Los Alamos NATIONAL LABORATORY

3N020A/WJ9H/IP2104MP:

Evaluation of Quantum Annealing Algorithms for Evaluation of Large Diffraction Datasets

Michael Pettes, MPA-CINT

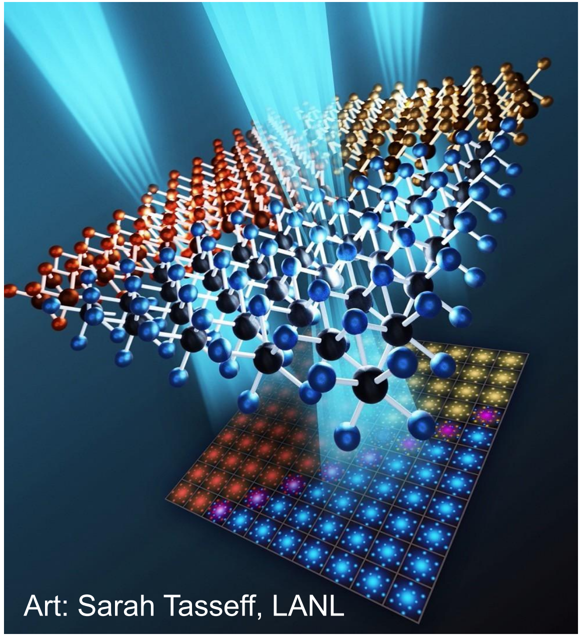
Nga Nguyen-Fotiadis, CCS-3

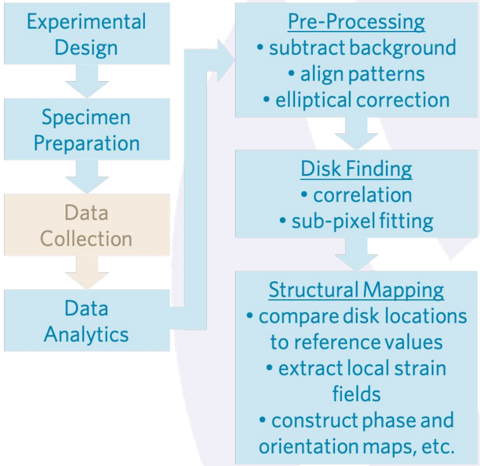
September 14, 2021

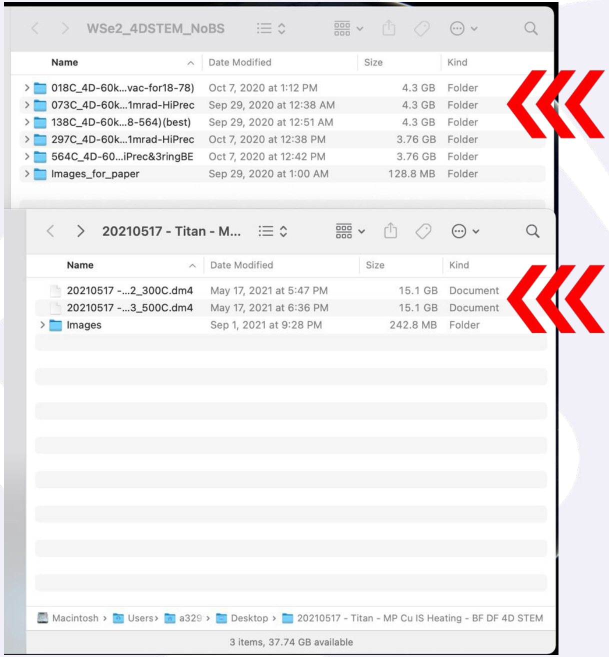
LA-UR-21-29046

Motivation: New Detectors Allow Unprecedented Information Rate … But at a Cost

- 4D-STEM … in principle
- 4D-STEM … in reality

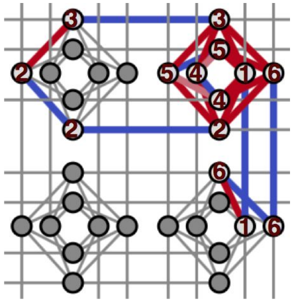






Proposed Solution: Methods Housed in LANL CCS for Large Data Analysis Problems

- Quantum Computation



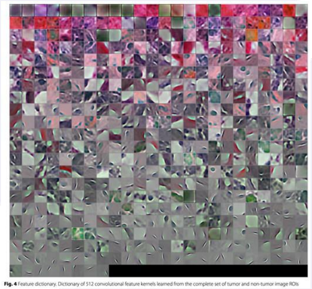
- Quantum Algorithms
  - Ising Model embedding algorithm

$$H = \sum_{i=1}^{N_q} h_i q_i + \frac{1}{2} \sum_{i<j}^{N_q} J_{ij} q_i q_j$$

  - Problems require sparse connectivity

- Precedence for Solutions by Nga
  - Classical (Darwin)

"Sparse coding of pathology slides compared to transfer learning with deep neural networks," Will Fischer, Sanketh S. Moudgalya, Judith D. Cohn, Nga T. T. Nguyen, and Garrett T. Ken-yon, *BMC Bioinfomatics* **19**, 489 (2018), https://doi.org/10.1186/s12859-018-2504-8



