Phase retrieval with the Ptychographical Iterative Engine

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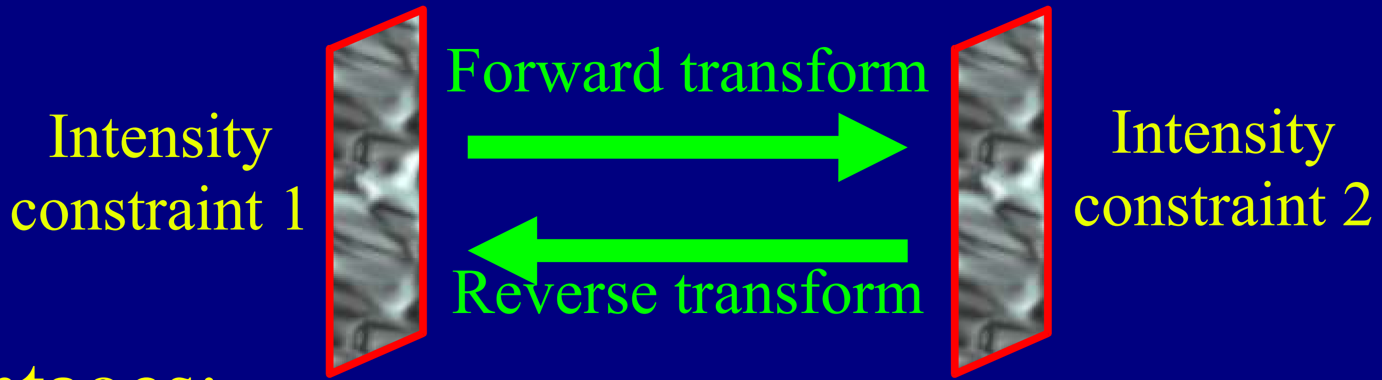
Outline

- Phase Retrieval
  - Iterative Algorithms
  - Ptychography
- Ptychographical Iterative Algorithm
  - Apparatus and Algorithm
  - Advantages of PIE
  - Experimental issues
- Conclusion

Iterative phase retrieval methods

- Gerchberg-Saxton method, Fienup method, etc



- Advantages:
  - Diffraction data can be easily measured at high resolutions
  - Image measurements are not necessarily required
  - Iterative algorithms are mathematically robust

- Disadvantages:
  - If images are required, lenses introduce aberrations
  - Alignment can be difficult
  - Not applicable to all specimens

