Artificial Intelligence for Scattering Experiments

Thomas Proffen

Neutron Scattering Division

ORNL is home to two world class neutron sources

High Flux Isotope Reactor (HFIR)

690 Scientific Publications in CY21*

685 Total Unique Users in FY21

95,469 Hours of Beamtime in FY21

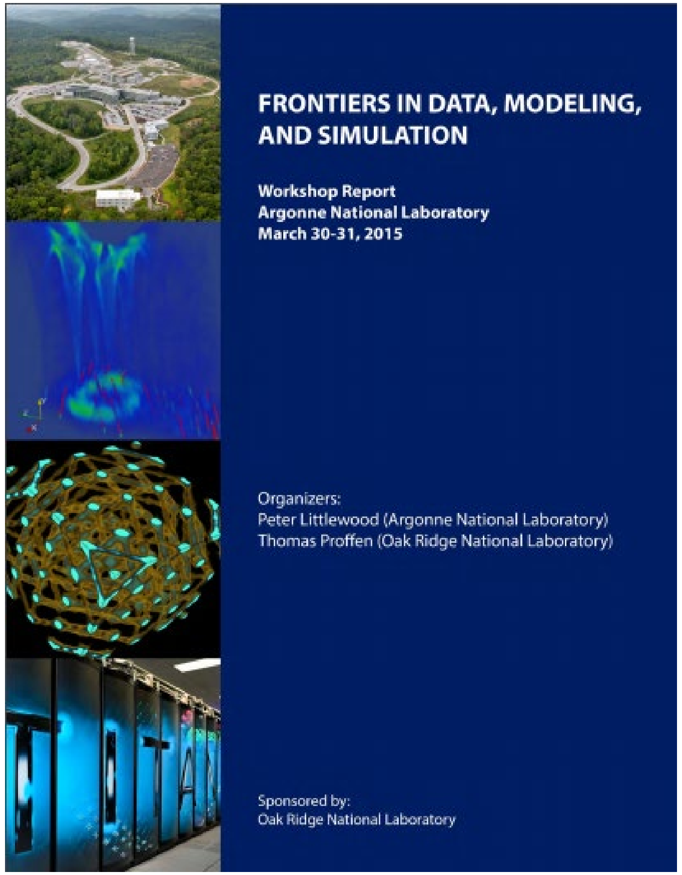
1,190 Total Experiments in FY21

Spallation Neutron Source (SNS)

Materials research crosses facilities

Opportunities

- Multimodal analysis
- Applied Math. concepts
- Advanced Materials Modeling



FRONTIERS IN DATA, MODELING, AND SIMULATION

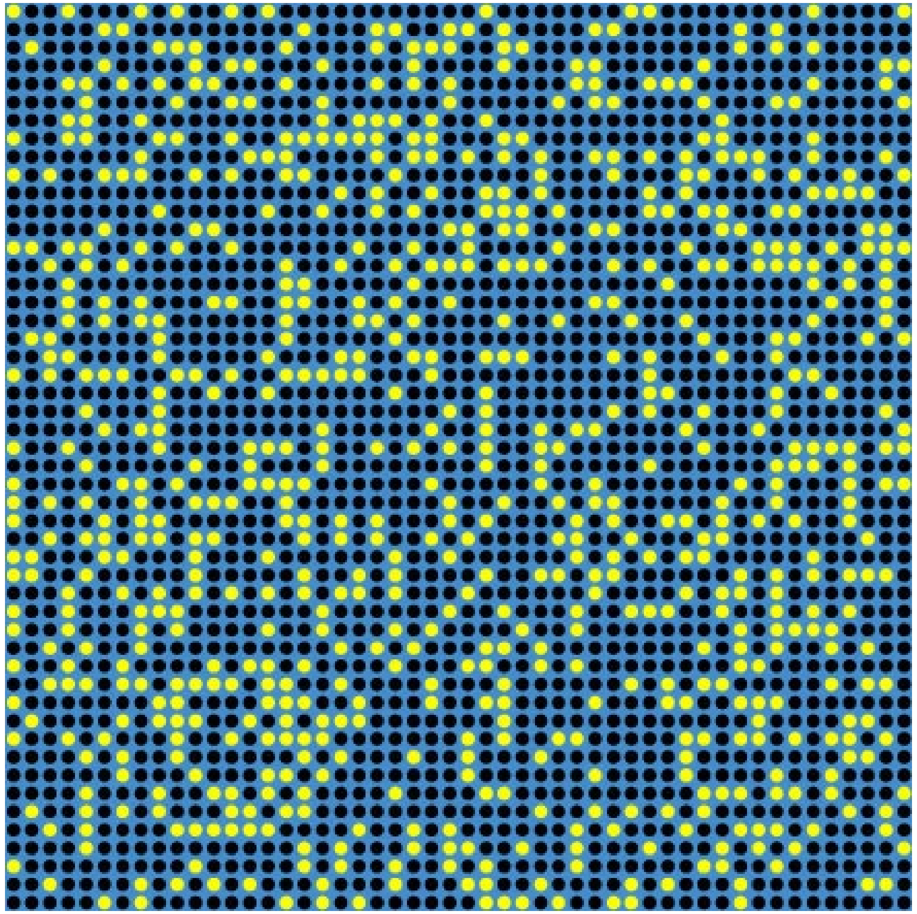
Workshop Report
Argonne National Laboratory
March 30-31, 2015

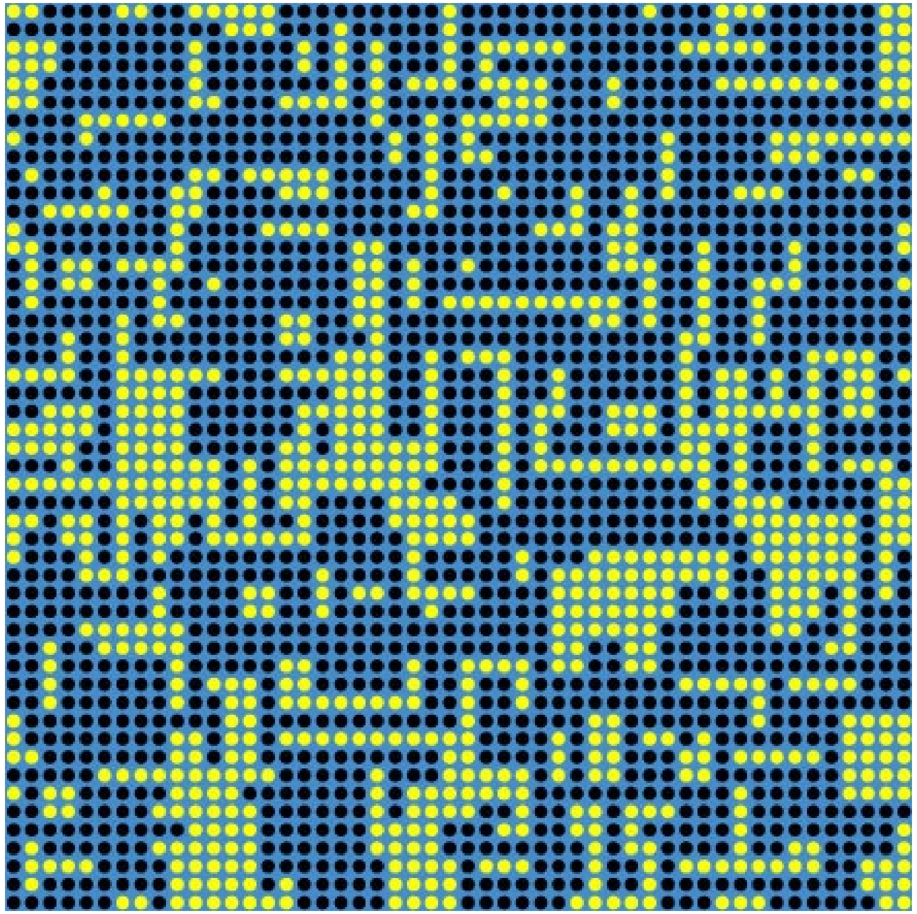
Organizers:
Peter Littlewood (Argonne National Laboratory)
Thomas Proffen (Oak Ridge National Laboratory)