  - Quantum (Ising)

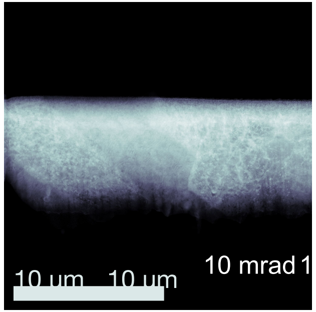
"Comparing Deep Learning with Quantum Inference on the D-Wave 2X," Nga T. T. Nguyen and Garrett T. Kenyon, in *Proceedings of 3rd International Workshop on Post Moore Era's Supercomputing (PMES)*, November, 2018, https://drive.google.com/file/d/1PCFNJuHLo2L3WeQnpyWd9ITlDNy4S4_M/view

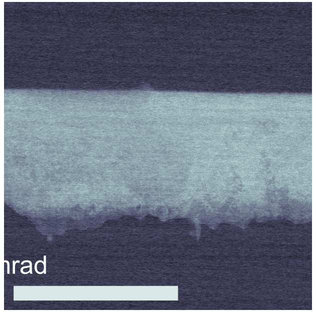
Fig. 1. Top: Original MNIST images downsampled to 12x12, Middle: Reconstructed images from bottleneck autoencoder, Bottom: D-Wave reconstruction from randomly selected imprinted features.

Information on Polycrystalline Metal by 4D-STEM

HAADF

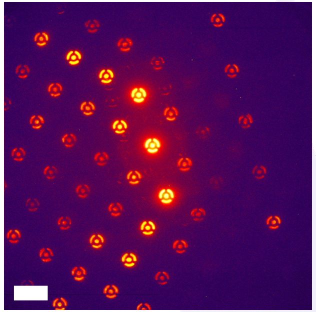
dm4 dm4
unscaled values [min = 4749 ; max = 21080] unscaled values [min = 4704 ; max = 4743]
processed values [min = 0 ; max = 1] processed values [min = 0 ; max = 1]

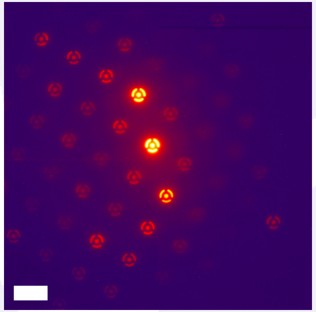




Mean and Max of 3200 Diffraction Patterns

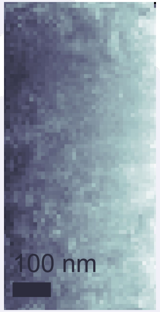
CBEDmax CBEDmean
unscalsd valus [min = 88.7045 ; max = 30907.9238] unscales values [min = -104.263 ; max = 3548.5671]
procsssd valus [min = 0.001 ; max = 1]processes values [min = 0.011 ; max = 1]