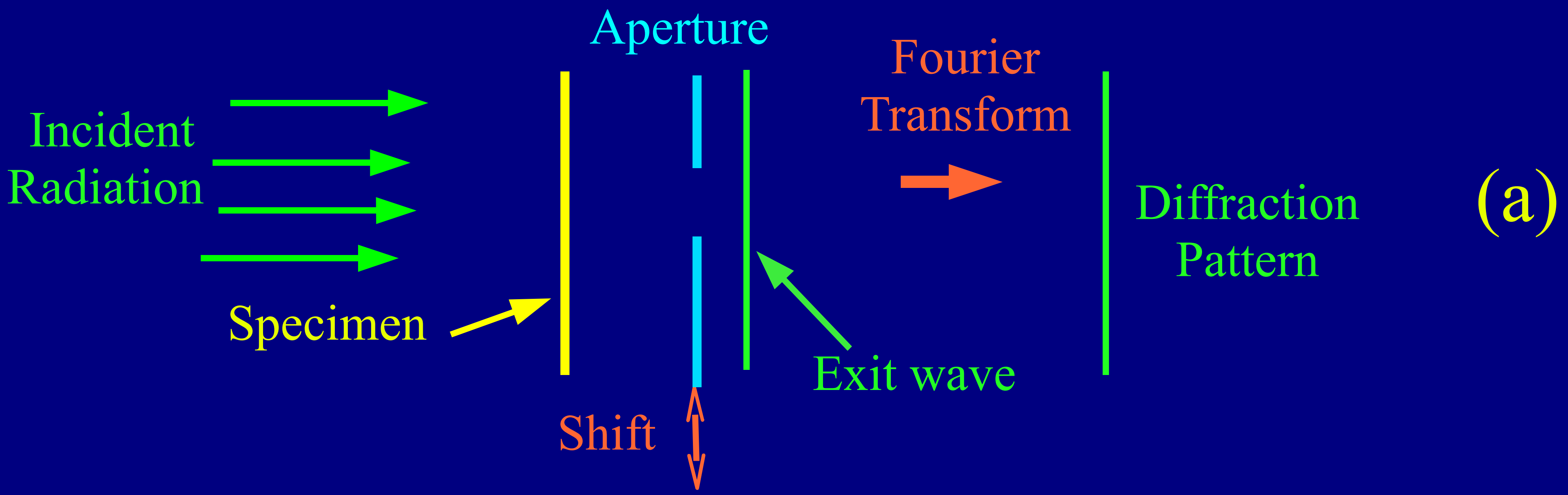
Ptychography

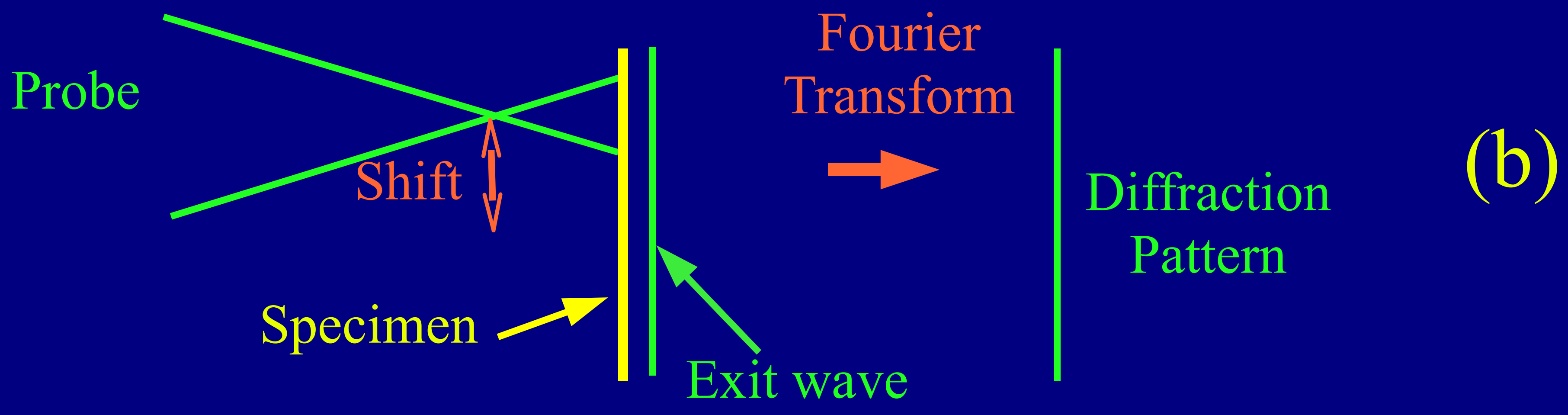
- Method:
  - Measure diffraction data from STEM at every probe position
  - Resulting 4D data set may be inverted to solve for the phase
- Advantages:
  - Uses only diffraction data
  - No limitations on specimen
  - Retrieves a wide range of view
- Disadvantages:
  - Very long data collection times
  - Specimen drift and contamination are a problem
  - Probe must be moved very accurately

A new approach to phase retrieval

- Combines the strengths of ptychography and the iterative methods
- Measure intensity only in the diffraction plane
  - Higher resolution is possible, since lenses are not required
  - Avoids alignment problems
- Vary the incident beam (eg STEM probe) position, or the position of a post-specimen aperture
  - This is experimentally easy to do without interfering with other parameters
- Only require a few measurements to have enough data
  - Specimen drift and contamination are reduced

