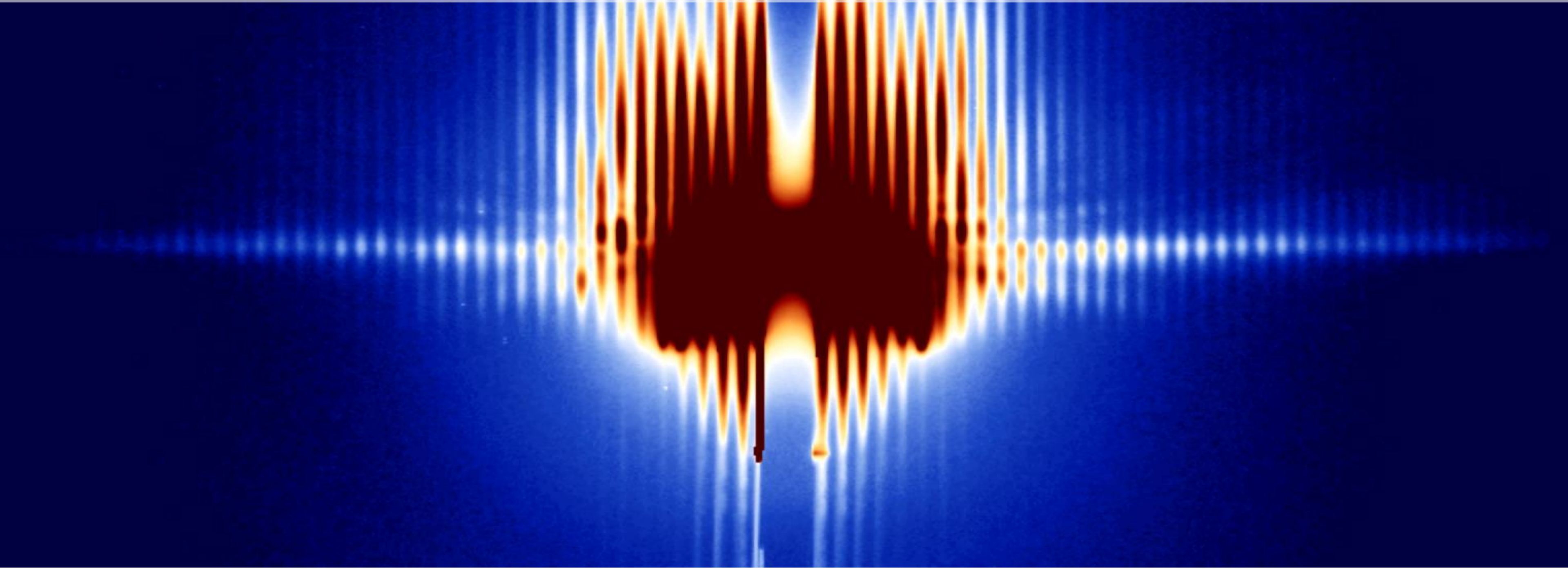
Deep Structured Analysis for Image Datasets from CFN and NSLS-II