Sponsored by:
Oak Ridge National Laboratory

http://neutrons.ornl.gov/grand-challenge-workshops

Diffuse scattering ?

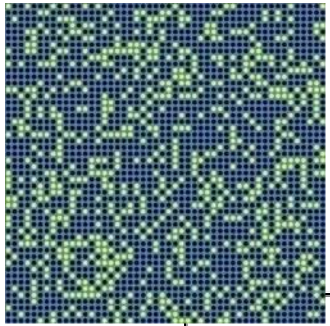




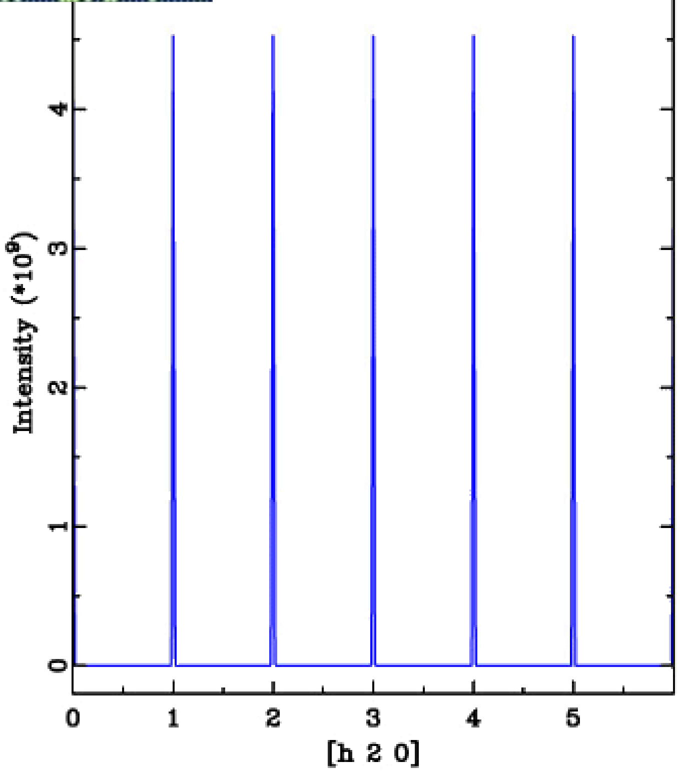
Cross section of 50x50x50 u.c. model crystal consisting of 70% black atoms and 30% *vacancies* !

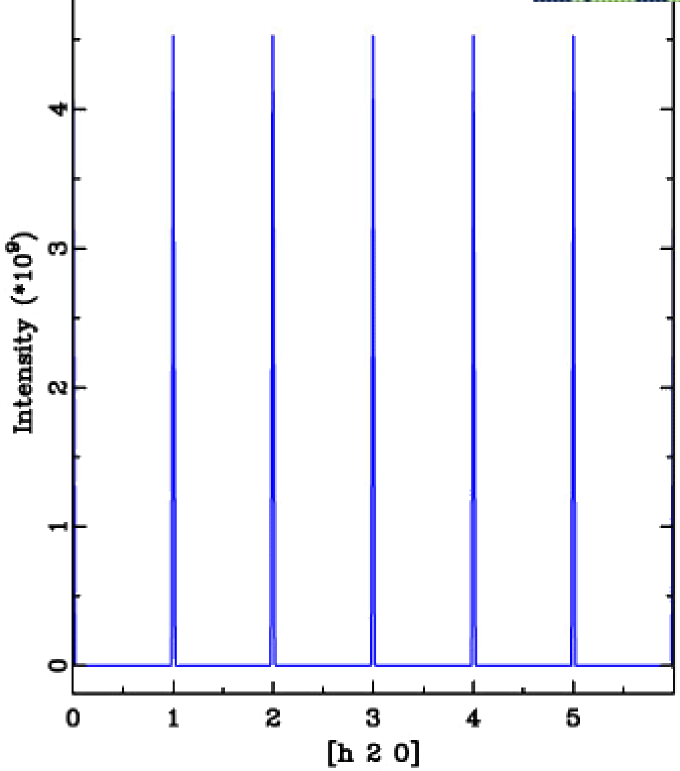
Properties might depend on vacancy ordering !!

Bragg peaks are blind ..

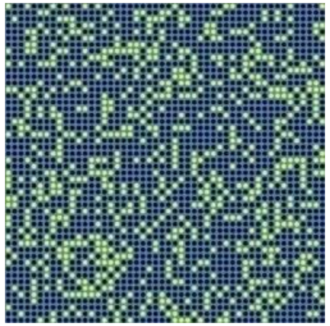


Bragg scattering: Information about the *average* structure, *e.g.* average positions, displacement parameters and occupancies.

