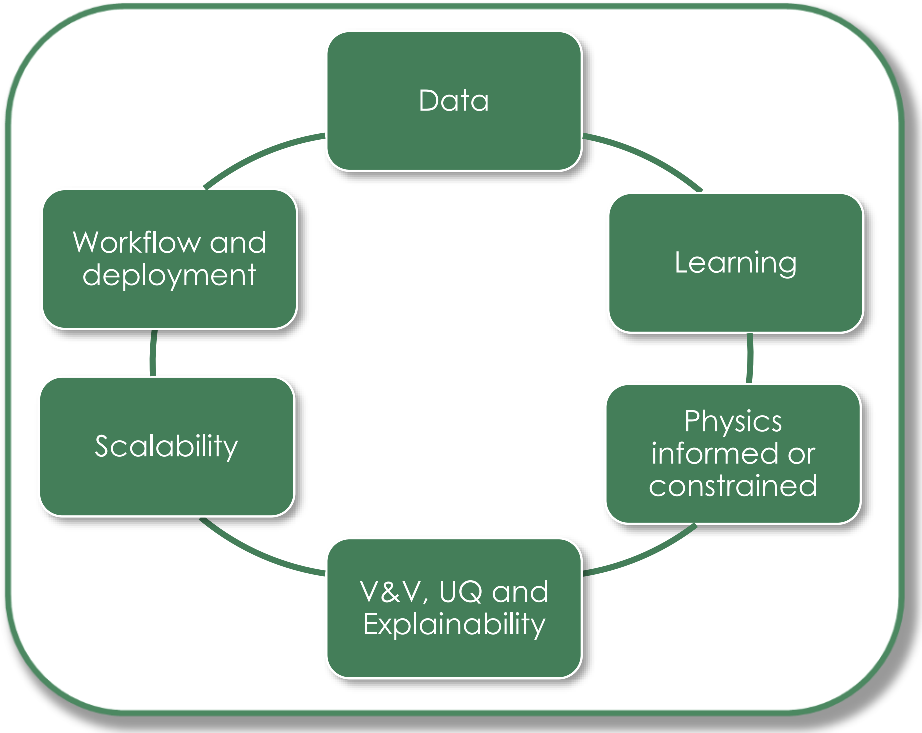


Observations to start a conversation

- Observations and issues
  - AI is effective at for narrowly defined tasks and only identifies correlations in (complex) data
  - Access to and availability of “good” and “labelled” data is one of the biggest challenges for AI
  - We need a sustainable data and compute infrastructure
  - While we have big machines, we don’t have scalable algorithms
  - Vulnerability threats for AI (hacking, intentional manipulation) are a huge concern for deployment
  - We don’t know how to do validation
  - HCI is an important component of the workflow, including explainability and interpretability
  - Deployment of AIs introduces a whole new set of challenges
  - Need to understand the ethics and human impact
  - AI is not synonymous with deep neural networks

Six Research Areas To Be Addressed

- Data quality and statistics
  - Even if we have enough data, it is not necessarily good data
  - Dealing with bias
- Machine learning
  - Needs to accelerate
  - Very model dependent
- Merging physics and AI
  - We can't violate the laws of physics
- Verification, validation and explainability
  - Is the answer right, is the model appropriate, and can we understand it
  - What is the human-computer interface
- Computing
  - How do we use "big" computers
  - How do we use accelerated nodes
- Workflow and deployment
  - Computing at the edge
  - privacy, ethics and regulations



Issue: “Syntactic” Space vs. “Semantic” Space

- Humans tend to think in semantic space, i.e., in terms of the meaning.

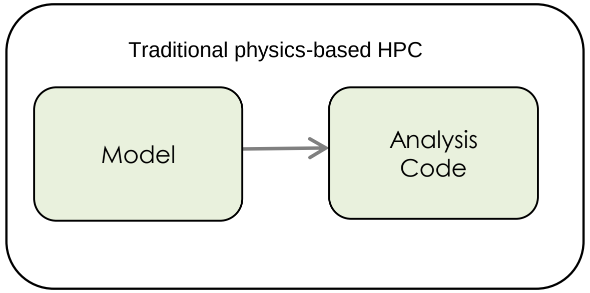

And metrics in semantic space are fundamentally different from those in syntactic space

- Implications
  - Easy to spoof classification systems
  - Transfer learning doesn’t map well.

    (Humans tend to transfer learning in semantic space, e.g., transfer what I learned about human behavior in kindergarten to how I drive. Most AI approaches transfer in syntactic space or transfer parts of the model (a sort of “gene transfer”).

