Computational Methods for Compressive Sensing driven Scanning Transmission Electron Microscopy

Jack Wells supervised by Yalin Zheng (UOL), Jony Castagna (Hartree Centre) and Nigel Browning (Sivananthan Laboratories)
EPSRC Centre for Doctoral Training in Distributed Algorithms, University of Liverpool, Liverpool, UK

Summary

- **Context and Motivations:** Compressive Sensing has been shown to reduce the total electron dose required to form a 2D scan in STEM.
  - ✔ Beam-sensitive materials may therefore be imaged without as much damage to the sample.
  - ✔ Complex (e.g. 3D) scans may be performed much faster with many fewer measurements.
  - ✗ Reconstructing images takes prohibitively long for the '*live*' operation of a microscope.
  - ✗ Microscope adjustment (e.g. Focus) would damage the sample before acquisition.
- **Contribution:** Development of efficient computational methods for subsampled STEM acquisition, dictionary learning and blind inpainting with the goal of 'real-time' reconstructions and operation of an Electron Microscope.

Over the last few decades, major developments in Scanning Transmission Electron Microscopy (STEM) such as modern aberration-correctors have enabled material scientists to analyse materials at the highest possible spatial resolution, allowing for atomic-scale observations of a materials structure, composition, and chemical properties. However, this unprecedented increase in achievable resolution has come at the cost of an increased operational probe current, now typically several orders of magnitude higher than many materials can withstand without significant damage to the sample. This has shifted the limiting factor from the properties of the instrument to that of the sample itself; in particular, the sensitivity of the sample to *electron beam damage*.

1. The Electron Microscope

Scanning Mechanism:

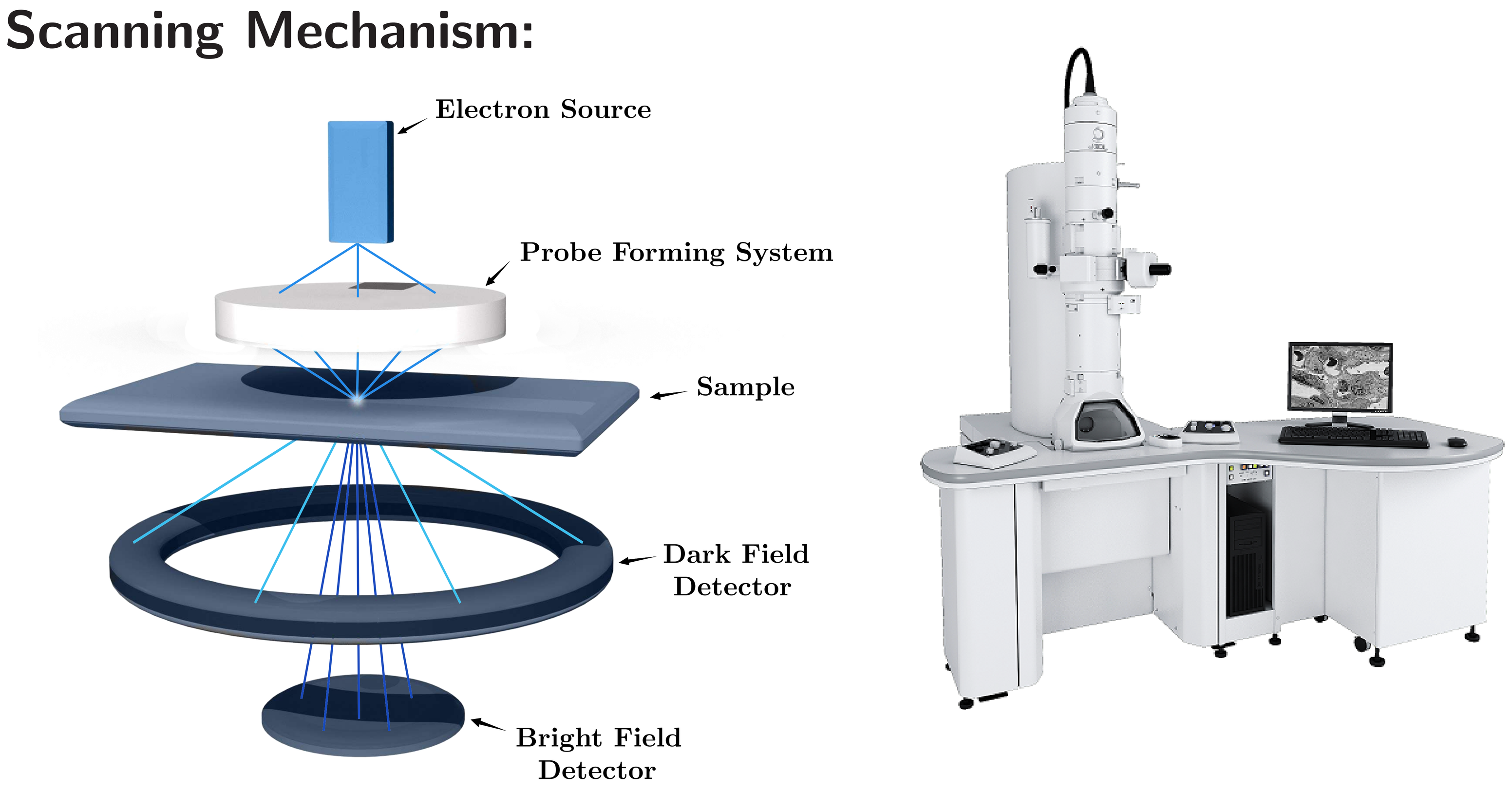


Figure 1: Electrons are emitted from the source and condensed by the probe forming system. The probe is then raster scanned over the sampling area and transmitted electrons are detected by either a dark field or bright field detector. The formed image is the intensity of the resulting electron wave-function at each pixel, corresponding to a certain set of coordinates.[1]

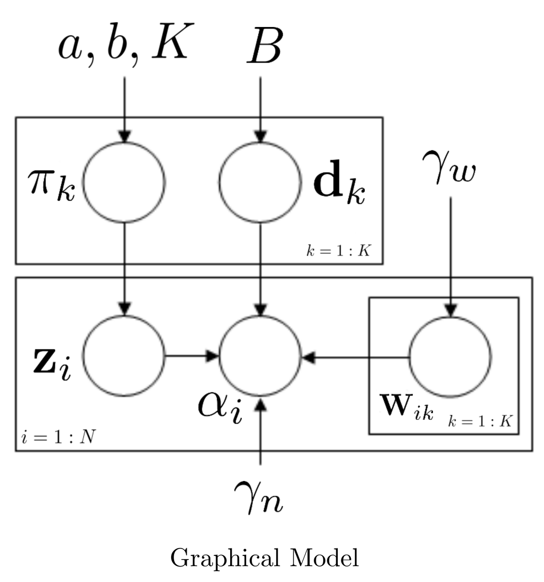
2. Compressive Sensing

In recent years, compressive sensing (CS) has been successfully applied to the field of low-dose STEM, where a deliberately subsampled (incomplete) scan is performed, acquiring an image with fewer pixels than in a regular raster scan, and reconstructing a fully sampled image from the reduced measurements. CS-STEM has been shown to reduce the dose, dose rate, and dose overlap necessary to recover a fully sampled image, all of which directly contribute to electron beam-damage.[2]

Theory:

BPFA model $$\mathbf{y}_i = \mathbf{P}_{\Omega_i}\mathbf{D}\alpha_i + \mathbf{n}_i$$ i^{th} signal (patch)

Dictionary of atoms:	$\mathbf{D} = [\mathbf{d}_1^\top, \cdots, \mathbf{d}_K^\top]^\top$
Distribution of atoms:	$\mathbf{d}_k \sim \mathcal{N}(0, B^{-2}\mathbf{I}_{B^2})$
Sparse weights:	$\alpha_i = \mathbf{z}_i \circ \mathbf{w}_i \in \mathbb{R}^K$
Distribution of weights	$\mathbf{w}_i \sim \mathcal{N}(0, \gamma_w^{-1}\mathbf{I}_K)$
Atom selection prob.:	$\mathbf{z}_i \sim \prod_{k=1}^{K} \mathrm{Bernoulli}(\pi_k)$
	$\pi_k \sim \mathrm{Beta}(\frac{a}{K}, \frac{b(K-1)}{K})$
Distribution of noise:	$\mathbf{n}_i \sim \mathcal{N}(0, \gamma_n^{-1}\mathbf{I}_{B^2})$