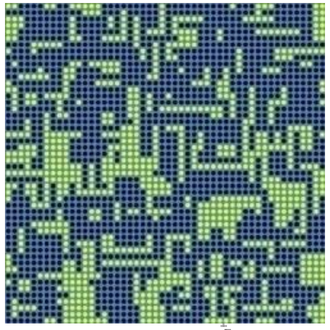


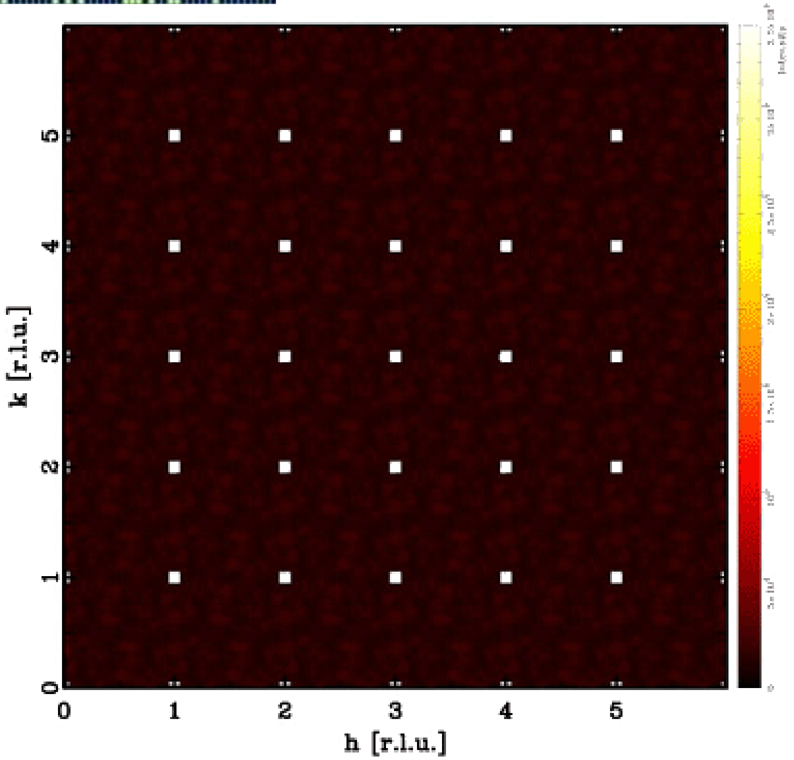


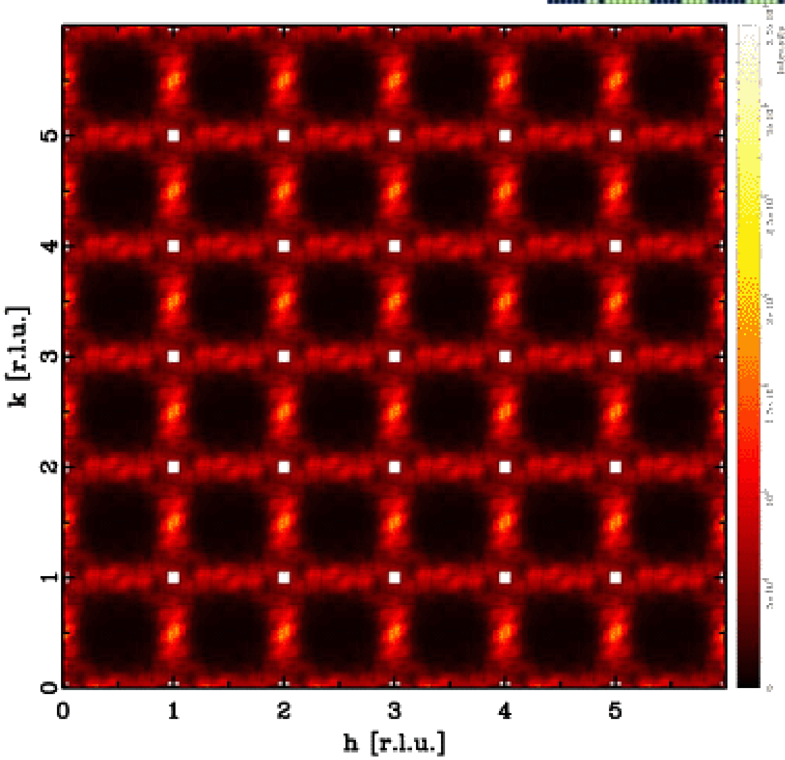
Diffuse scattering to the rescue ..



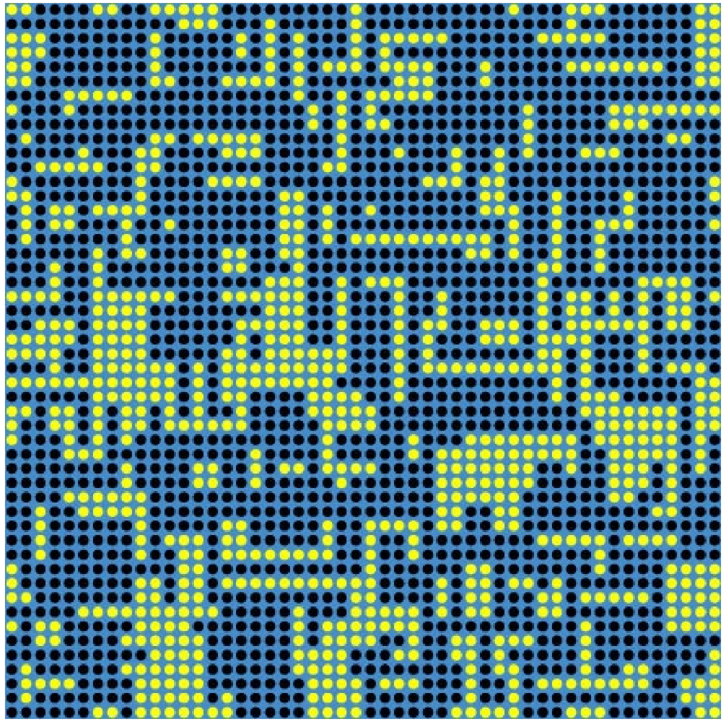
Diffuse scattering: Information about *two-body correlations*, *i.e.* chemical short-range order or local distortions.