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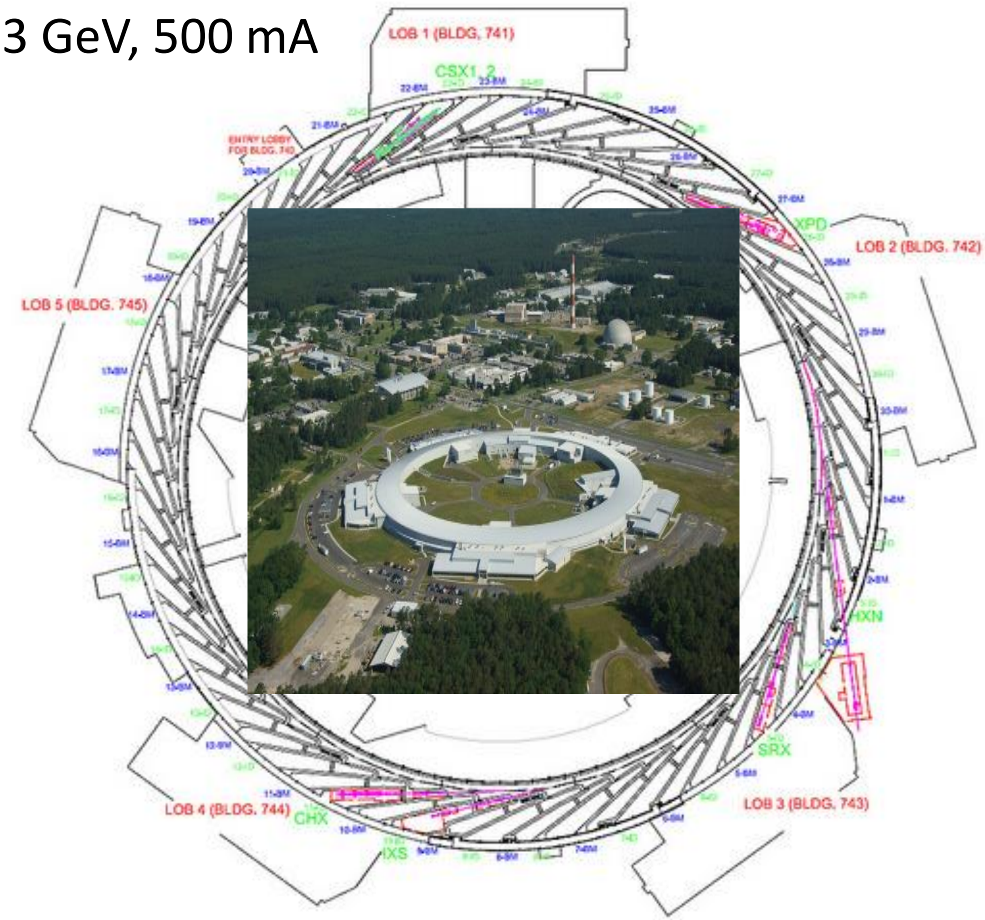
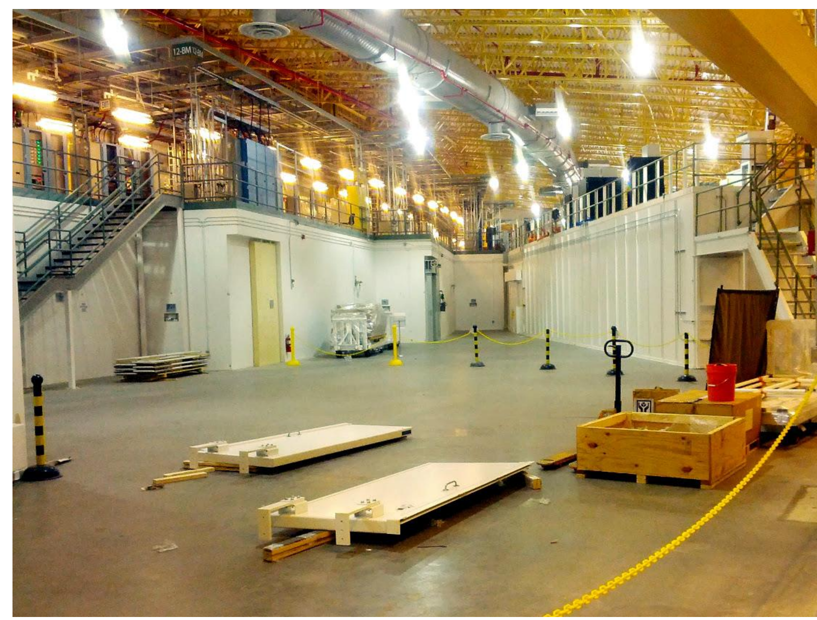
NSLS-II

- $912M
- 791 m circumference
- 58 beam ports
- 3 GeV, 500 mA



- Each x-ray beam is ~10^{13} ph/s



Motivation

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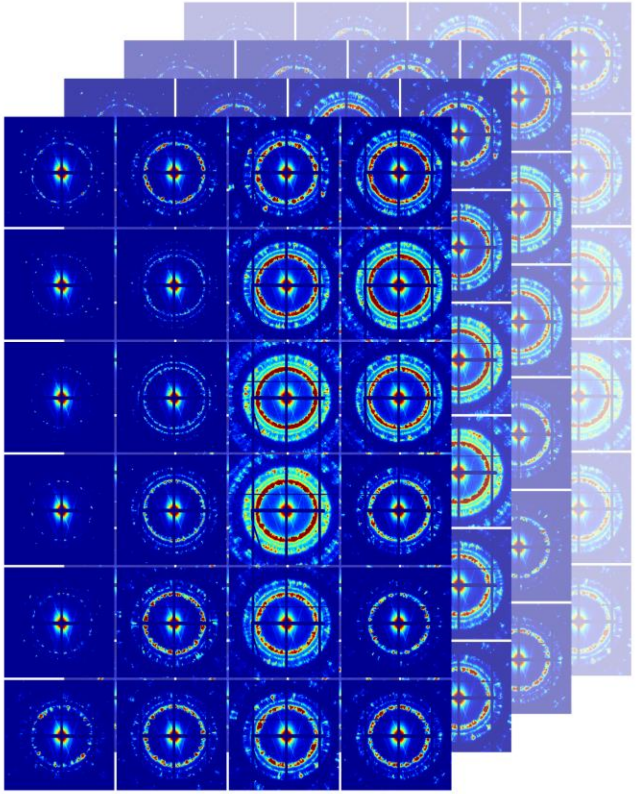
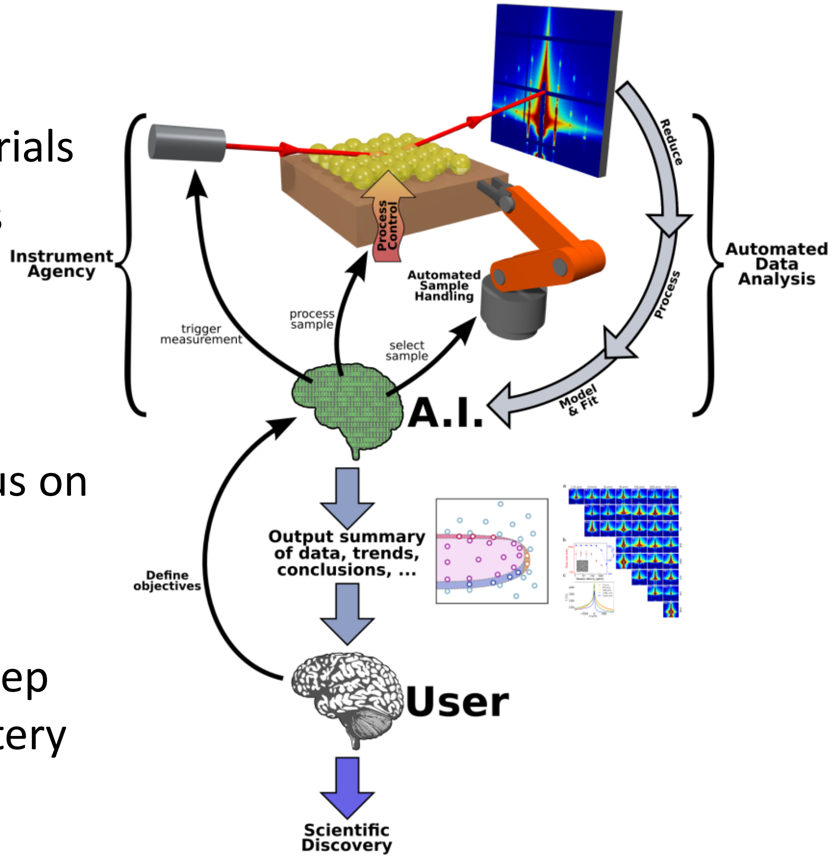
- Modern scientific experiments generate massive amounts of data
- Complex data analysis consumes scientists' precious time, distracting from deep scientific questions
- We can train machines to perform much of the workflow
- **Deep learning** can extract meaningful insights and detect patterns from massive amount of data; well-suited to image-like datasets