Issue: Verification, Validation, Explainability and Interpretability

- Verification
  - Is the model implemented correctly?
- Validation
  - Is the model (including training data) appropriate for the decisions being made?
  - Must be evidence based
  - Requires some form of UQ, robustness guarantees and bounds on “distortion”



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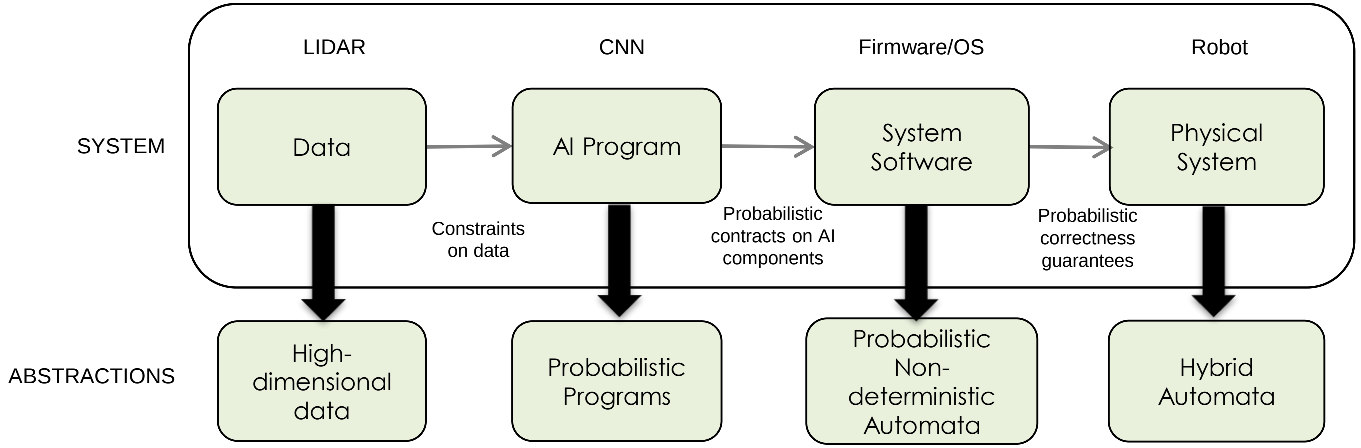

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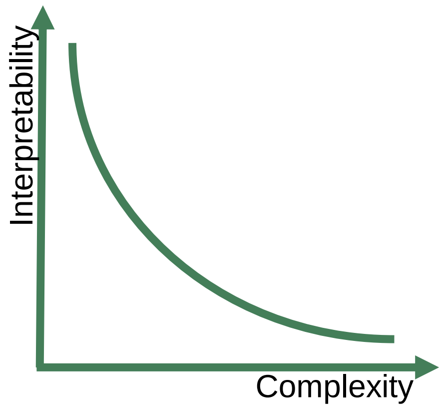
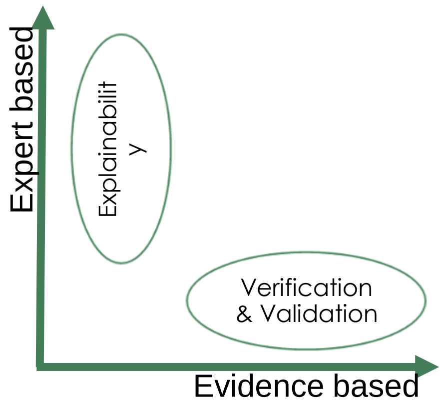
Issue: Verification, Validation, Explainability and Interpretability

- Interpretibility
  - Can a human understand the model? For example, do the basis vectors in a dimension reduction algorithm have a physical meaning?
- Explainability
  - Can the model present a sequence of steps that can justify the answer to an expert?
  - Expert based
- Reproducibility
  - Does the same experiment lead to the same conclusion?
  - Can we run different experiment and not contradict our conclusion?
  - If we create a new model with the same data, do we get the same conclusions?
  - Required for good science
-