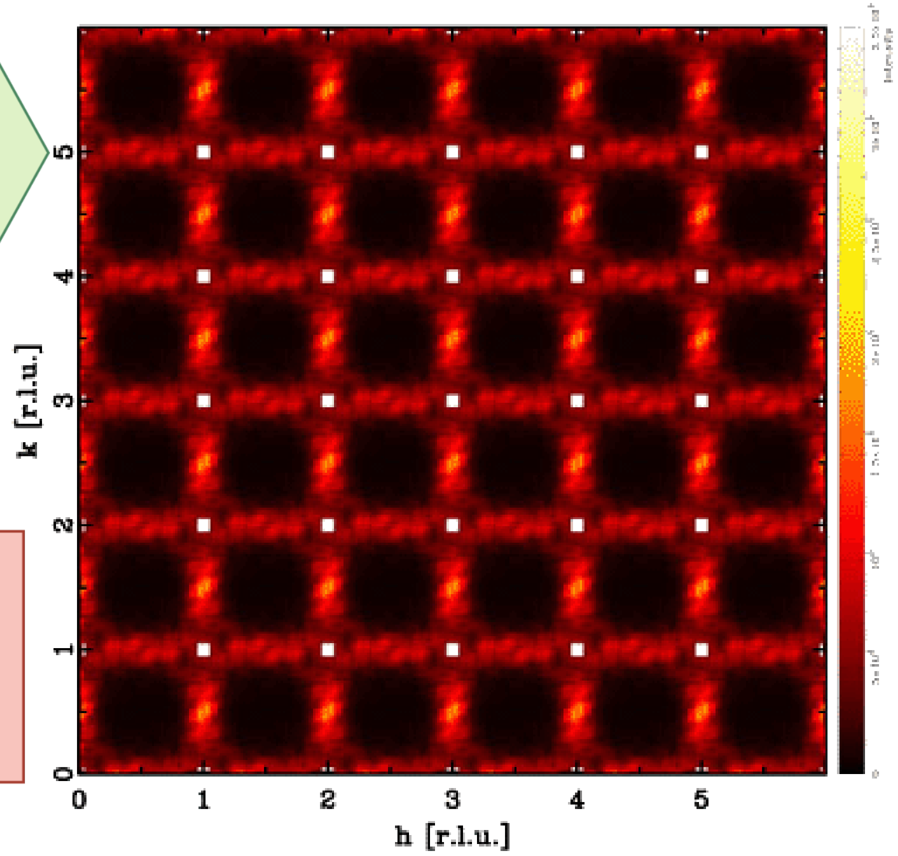




Inverse Problem *aka* Crystallographic Phase Problem



$$F(\mathbf{h}) = \sum_{i=1}^{N} f_i(\mathbf{h}) e^{2\pi i \mathbf{h}\mathbf{r}_i}$$



Intensities measured only give |**F**| and not the phase

☹

Analyzing diffuse scattering

- **Correlation approach**: Expansion of kinematic scattering equation in terms of displacement. Yields set of two-body correlations.

- **Monte Carlo based computer simulations**: Scientist might "win" solution to the problem ..
  - Minimize total energy E: AMC
  - Minimize (observed – calculated)^2: RMC

- More: "Diffuse Neutron Scattering from Crystalline Materials" by Nield and Keen, Oxford University Press

Table 1. Summary of the properties of the different components of the diffuse intensity.

Term	$\mathbf{I_0}$	$\mathbf{I_1}$	$\mathbf{I_2}$	$\mathbf{I_3}$
Description	Short-range order (SRO) term	Warren Size-effect	Huang Scattering 1st order TDS	3rd order size term
Lattice averages involved	SRO parameters α^{ij}	$\langle X^{ij}\rangle, \langle Y^{ij}\rangle$ *etc.*	$\langle (X^{ij})^2\rangle$, $\langle X^{ij} Y^{ij}\rangle$ *etc.*	$\langle (X^{ij})^3\rangle$, $\langle (X^{ij})^2 Y^{ij}\rangle$ *etc.*
Type of Summation	cosine	sine	cosine	sine
Symmetry	symmetric	anti-symmetric	symmetric	anti-symmetric
Variation in $\boldsymbol{k}$–space	nil	linear, *i.e.* with h_1, h_2 *etc.*	quadratic, *i.e.* with $h_1^2, h_1 h_2$ *etc.*	cubic, *i.e.* with $h_1^3, h_1^2 h_2$ *etc.*
Dependence on f_A, f_B for binary	$(f_A - f_B)^2$	$f_A(f_A - f_B)$, $f_B(f_A - f_B)$	$f_A^2, f_A f_B, f_B^2$	$f_A^2, f_A f_B, f_B^2$
Number of components for binary	1	6	18	30

The Automatic Monte Carlo Method

Input:

- Observed diffuse scattering
- Starting structure (e.g. average)
- Model for disorder in terms of interaction energies for MC simulation.

Result:

- Set of interaction energies for given model that best match the data.

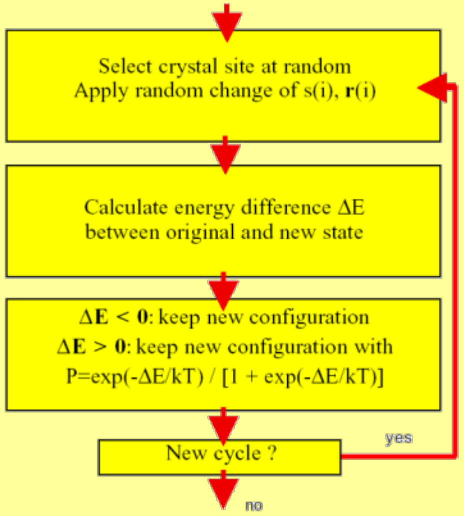
Questions:

- Finding the right model ..
- It is very slow ..