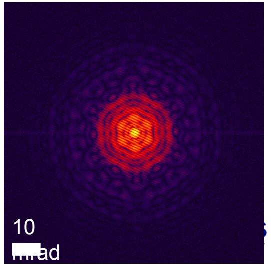
“virtual” image

sigBF
unscaled values [min = 22.7897 ; max = 46.0698
] processed values [min = 0 ; max = 1]

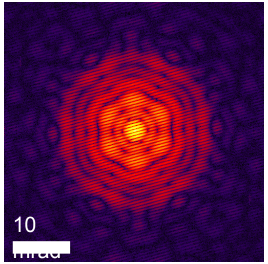


Information Contained in Diffraction

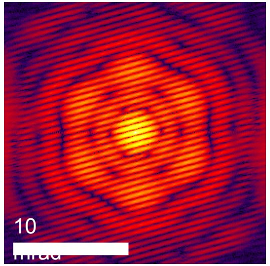
1024×1024



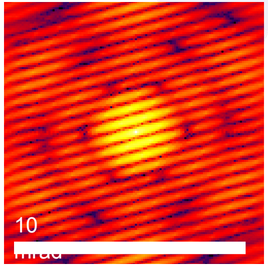
512×512



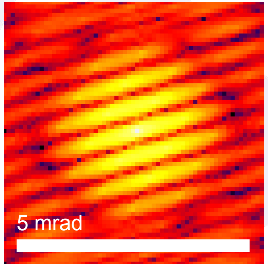
256×256



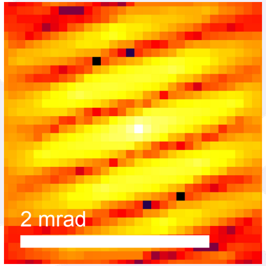
128×128



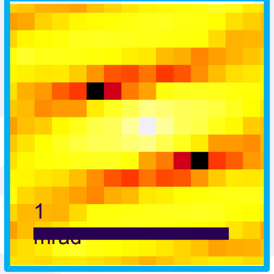
64×64



32×32



16×16



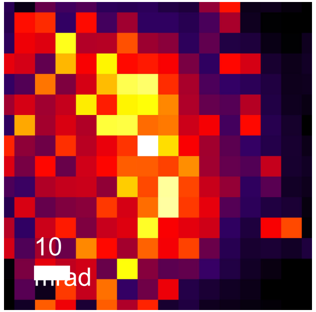
Preparation for Analysis

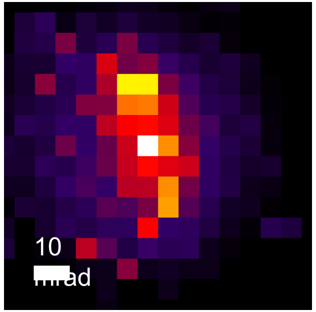
Mean and Max of 3200 Diffraction Patterns (bin 2^6)

CBEDmaxbin12 CBEDmeanbin12

nscaled valnes [min = 79536.1637 ; max = 12804694.2029] inscaled valies [min = 44436.2188 ; max = 3249906.0815]

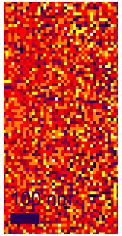
processed valnes [min = 0.001 ; max = 1] processed valies [min = 0.011 ; max = 1]