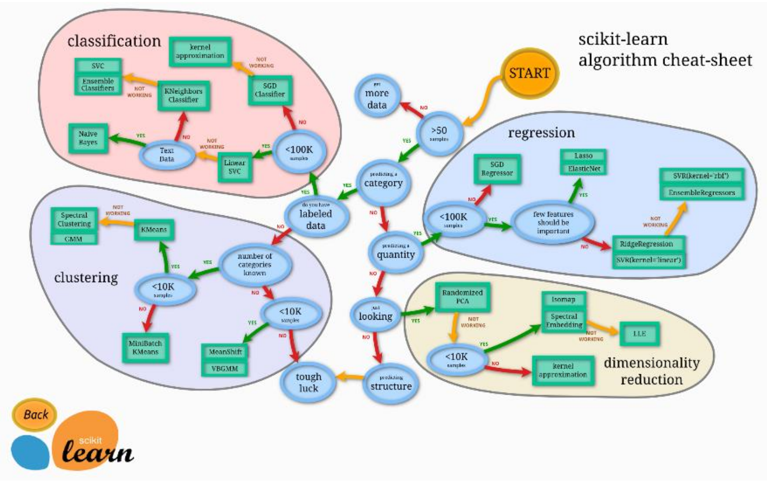


Issue: Big Data Is A Big Problem

- Need more data than was imagined just a few years ago
  - We are looking for complex correlations
  - Using primarily statistical methods
- Labelled data is a problem
  - Generating labels is expensive and labor intensive (e.g., Mechanical Turk)
  - Need to move toward reinforcement learning
- Noisy and missing data is a problem
- Data needs to be curated
- Synthetic data and simulated environments are partial solutions
  - But an AI can learn the flaws in these systems

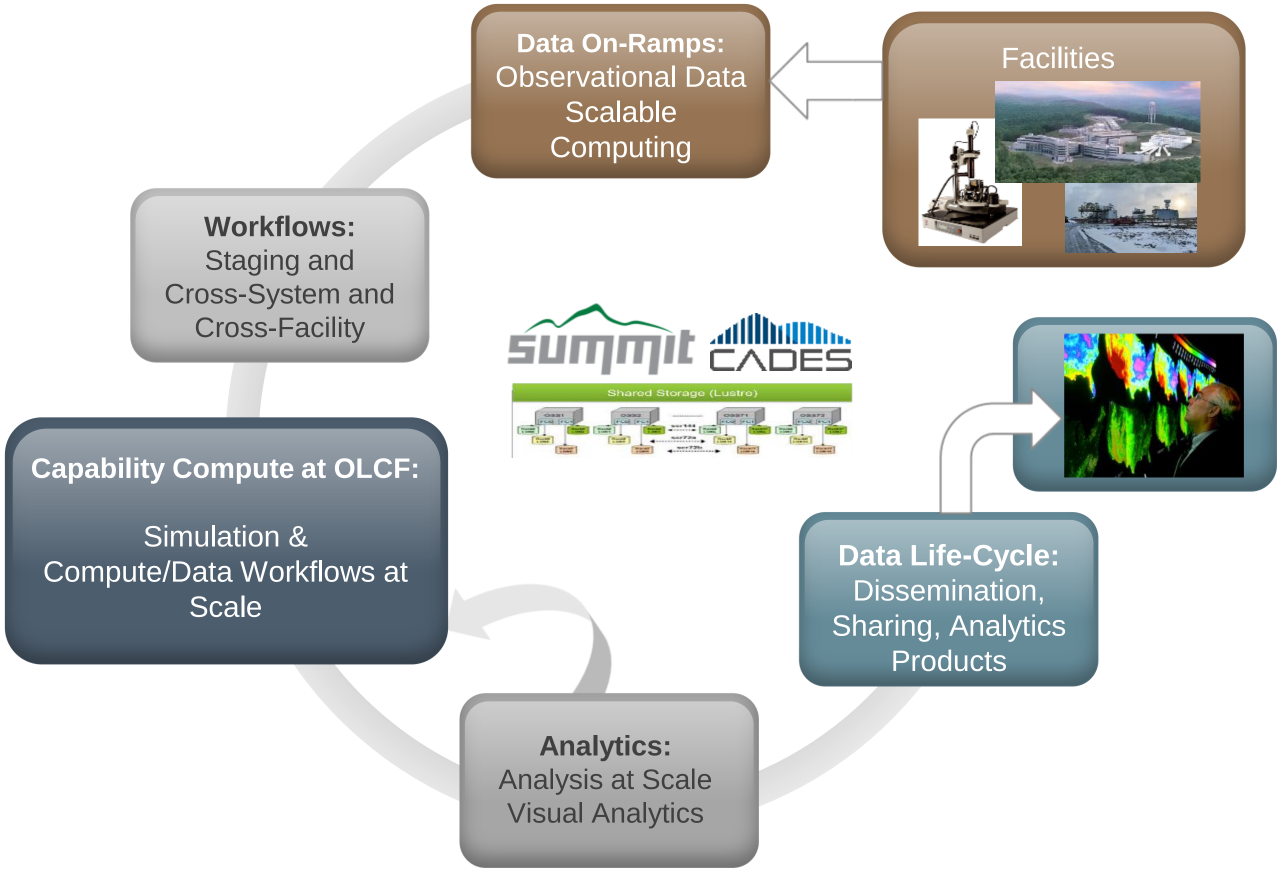
Issue: AI Is An Art

- Choosing the model form and hyper parameters is often ad-hoc and requires experience and insight
- AI models must be tuned
- Neural networks design is difficult and often requires tuning
- Interpreting the results requires expertise