Least Squares

For each parameter in MC model

Run MC



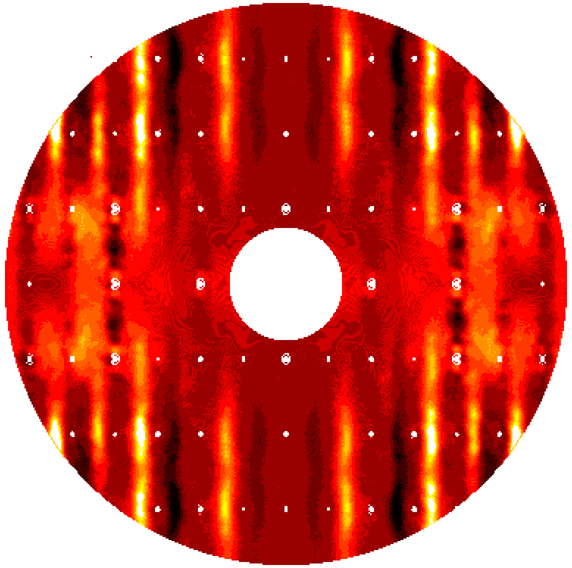
Calculate diffuse scattering

Obtain derivatives

Disorder in $Fe_3(CO)_{12}$ – AMC refinement

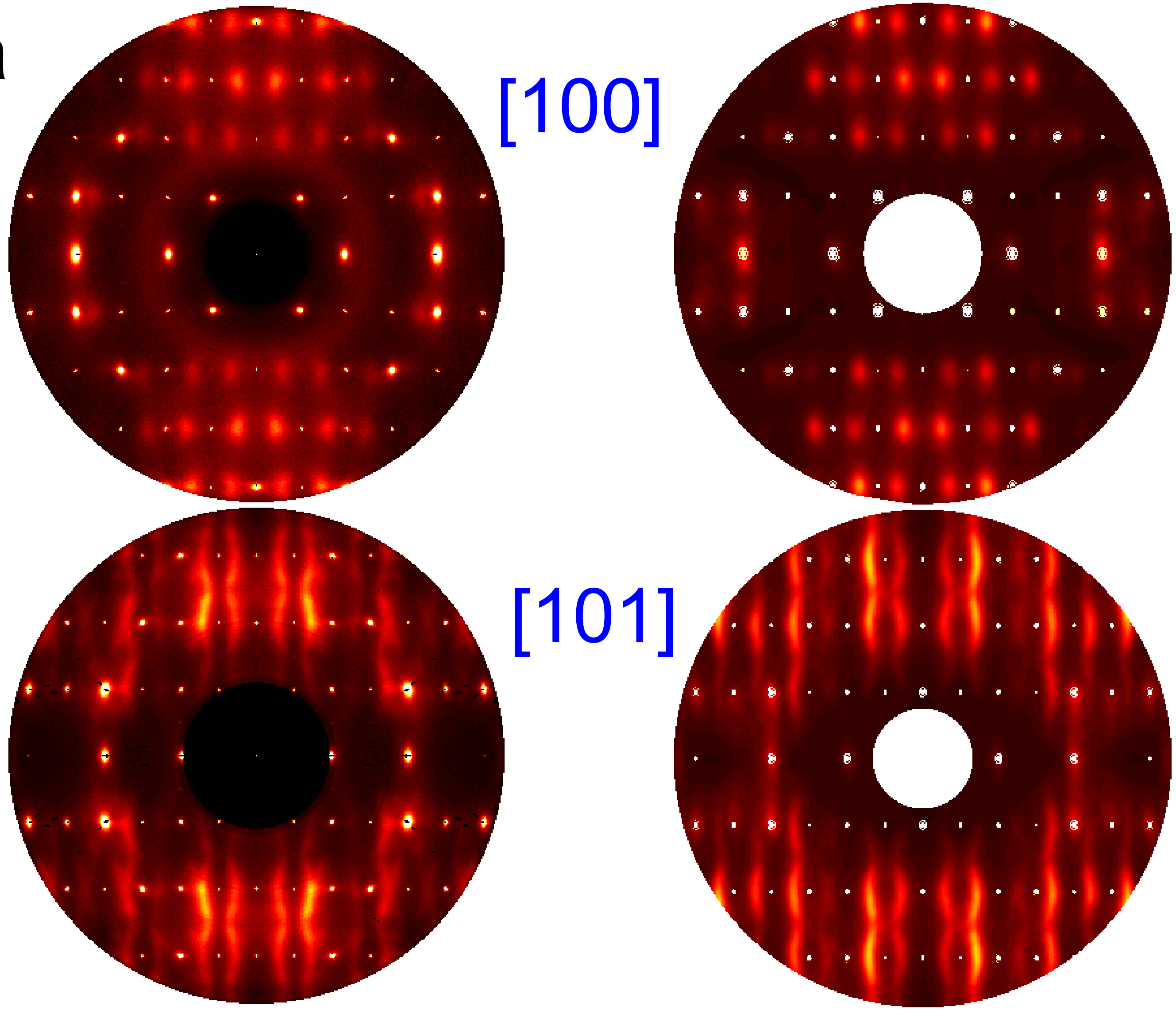
Numerical estimates of Differentials

$$\frac{\partial \Delta I}{\partial p_i} = \sum_{hklm} \frac{\left(\Delta I_{p+} - \Delta I_{p-}\right)}{2\delta_i}$$



Difference between two calculated diffraction patterns

Data **calculated**

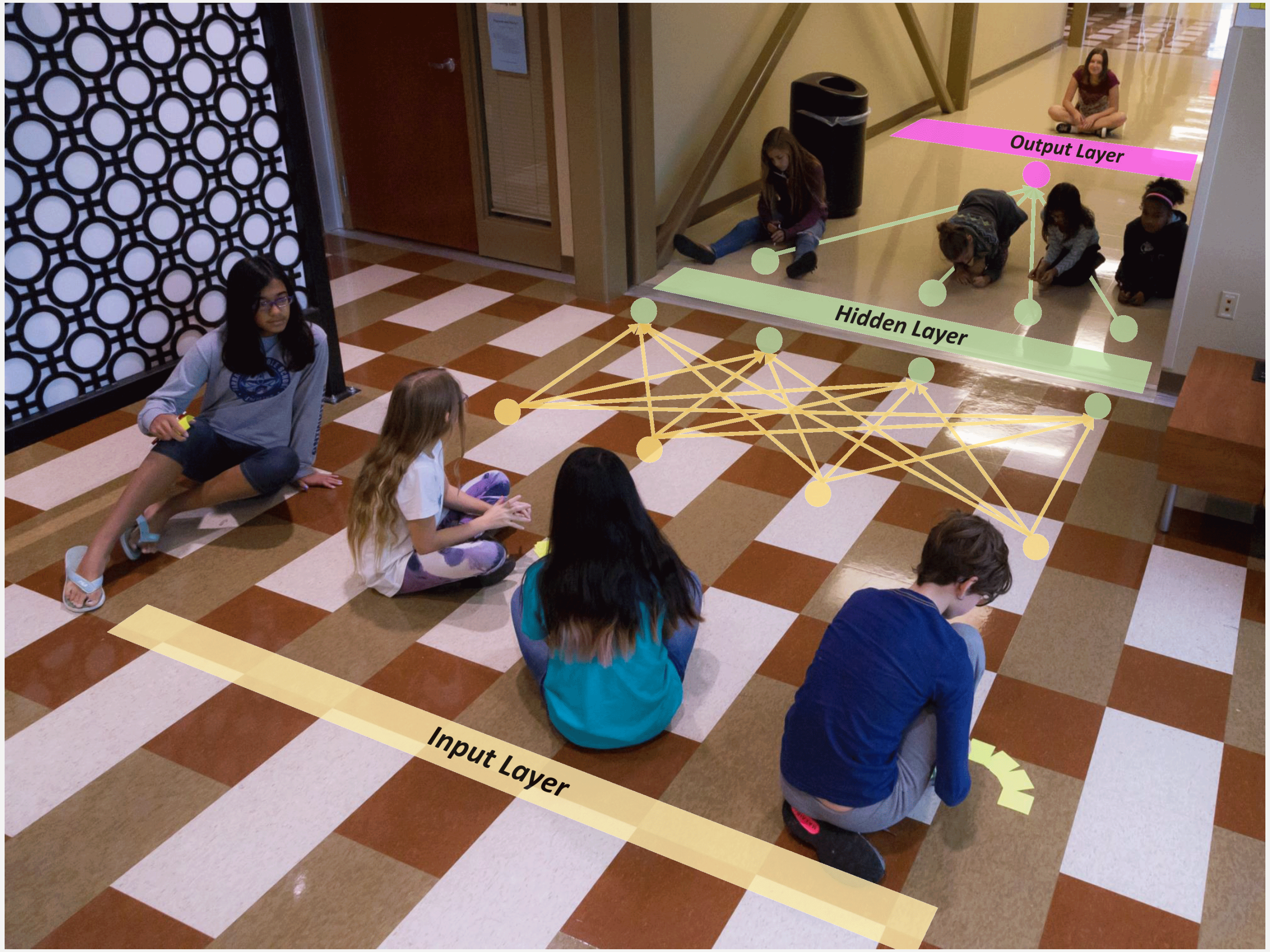


Opportunities using Machine Learning

AI is about how we use and process data. It will be, and is, transformative in knowledge-based disciplines. AI will not replace scientists, but scientists who use AI will replace those who don't.*

*Modified from a quote in the Microsoft report, "The Future Computed: Artificial Intelligence And Its Role In Society"

MACHINE LEARNING



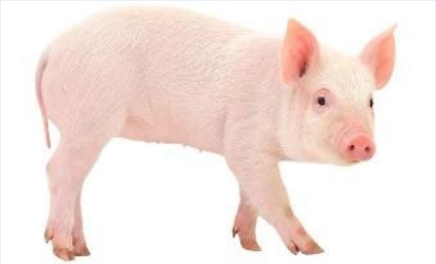
www.orcsgirls.org

MACHINE LEARNING

A machine learning method takes a bunch of data and "learns" from it!