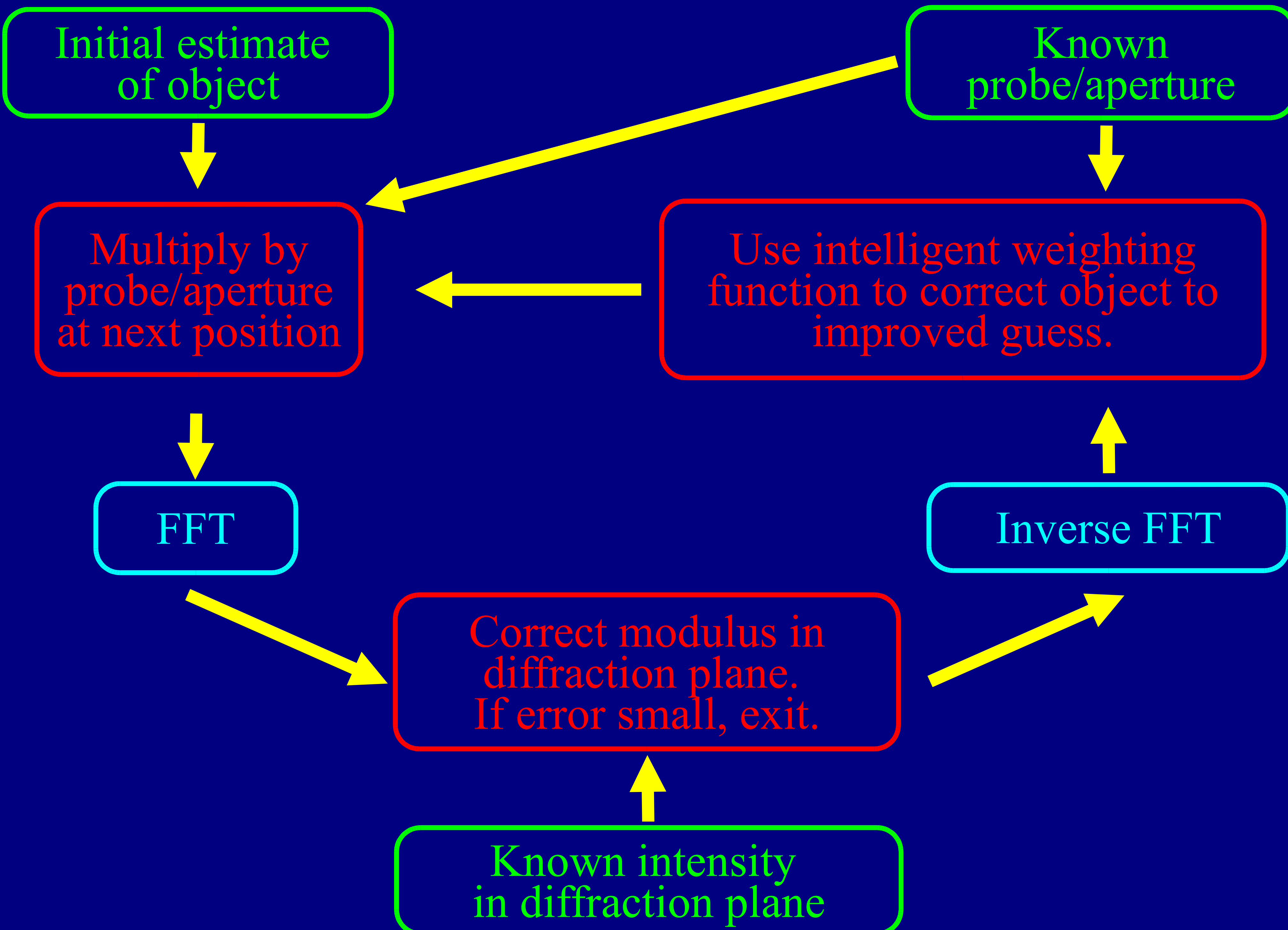
Potential experimental arrangements





Ptychographical Iterative Engine

- Works for general incident radiation or a general aperture
- Applicable to a very wide range of experimental situations:
  - STEM
  - X-ray diffraction
  - Light-optical experiments
  - ...


Initial estimate of object
Known probe/aperture
Multiply by probe/aperture at next position
Use intelligent weighting function to correct object to improved guess.
FFT
Inverse FFT
Correct modulus in diffraction plane. If error small, exit.
Known intensity in diffraction plane