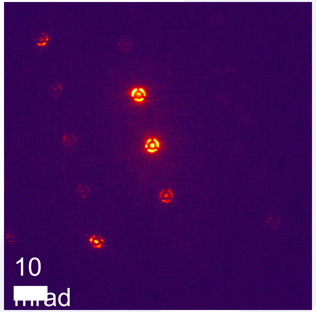
scaled values [min = 0.00024414 ; max = 0.00024414] processed values [min = 0 ; max = 1]

HAADF / HAADF(bin 2^6)



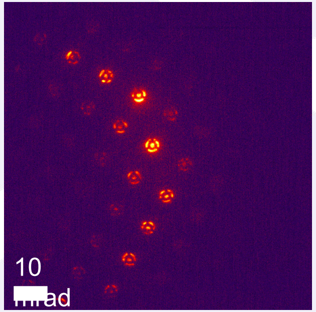
Class A

CBED2825
unscaled values [min = -246.5895 ; max = 8822.0088]
processed values [min = 0.01 ; max = 1]



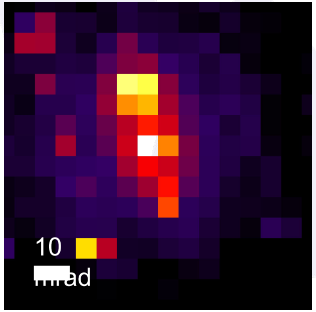
Class B

CBED8030
unscaled values [min = -230.031 ; max = 7817.2363] processed values [min = 0.01 ; max = 1]



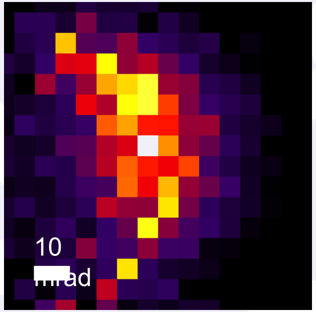
Class A (bin 2^6)

CBED2825bin12
unscaled values [min = 32030.69 ; max = 3941807.5512] processed values [min = 0.01 ; max = 1]



Class B (bin 2^6)

CBED8030bin12
unscaled values [min = 42250.4962 ; max = 2764122.4098]
processed values [min = 0.01 ; max = 1]



Next Steps / Opportunities

- AI/ML

https://ieeexplore.ieee.o rg/stamp/stamp.jsp?tp= &arnumber=8638596&ta g=1

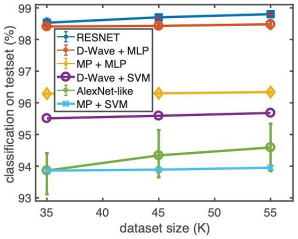


Fig. 5: (Color online) Image classification on the D-Wave 2X, near state-of-the-art DCNN (AlexNet-like) built with TensorFlow, and matching pursuit for our reduced dimensional

- Sparse Feature Identification (can be done with quantum-friendly algorithms)