Data

Label: Not a pig



Label: Pig

Label: Pig

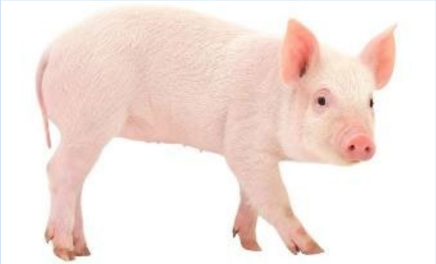
Label: Not a pig

Machine Learning Method

Machine's rules for determining whether or not an image is a pig

DID IT "LEARN" SOMETHING?

Label: Not a pig



Label: Pig

Label: Pig

Label: Not a pig

Training Data

The data we give to the machine learning method to learn from

Label: Not a pig

Label: Pig

Testing Data

The data we hold out and use to check to see if the method actually learned something!

DEEP LEARNING

Simulated scattering 'images'

- Small Angle Scattering
- Diffraction
- Diffuse Scattering
- Quasi Elastic Scattering

Labels

- Relate to model / parameters
- Related to topology
- Good/Bad

Training Data

The data we give to the machine learning method to learn from

Testing Data

The data we hold out and use to check to see if the method actually learned something!

Machine Learning for classification

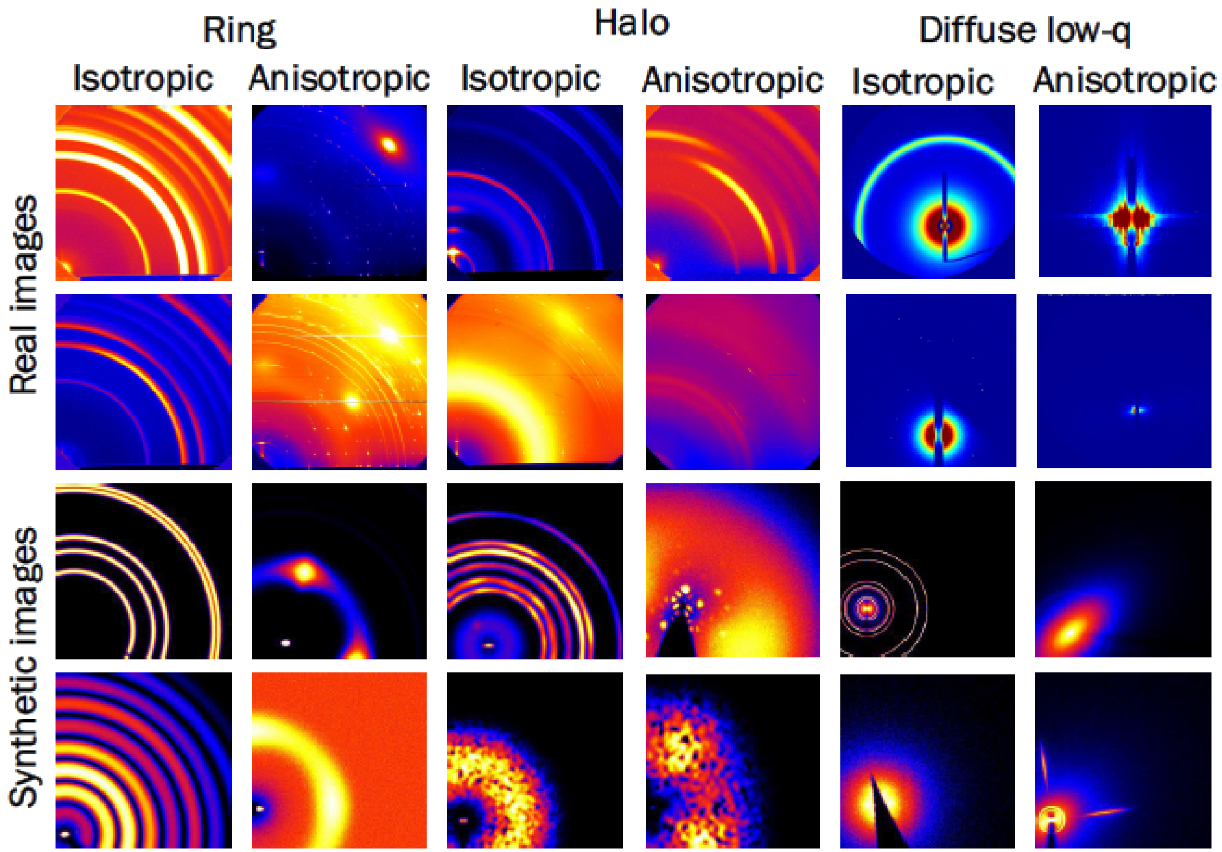


Figure 2: Comparison between synthetic images and real experimental images. The first and second rows are real experimental images, while the third and forth rows are synthetic images. Images in the same column have the same attribute. From left to right, the attributes are: Ring: Isotropic, Ring: Anisotropic, Halo: Isotropic, Halo: Anisotropic, Diffuse low q: Isotropic, and Diffuse low q: Anisotropic. Visually, synthetic and real images are indiscernible.

2017 IEEE Winter Conference on Applications of Computer Vision

X-ray Scattering Image Classification Using Deep Learning

Boyu Wang[1], Kevin Yager[2], Dantong Yu[2], and Minh Hoai[1]
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{boywang, minhhoai}@cs.stonybrook.edu
[2]Brookhaven National Laboratory, Upton, NY, USA
{kyager,dtyu}@bnl.gov

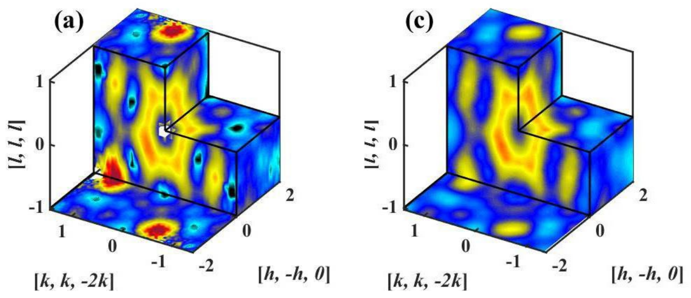
AI accelerating neutron scattering research

Automatic model selection for neutron reflectivity

- Prototype allows to automatically detect and refine multi-layer models from experimental neutron reflectivity data.
- Training data set was calculated using **refl1d** for 1, 2- and 3-layer models.
- Future:
  - Expand to more models and deploy for users.
  - Integrate in automatic reduction and (initial) analysis workflow.