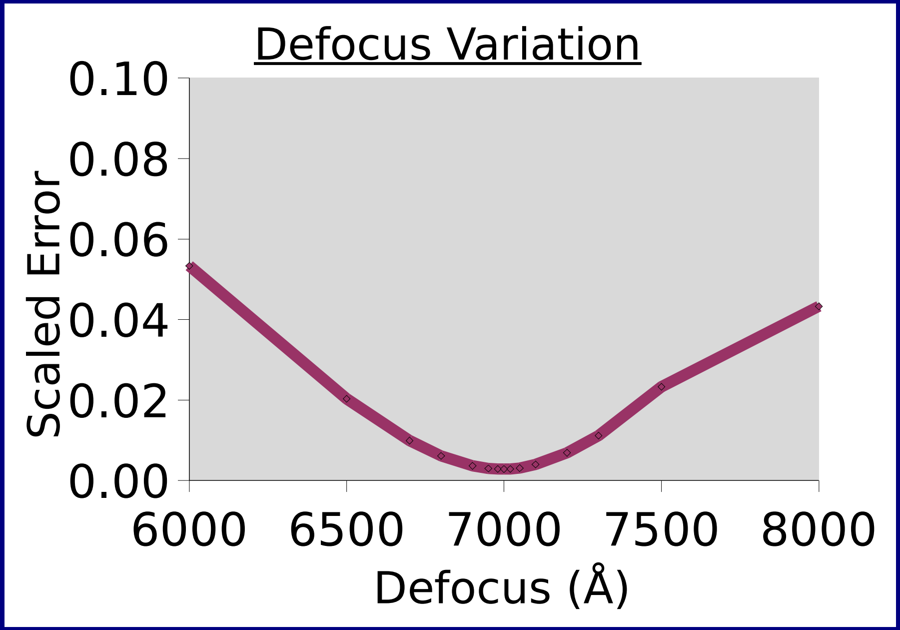
Weighting function makes the difference

$$object_{new} = object_{old} + \frac{|probe|}{|probe_{max}|} \times \frac{probe^*}{\left(|probe|^2 + \alpha\right)} \times \beta\left(\Psi_{corrected} - \Psi_{guessed}\right)$$

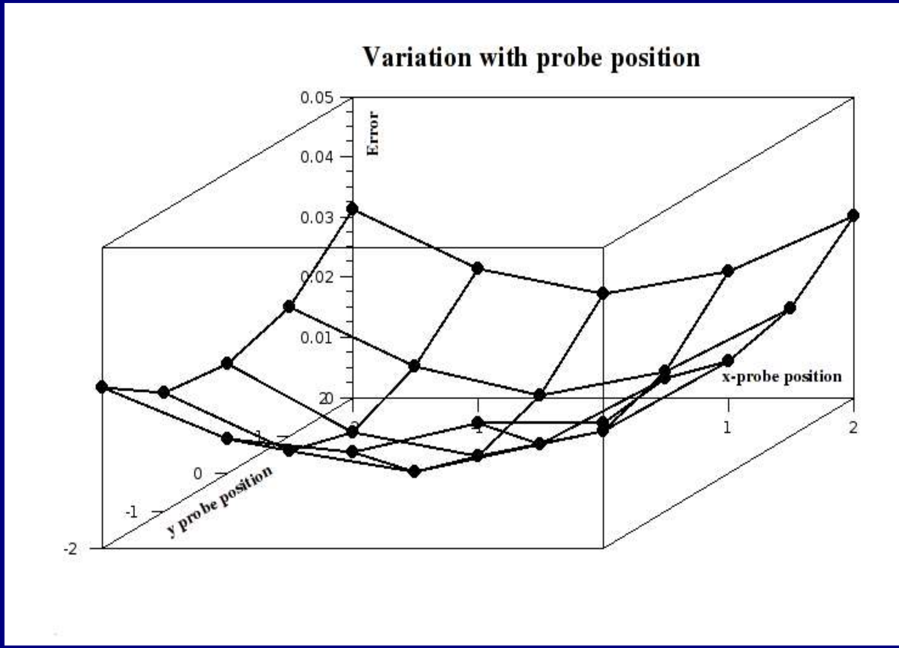
- The weighting function achieves the following:
  - Maximises contribution from regions where incident radiation is strong
  - Minimises contribution from regions where incident radiation is weak or non-existent
  - Allows varying contribution from the previous guess at the object
  - Reduces to dividing by the probe for correct choice of parameters, therefore making physical sense

Demo of PIE...

What if the probe is incorrectly known?