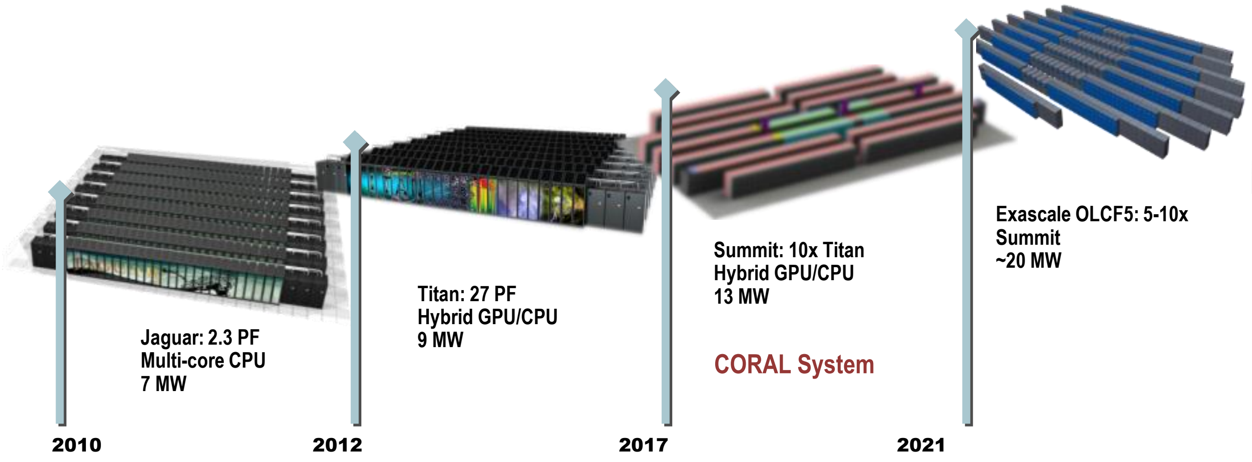
> "Machine learning methods are often described in papers at an abstract level, for maximum generality. However, a good choice of hyperparameters is usually necessary to make them work well on real-world problems, and tricks are often used to make most efficient use of these methods and extend their capabilities."
>
> G. Montrevan, et.al., "Methods for Interpreting and Understanding Deep Neural Networks."

Infrastructure is critical to a good workflow



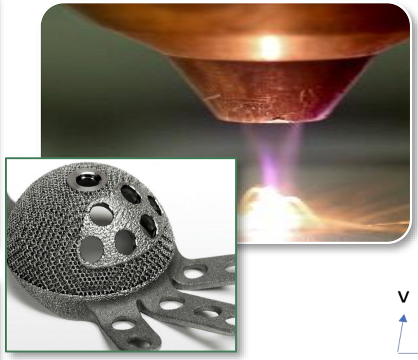
New HPC capabilities enable AI

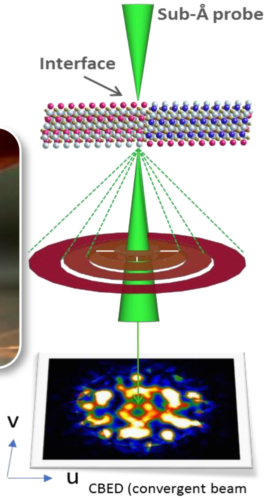
- We have the ability to collect and store large amounts of data
- Computational power continued to increase, with architectural improvements that are amenable to neural networks and AI more generally
  - For example, GPU became practical for accelerated computations.
  - Reduced-precision tensor core units are included



AI is changing the way we do science and engineering

- Science and national security drive the applications at ORNL
  - New materials and processing
  - Autonomy and control
  - Predictive and personalized health systems
  - Energy and the environment
  - Disaster response and security
  - Unique data sets and user facilities
- Research in AI and machine learning establishes the capability
  - Scalability for world-class facilities
  - Innovative learning algorithms
  - Bringing together mathematics, statistics, computer science and data science





CBED (convergent beam electron diffraction)