1 Application: xia2setup

1.1 Introduction

xia2setup is a new application which will "trawl" a directory and construct a .xinfo file to reduce the data that is found, with the following assumptions:

- All data in a directory is measured from one crystal.
- The date and time of data collection is in the image header.
- If a sequence (.seq) file is found in the directory this corresponds to the sequence of that crystal.
- If a scan (.scan) file is found this corresponds to the wavelengths of the data which were collected.
- Heavy atom information will be passed in on the command line.

This will give a command line something like:

xia2setup -atom se /path/to/directory

This will generate a .xinfo file called automatic.xinfo which should be inspected and perhaps updated before being used. If heavy atom information and a scan are supplied then the system will try to identify PEAK, INFLECTION, LOW and HIGH REMOTE data sets, or SAD if appropriate, else for sigle wavelength sets this will be called "NATIVE" or WAVE1