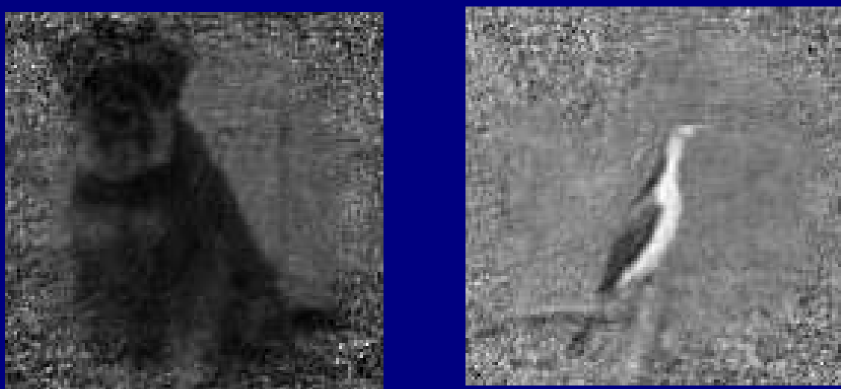
Defocus of STEM probe incorrectly known



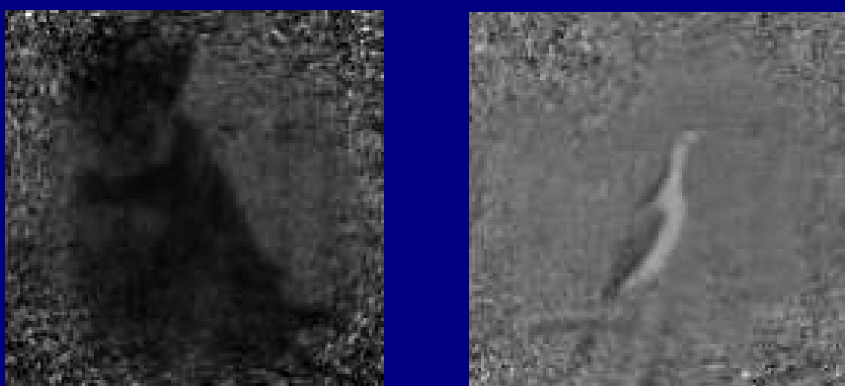
Position of STEM probe incorrectly known

- The PIE algorithm can be used to improve the characterisation of the incident radiation

What if the data is noisy, or the incident beam incoherent?



Poisson noise (10pA, 0.1s exposure)
plus 10% random noise



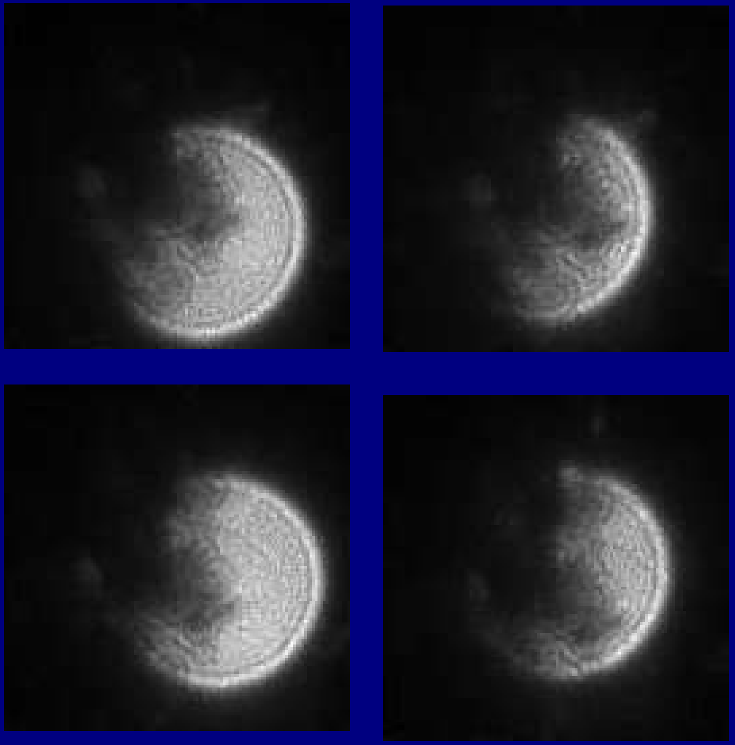
Poisson noise (10pA, 0.05s exposure)
plus 20% random noise

- Similar "graceful" degradation of performance as incoherence increases.

Why no experimental results yet?

- Good question!

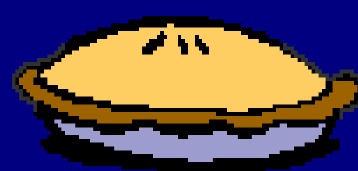
Gold on thin carbon film, with 200keV defocussed probe



- Data is not
  - Too noisy
  - Too incoherent
  - Too similar or disimilar
  - Assuming too incorrect characterisation of the probe
- Any suggestions?

Conclusion

- The PIE algorithm combines the best aspects of iterative algorithms and ptychography
- It is effective for general incident radiation and a general, complex specimen
- It allows close examination of whichever region/s of the specimen are of interest
- It allows more accurate characterisation of the incident radiation
- Experimental results soon...



The end