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The imaging methods being developed by this group all depend on the existence of a unique relationship between a diffraction pattern and an over-sampled periodic diffracting object. The program has found success in the past year in developing techniques adapted to imaging using beams of X-rays focused by zone-plates, and iterative phase retrieval algorithms derived from Fresnel propagators.

All methods of this type use whatever a priori information that is available about the diffracting object to assist in obtaining a representation of its image from diffracted intensity data. Such information includes its spatial extent (support), its material composition, the phase and intensity structure of the illuminating source, and the geometrical parameters of the experiment. With this must also be handled sources of systematic and random error, such as sources of noise, detector response functions and errors in determining the geometrical parameters on which the reconstruction algorithms critically depend. Two general approaches are being explored in the algorithm development program. The first of these are based on numerical propagation of the electromagnetic information between planes that are subject to known constraints. To this are currently being added a second layer of statistical methods, in which Bayesian hypothesis testing is used to assess the information content in the reconstruction on the basis of models of the diffracting object and the sources of error. This second line of attack will involve the detailed modelling of the experiment, including treatments of the partial coherence of the source, the detector response function the characteristics of the focusing zone-plate optics and the influence of scatter from intermediate apertures in the system. As well as these physical effects, detailed electronic models of the scattering materials are to be used to formulate tests against which to measure the likely accuracy of the reconstruction to the experimental data.

In preparation for the availability of highly coherent X-ray sources from high harmonic generation or free-electron lasers, preliminary work has begun on modelling the interaction between molecules and intense electromagnetic fields. This is very much frontier territory in theoretical research because of the need to obtain a detailed description of the time-dependent response of a complex system to a rapidly varying external perturbation that is sufficiently strong to cause secondary effects such as ionization and the cleavage of bonds. Since it is envisaged that the interaction between a molecule and such a source will occur over the lifetime of a pulse lasting of order a femto-second, the possibility exists that it will be possible to extract structural information from the diffracted intensities resulting from these encounters. Success in this part of the program will require a fundamental reappraisal of methods currently used in coherent diffractive imaging because of the non-linear response of the target to the illumination.