Impact to Materials Science

- NSLS-II beamlines study materials from many perspectives:
  - Complex, multi-component, hierarchical materials
  - Diffraction, scattering, coherence experiments
  - Structure & dynamics across many scales



- If machine automation/learning become part of experimental workflow, scientist is liberated to focus on scientific discoveries

- Will shorten the latency between experiment to deep scientific insight, Impact for material design of battery components, solar PV, etc.

- Develop at CMS and CHX; and extend to other beamlines (SMI, LiX, FXI, HXN)

- To enable **automated materials discovery** across many synchrotron beamlines (Multimodal Analysis)

Objectives

- Low-level: identifying characteristic features in a diffraction image;
- Intermediate-level: detecting the occurrence of a physical process from a sequence of images;
- and 3) High-level: learning and predicting scientifically-meaningful trends.
- On-line Recognition and Prediction with Incremental Information
- The velocity of processing must be commensurate with that of data generation.

Preliminary Work

- Initial work has demonstrated the viability of applying machine-learning methods to synchrotron data

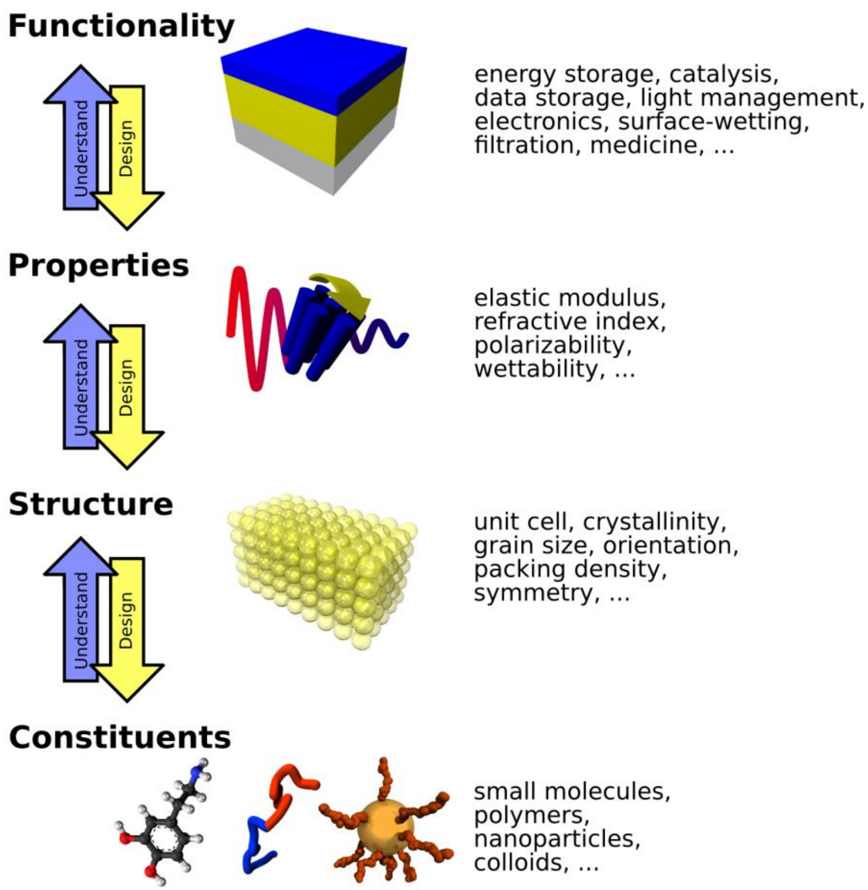
- Applied machine-vision methods to tagging and classifying x-ray scattering images
  - *Materials Discovery: Fine-Grained Classification of X-ray Scattering Images* Kiapour, M.H.; Yager, K.G.; Berg, A.C.; Ber, T.L., Winter Conference on Applications of Vision (WACV) 2014 (Steamboat Springs)