- Hybrid algorithms

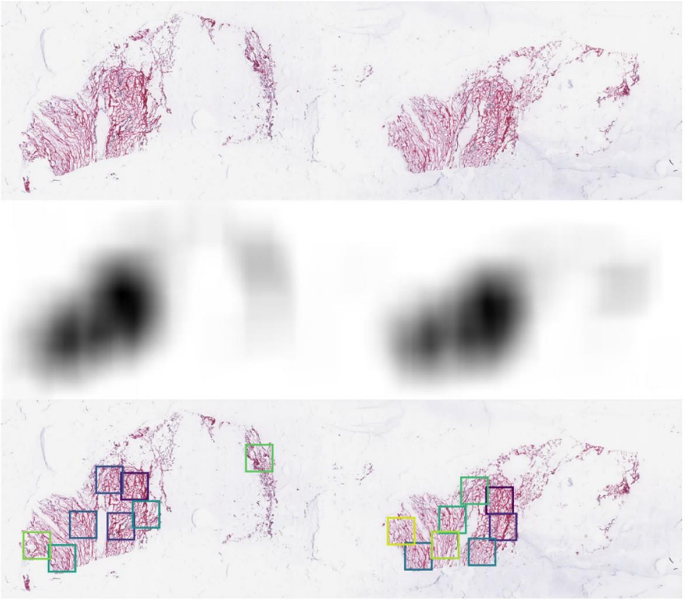
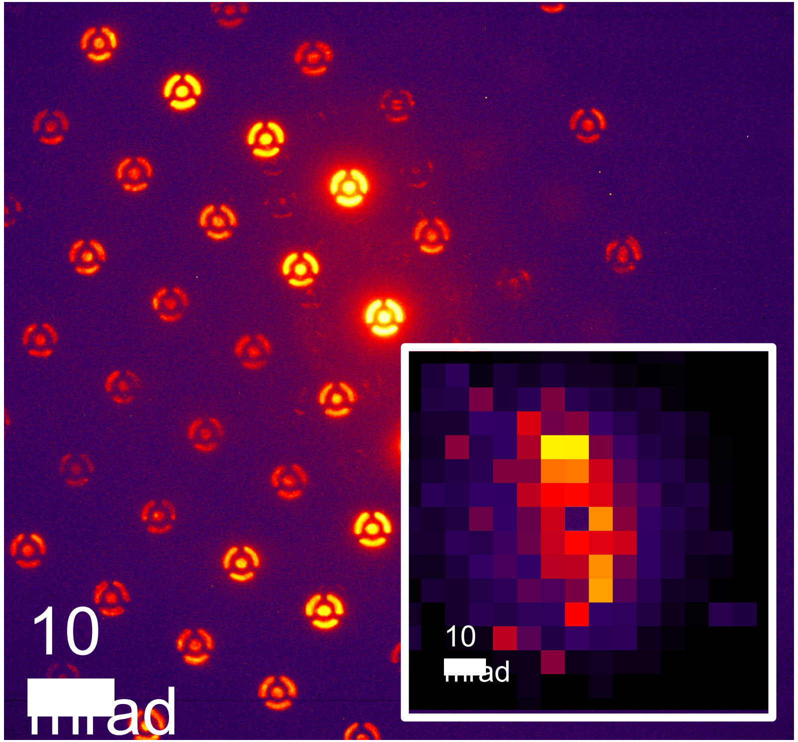


Fig. 1 Preprocessing of TCGA pathology slides. Full-extent low-resolution images were used to determine image coordinates; full-resolution image slices were used to generate sparse representations. Top: initial image; center: fast Fourier transform versus all-white, to determine optically dark regions of the image; bottom: non-overlapping image slices representing a succession of darkest remaining portions of the image. Full resolution regions of interest (ROIs; colored boxes) were extracted from the SVS file; the four darkest ROIs from each image were used for the analyses reported here

https://doi.org/10.1186/s12859-018-2504-8

Evaluation of Quantum Annealing Algorithms for Evaluation of Large Diffraction Datasets



High resolution image of electron diffraction of a polycrystalline metal used with classical image processing algorithms. (inset) Sparse representation of the same diffraction data used with quantum algorithms.

Project Description. The goal of this project is to explore the possible ways and practicality of using a quantum annealer for a currently important and hard problem of materials characterization and design, namely searching for a material's local orientation and structure, and identifying signatures of defects such as grain boundaries using unsupervised machine learning.

This is an image analysis problem tied to machine learning in a very high-dimensional space, thus being difficult for conventional computer algorithms as the datasets become increasingly larger.

Project Outcomes.

- New Collaboration between MPA and CCS bringing together researchers from very different parts of the lab.
- Pre-processing routine for image analysis by quantum annealer.
- Preliminary data for more thorough follow on studies involving methods built in CCS, i.e. AI/ML.

PI: Michael Pettes (Co-PI: Nga Nguyen-Fotiadis) Total Project Budget: $30,000

ISTI Focus Area: 2) Computing Platforms (including Quantum and Novel Computing)

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END