DIALS for ED: Adapting X–ray software for electron diffraction integration

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DIALS is a new diffraction integration package, designed as a flexible toolkit that can be used for a wide variety of tasks in single crystal diffraction analysis. Recently, efforts have been made to use DIALS to integrate electron diffraction data from 3D crystals of both small molecules and proteins. This presentation will report on some of the features of DIALS that have proven useful in this task, such as a plug-in system for new image data formats, 3D FFT indexing using all available data, joint refinement of multiple experiments with crystal unit cell restraints and multiple panel detector modelling. Some of the challenges inherent in processing ED data will be discussed, in particular those related to the refinement of diffraction geometry and the crystal unit cell in the presence of high parameter correlations and possibly unmodelled distortions. Nevertheless, it is seen that data processing is not typically the limiting factor and reasonable results can be obtained with simple data processing protocols when the experimental data is of good quality.