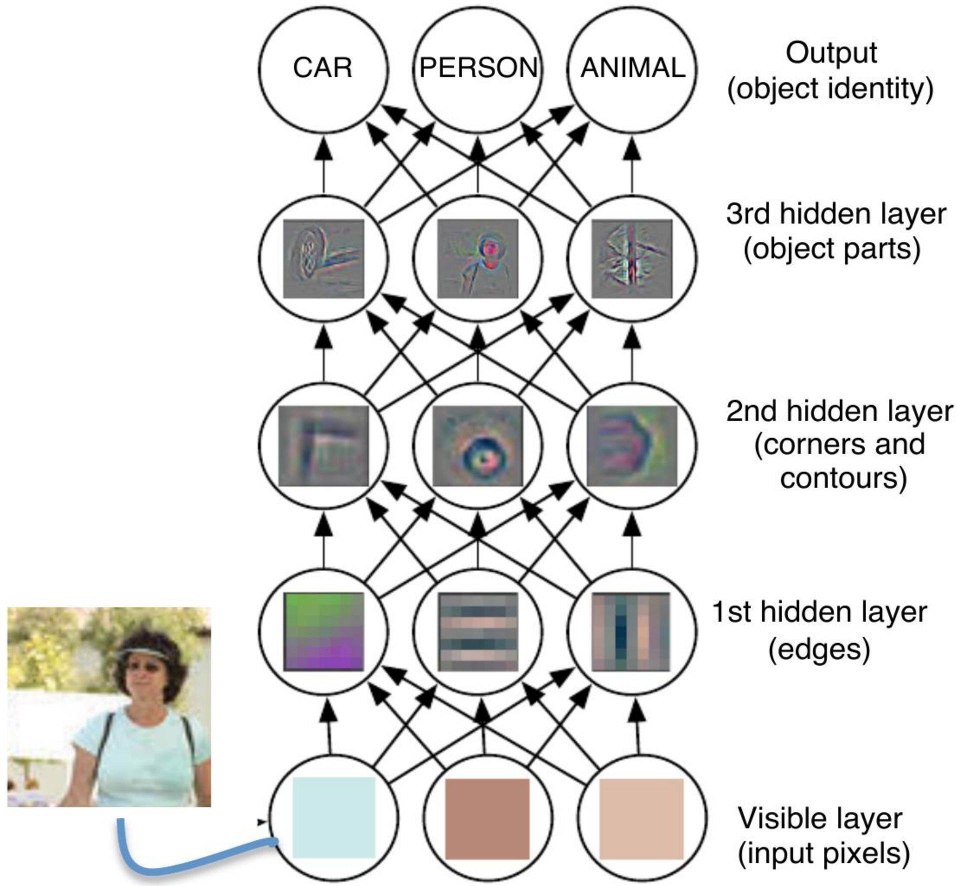
- Used advanced clustering methods to organize synchrotron data
  - *Diffusion-based Clustering Analysis of Coherent X-ray Scattering Patterns of Self-assembled Nanoparticles* Huang, H.; Yager, K.G.; et al., 29th Symposium On Applied Computing (SAC'14) March 24-28, 2014, Gyeongju, Korea

- Exploring machine-video methods to identify events in time-sequence scattering data
  - Ongoing collaboration with M.H. Nguyen, Stony Brook University