A full image inpainting algorithm (which takes only a *subsampled* measurement as its input) typically consists of a 'blind' dictionary learning algorithm such as Beta-Process Factor Analysis (BPFA) (developed in [3]) which learns the representative patterns within the target image, followed by a sparse-coding algorithm which aims to find the optimum combination of the learned dictionary 'elements' to best represent each overlapping patch of the image provided in the target batch.

Dictionary Transfer:

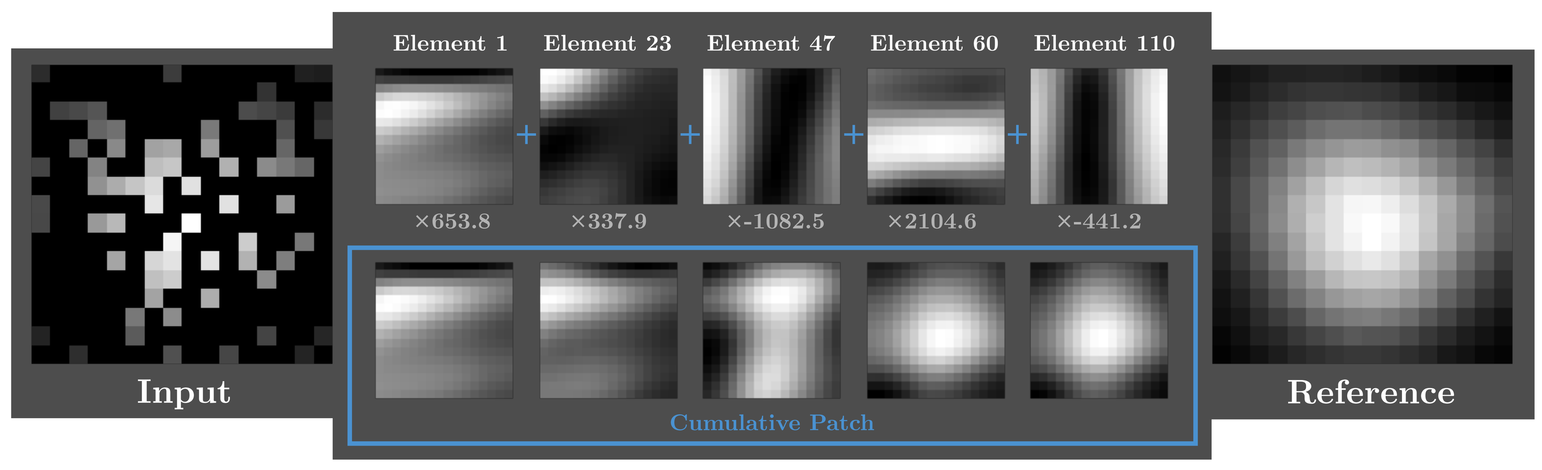


Figure 2: Illustration of the formation of a [16×16] patch containing a circular atom from seemingly inappropriate dictionary elements.

Image Reconstruction:

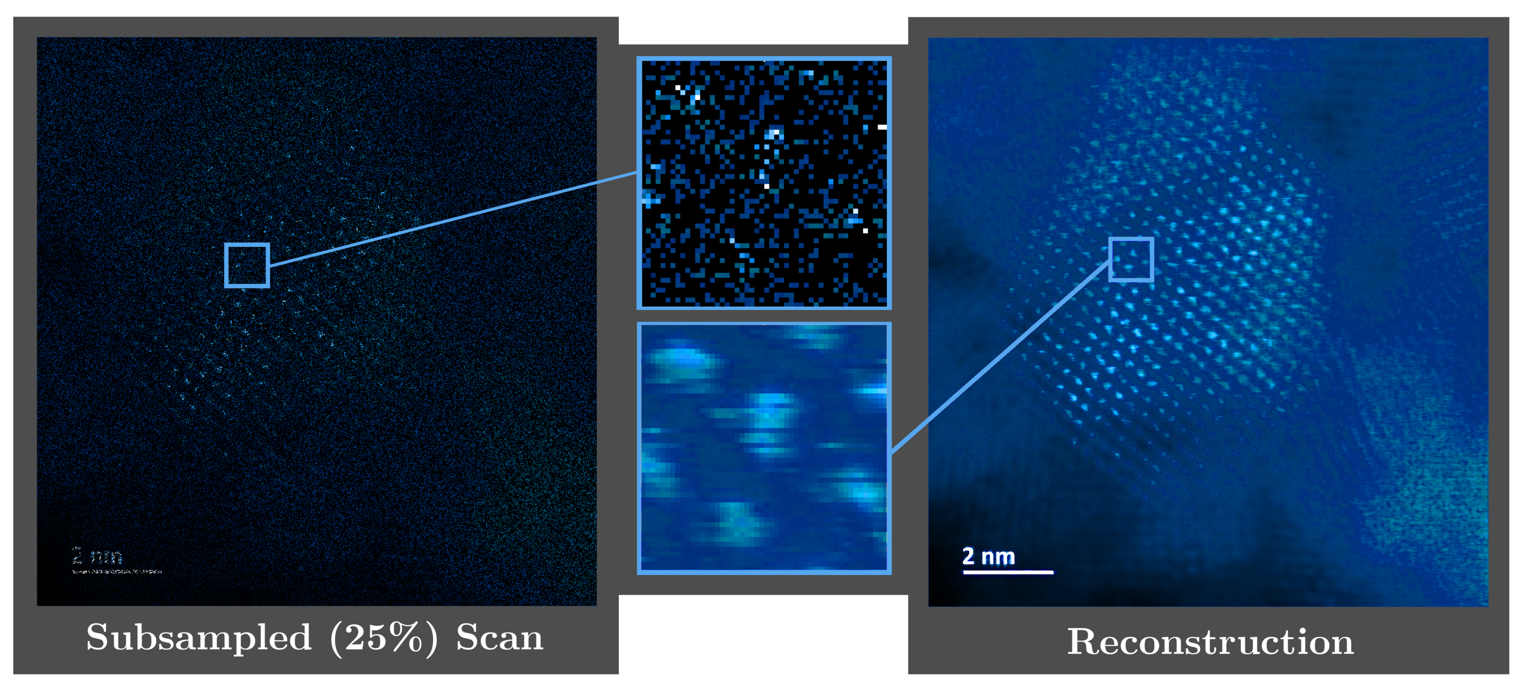


Figure 3: An example reconstruction of a STEM image subsampled to 25% of the pixels.

3. Time-to-Solution

One way to speed up reconstructions is to leverage the independence of the steps in the dictionary learning and sparse-coding process. In both cases, a separate algorithm is performed for each element or signal in the given batch, making the process highly parallelisable. By developing a method for generating batches of signals from an image on-demand (rather than attempting to build a full matrix), the amount of RAM required can be drastically reduced, and time-to-solution decreased further due to less time spent creating and copying memory.