Machine learning insight into spin ice

- Model Hamiltonians for spin ice were selected from experimental neutron scattering data.
- Approach used machine learning and training data were calculated using forward models.



(a) Scattering data and (b) simulated data of $Dy_2Ti_2O_7$ [arXiv:1906.11275]

Future opportunities

- Machine learning generated meta-data enabling automation (e.g. marking data from misaligned samples)
- Feature identification in elastic and inelastic neuron scattering data allowing automation and selecting modeling approaches

Analysis and feature detection in large volumes of diffuse x-ray and neutron scattering from complex materials

Thomas Proffen, Ray Osborn, Rick Archibald, Stuart Campbell, Ian Foster, Scott Klasky, Tashin Kurc, Dave Pugmire, Michael Reuter, Galen Shipman, Chad Steed, Chris Symons, Ross Whitfield, Doug Fuller, Guru Kora, Mike Wilde, Justin Wozniak

Facilities/Resources
SNS, APS, ALCF; OLCF; and CADES at ORNL

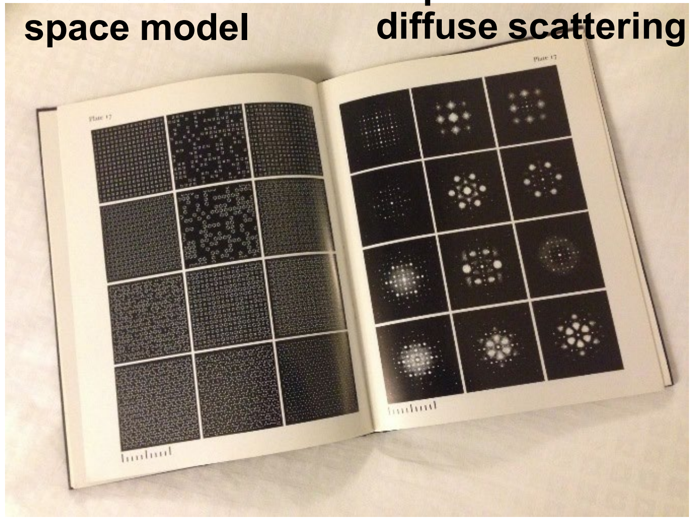
Argonne NATIONAL LABORATORY

OAK RIDGE National Laboratory | HIGH FLUX ISOTOPE REACTOR | SPALLATION NEUTRON SOURCE

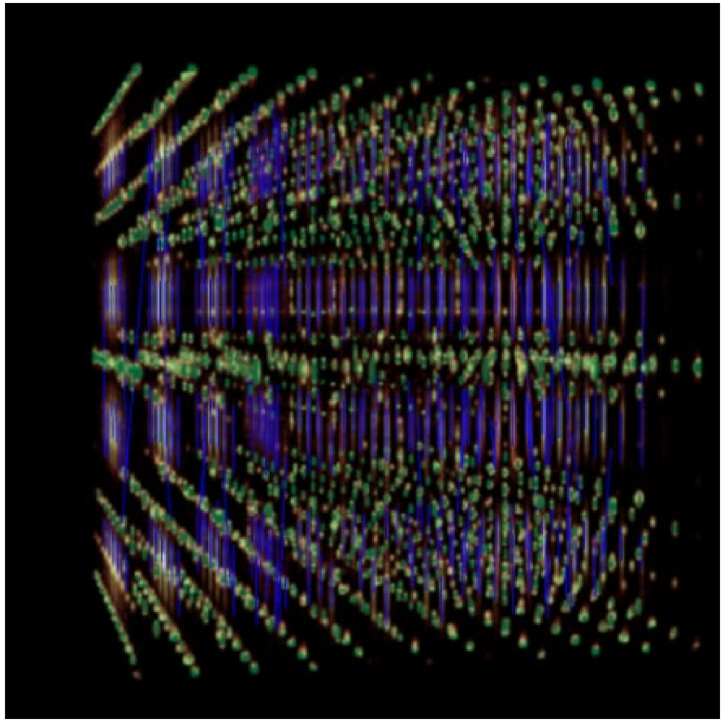
DOE Science Data Pilot Project

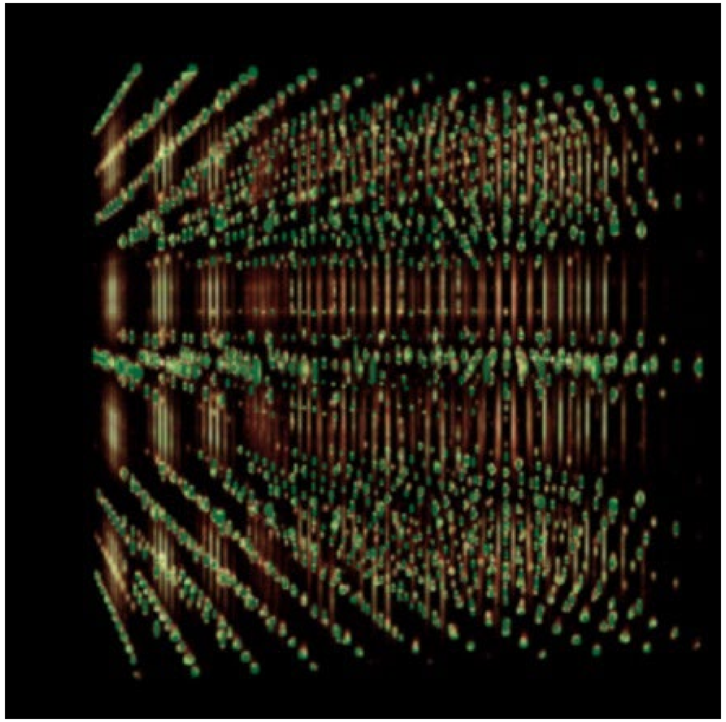
- **Diffuse scattering** contains information about **disorder in materials** which is critical to understand function.
- **Novel approach using pattern recognition and machine learning**.
- Aligned with science needs of CORELLI and TOPAZ.