New Ideas

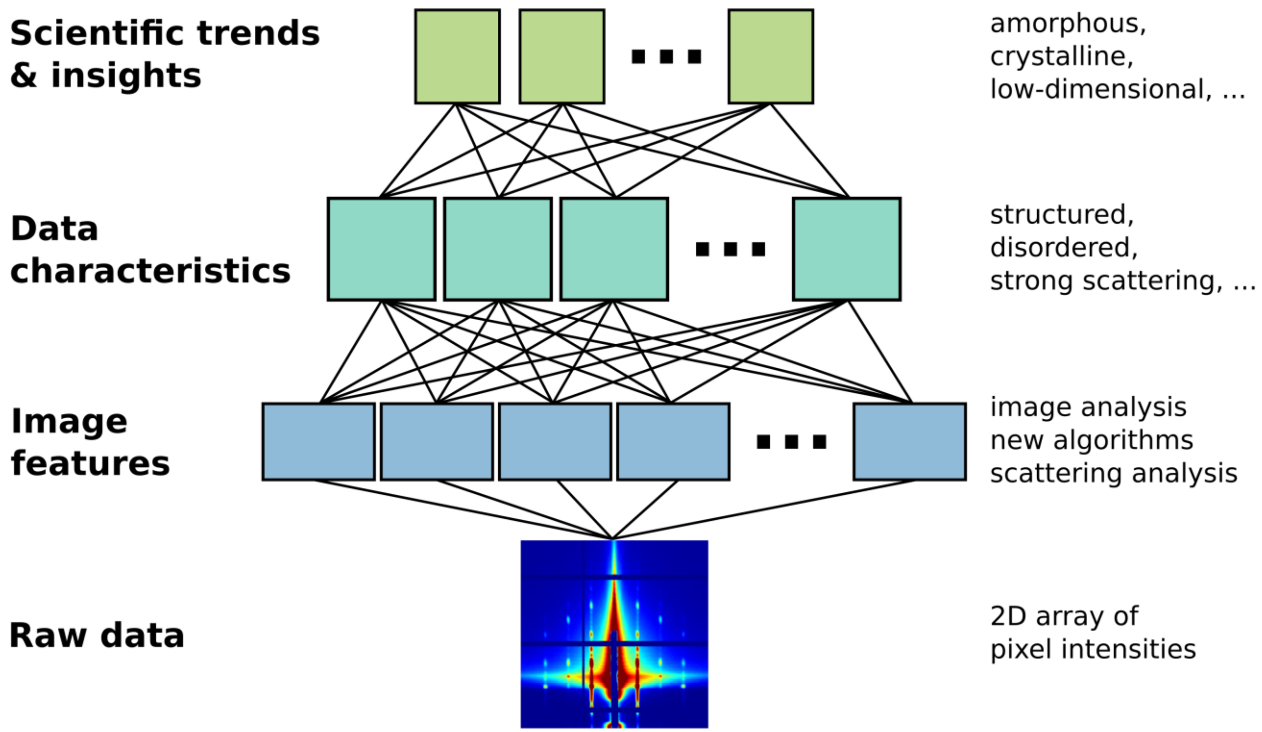
- Physical systems have natural hierarchies
- Deep-learning trains multiple levels of features/representations to extract meaning from data
- We will explore machine-learning hierarchies tuned to extract physics layers and meaning from scientific datasets





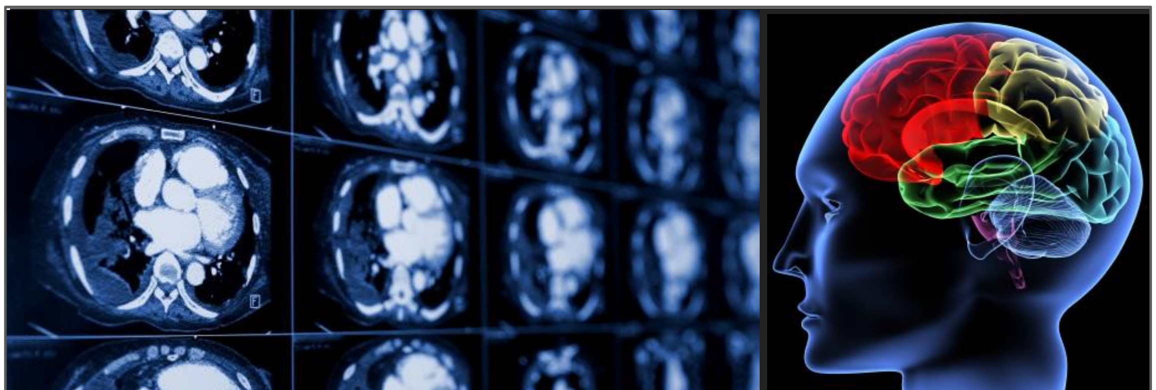
Technical Approach

- Synchrotron images analyzed using a combination of existing domain and image-analysis techniques, as well as new algorithms
- (Supervised/Unsupervised) Cluster and tag the data with physically-meaningful attributes
- Attributes/features used to extract higher-order trends, and to extract scientifically-relevant insights
- For example, this procedure could be mapped to a four-layer convolution neural network for trend analysis