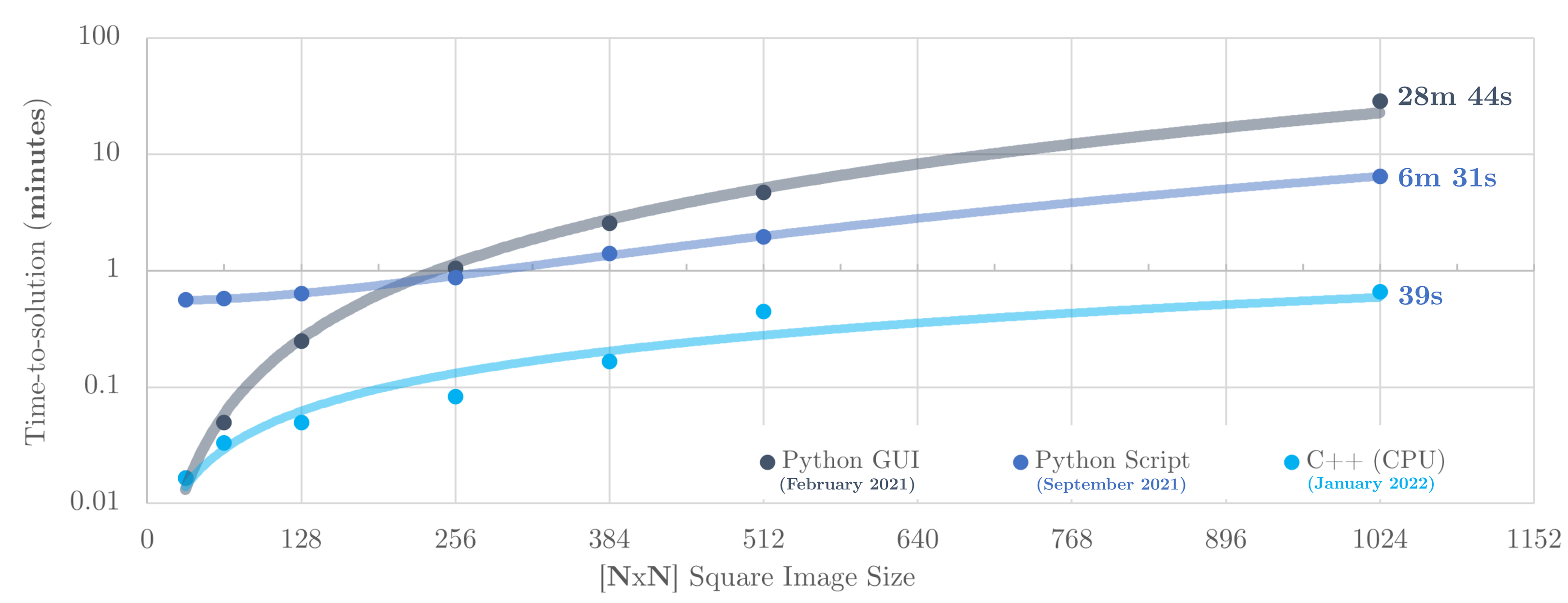


Figure 4: Time-to-solution vs Square (NxN) image size for a length 64 dictionary of [10x10] patches showing recent progress in computational efficiency

Future Work

This speed improvement from minutes/hours down to a matter of seconds provides a *pathway* to 'real-time' reconstructions of subsampled STEM images and/or each frame of a live feed from an electron microscope, allowing the operator to preview a beam-sensitive sample under low-dose conditions and make appropriate adjustments to the microscope. While currently implemented in parallel on a CPU, this implementation lends itself well to being performed on a high-performance GPU to reach even faster speeds and enable true real-time CS-STEM (frame-by-frame) video reconstruction.

Goals:

- ✔ Achieve 'Real-Time' reconstructions and subsampled operation of the microscope
- ✔ Investigate the most effective sampling strategies to obtain the best reconstruction quality for the least beam damage (including mask design, sequence and dwell-time).
- ✔ Apply these new methods to other data-sets, such as Hyperspectral (3D) data-cubes, Ptycography, STEM video etc.

References

[1] D. Nicholls et al., ICASSP **2022**, 2022, pp. 1586-1590
[2] A. Stevens el. al, Microscopy, **63** (2014), pp. 41–51.
[3] S. Sertoglu et. al, **23**rd European Signal Processing Conf. (2015), pp. 2771–2775.

Daniel Nicholls (UoL) is recognised for his work in acquiring data used in Figure 3.

Contact: Jack Wells (sgjwells@liverpool.ac.uk)

Engineering and Physical Sciences Research Council

UNIVERSITY OF LIVERPOOL

Sivananthan LABORATORIES