Disordered real space model **Compare to observed diffuse scattering**

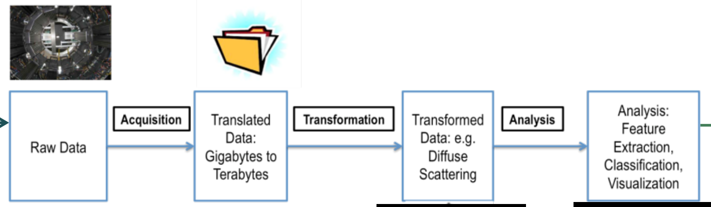


Atlas of Optical Transforms, Harburn, Taylor and Welberry (1975)

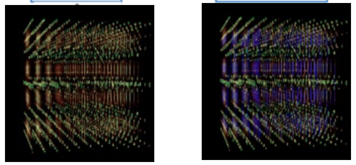




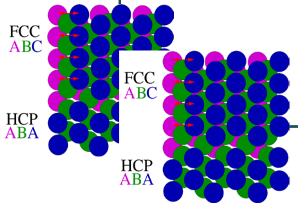
High Level Demonstration Workflow



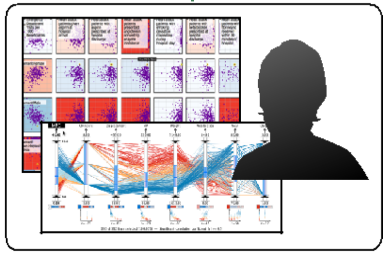
SNS – TOPAZ
Neutron Scattering



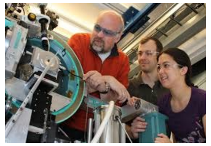
Feature detection “Streaks” in Diffuse scattering data



Classification of “streaks” into candidate stacking faults

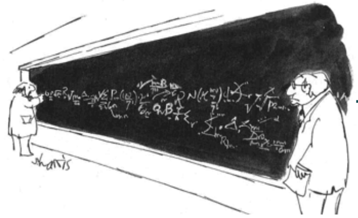


Scientific visualization and visual analytics interface presenting detected features and candidate stacking faults based on classifiers



APS - X-ray Scattering coming soon

Diffuse scattering simulations over parameter space



Knowledge base of experiments and simulations

Data sharing and catalog of results

DISCUS SIMULATION PACKAGE

EDEN
Exploratory Data analysis ENvironment

swift

globus online

VisIt

ADIOS

Challenges

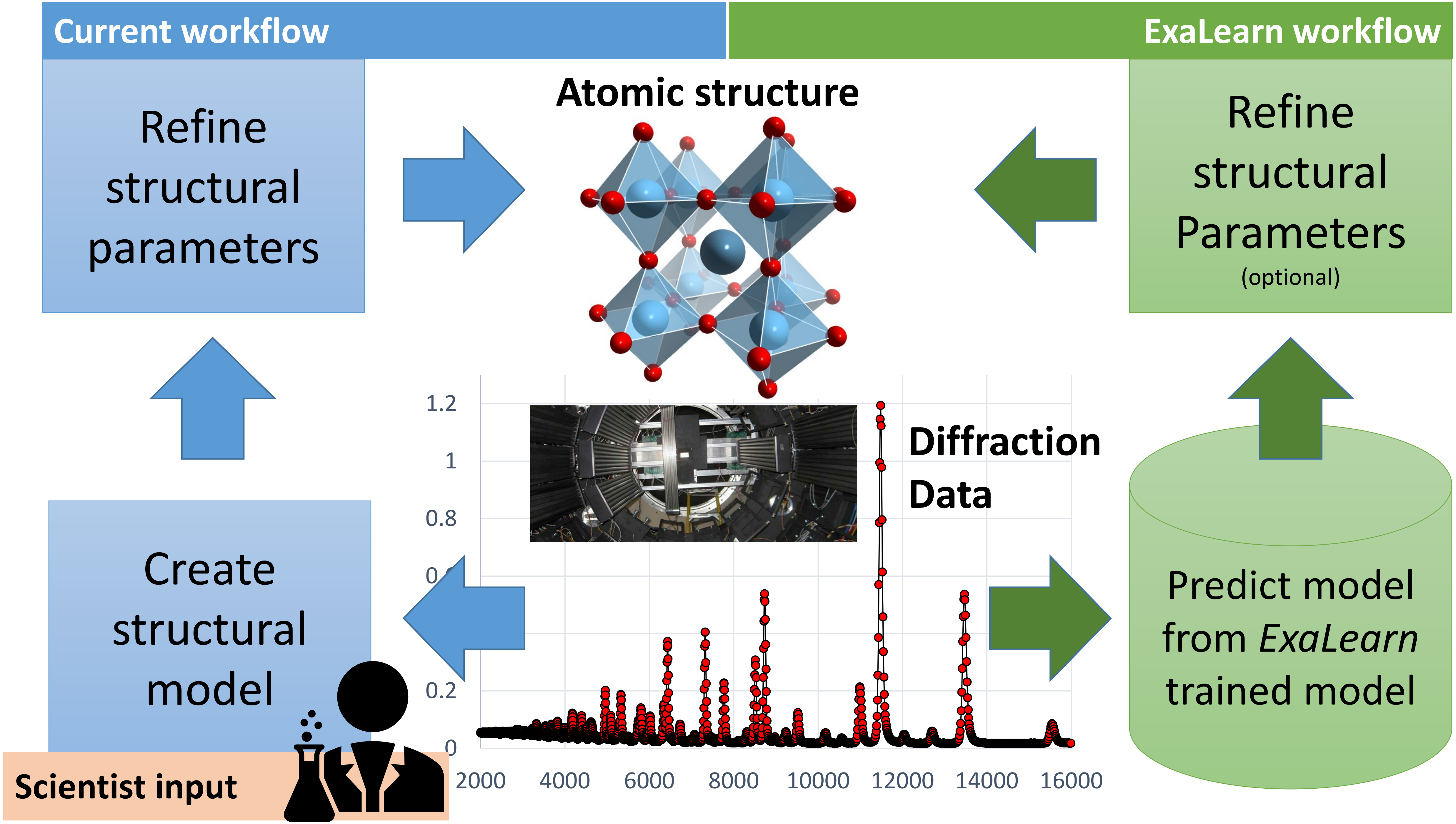
- What are the correct labels?
- Sparse data.
- Data management and 'ML friendly' metadata.
- Correct normalization for scientific data.

Machine Learning for Inverse Problems

Cristina Garcia Cardona (LANL), Ramakrishnan Kannan (ORNL), Thomas Proffen (ORNL), Travis Johnston (ORNL), Katherine Page (ORNL/UTK), David Womble (ORNL), Sudip K Seal (ORNL, POC)

ECP EXASCALE COMPUTING PROJECT

OAK RIDGE National Laboratory | HIGH FLUX ISOTOPE REACTOR | SPALLATION NEUTRON SOURCE


Current workflow
ExaLearn workflow
Refine structural parameters
Atomic structure
Refine structural Parameters
(optional)
1.2
1
0.8
0.2
0
2000
4000
6000
8000
10000
12000
14000
16000
Diffraction Data
Create structural model
Predict model from *ExaLearn* trained model
Scientist input

Thank you

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