On-Line Detection

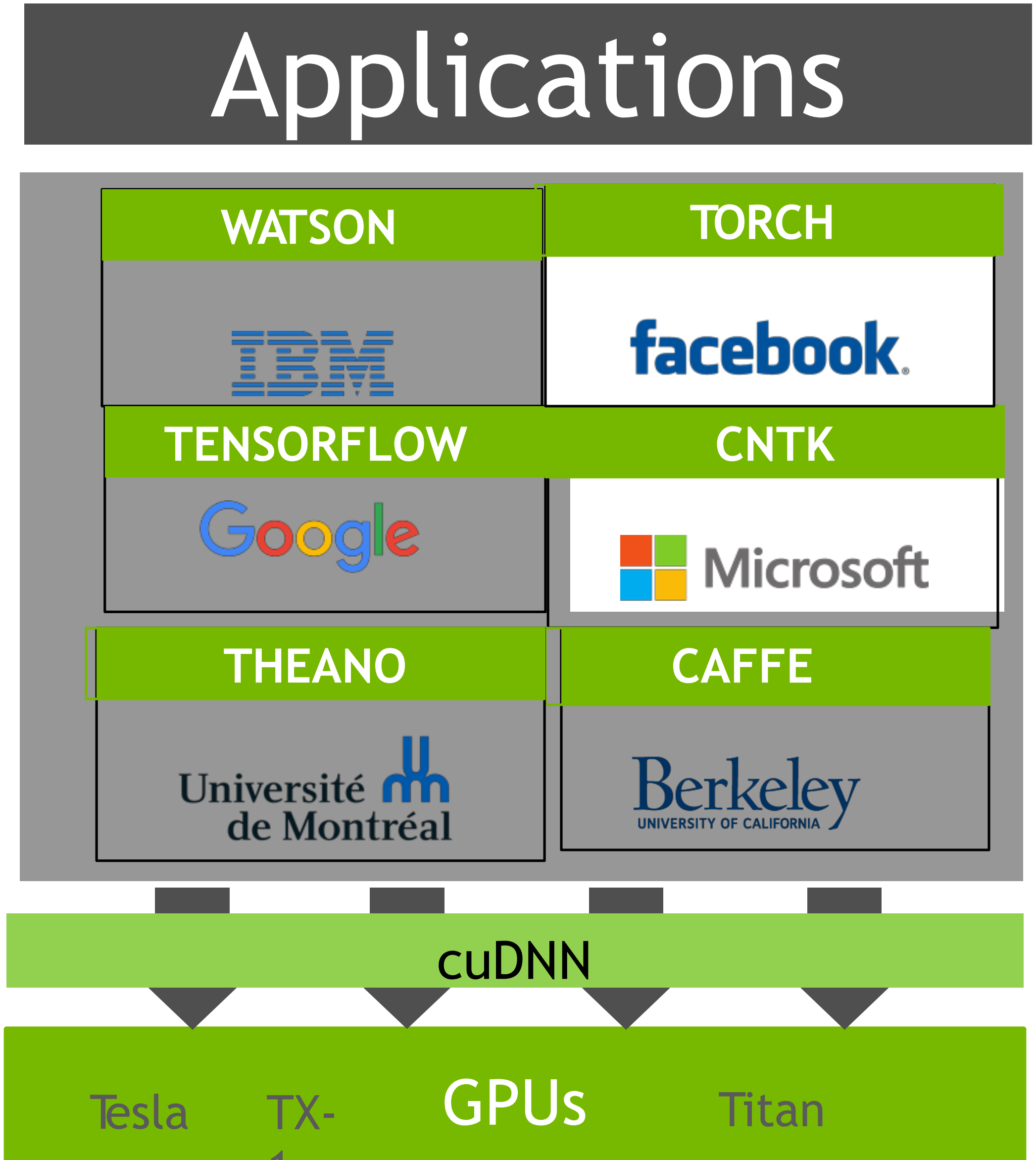
Pedestrian Detection, Traffic Sign Recognition

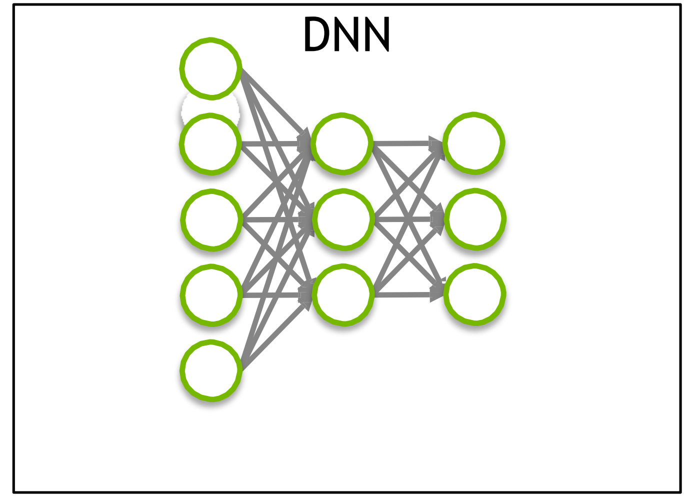


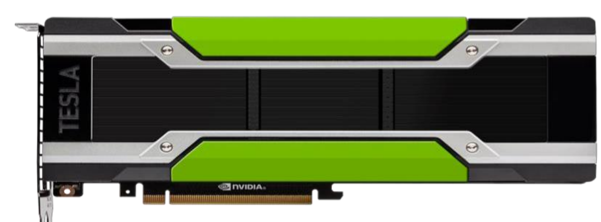
Breast Cancer Cell Mitosis Detection,
Volumetric Brain Image Segmentation

- Off-line Training, On-line detection → On-line Training, on-line detection
- Incremental Update to Existing Training Model
- On-line optimization

Co-Design Deep Learning Applications





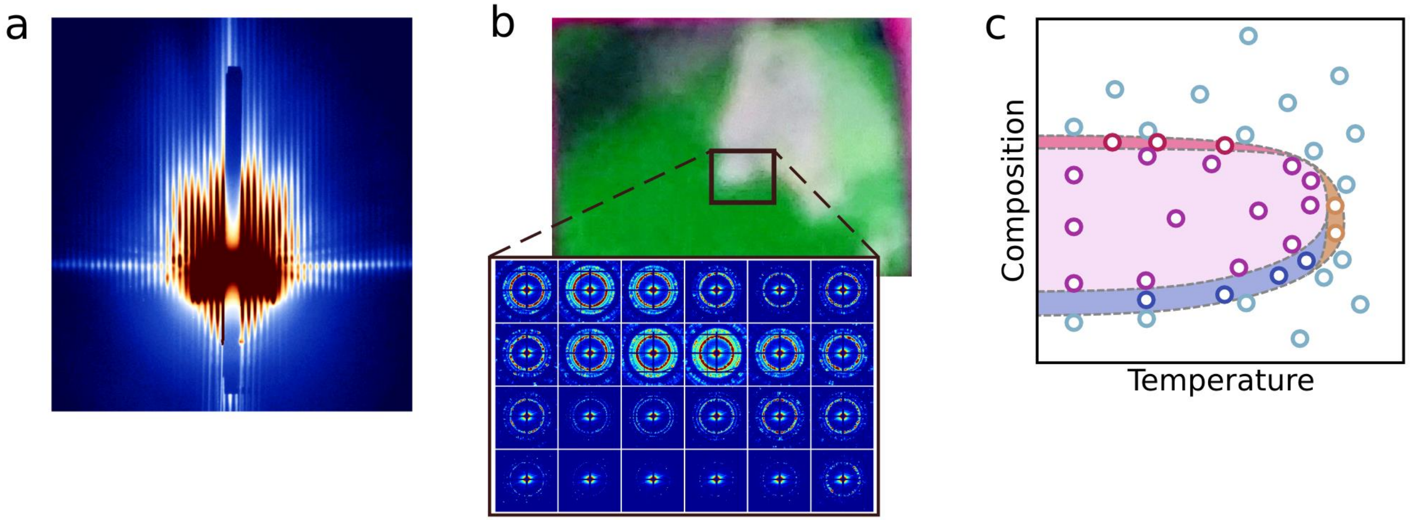


cuDNN is a library of primitives for deep learning

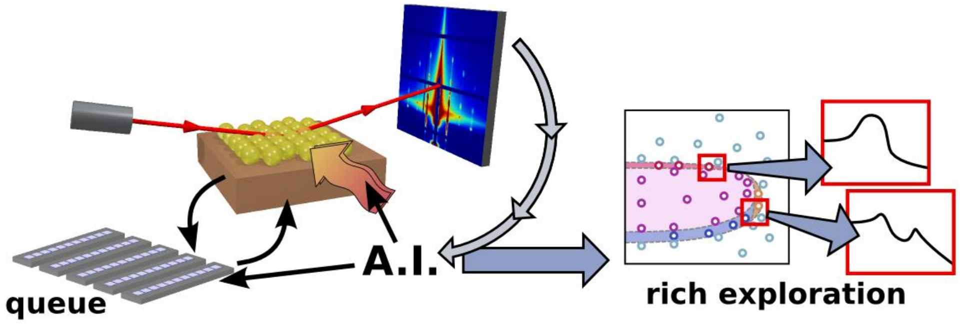
Future Machine Learning Aided Material Design

- X-ray scattering generates various 'images' that can be analyzed using machine-learning

Processed area detector frame | **Grid of data forms map of sample** | **Physical phase-diagram for experimental system**

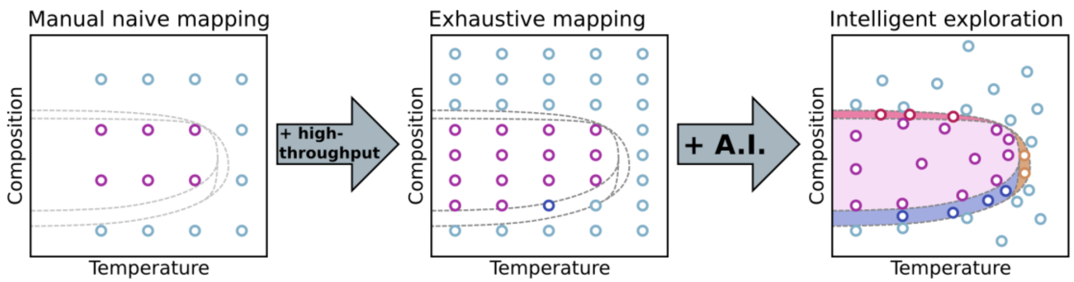


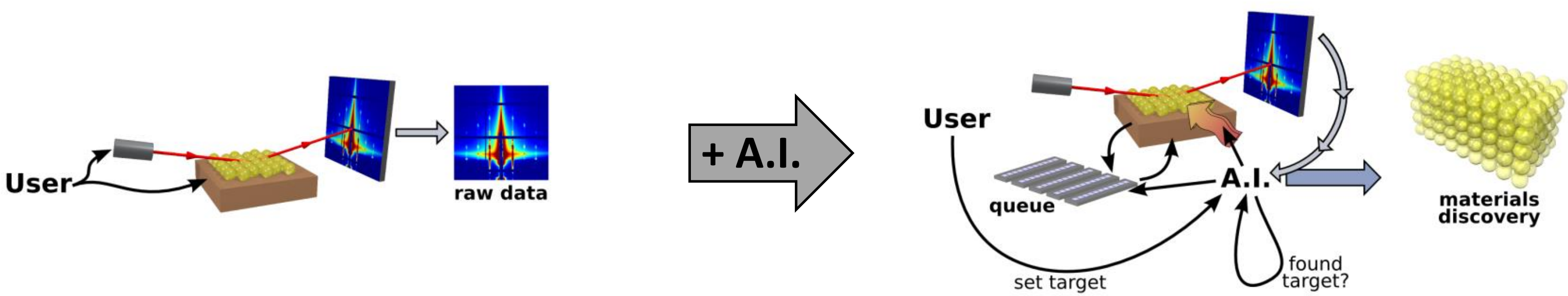
- Computer-directed beamline experiments would allow the instrument to explore physical parameter spaces, without human intervention



Conclusion

- Machine-learning is a critical component of **automated materials discovery**; a new experimental mode that:
  - Liberates scientists to work on science
  - Enables computer-controlled ‘intelligent’ exploration of materials questions
  - Accelerate scientific discoveries





- Deep-learning is a crucial tool, allowing the computer to extract physically-relevant meaning from abstract datasets

CFN/NSLS-II Beamline: CMS

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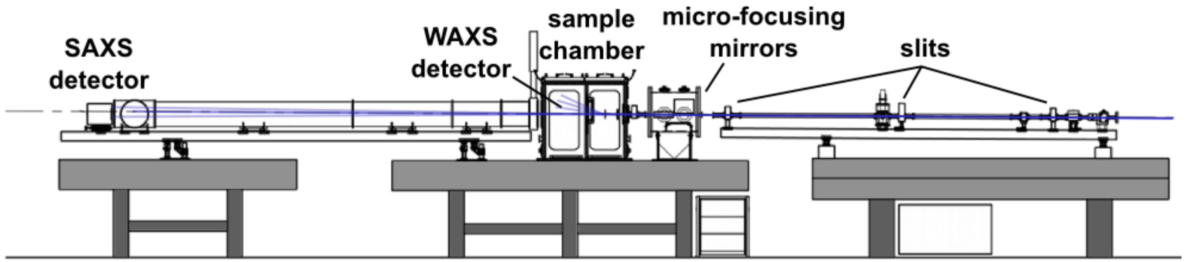
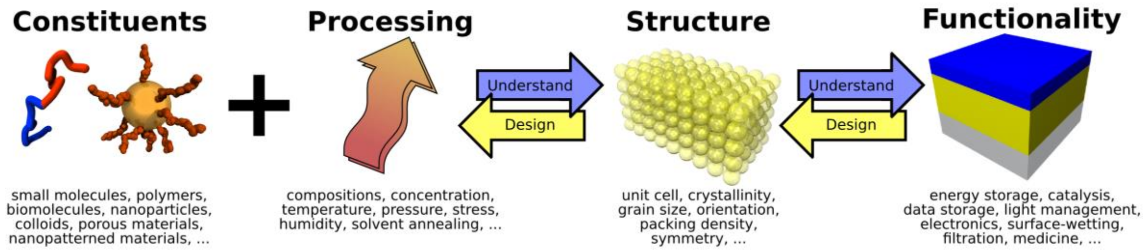
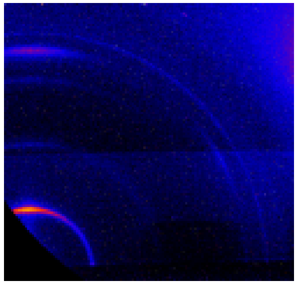
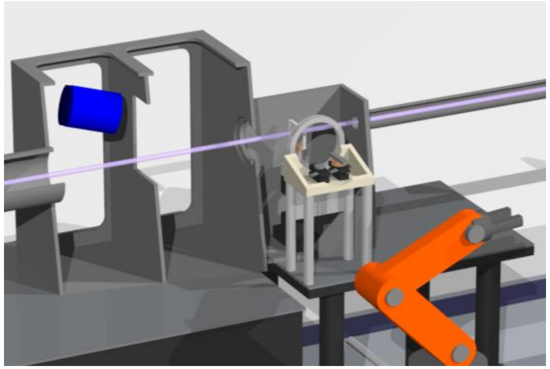
- CFN/X9 program has been extremely successful: premiere, highly-sought (>2:1) scattering instrument; highly productive (>25 publications/year)

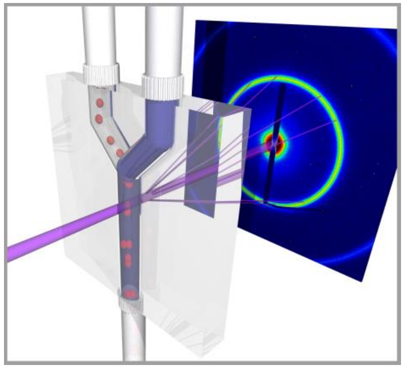


- **Complex Materials Scattering** beamline will provide:
  - Sample environments for **in-situ** and stimuli-responsive studies of (non-equilibrium) nanomaterials
  - Automation and software for **intelligent exploration** of multidimensional parameter spaces
  - New paradigm for rapid **materials discovery**









CFN/NSLS-II Beamline: SMI

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- **Soft Matter Interfaces** beamline: high-flux and high-resolution grazing-incidence scattering instrument
  - Wide energy range (2 to 24 keV) for resonant scattering on hybrid (soft/hard) materials, including edges relevant to soft matter (P, S, K, Ca)
  - Wide *q*-range for studies of hierarchical materials
  - Microbeams (~2 μm) for mapping of heterogeneous samples
  - High-flux and fast detectors for kinetic, in-situ, and in-operando experiments

SMI