The State of CHART

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1 Recap

CHART was initially conceived to be a interventionless attempt at structure solution MAD/SAD/MIR/SIRAS data to initial atomic model[1].

It was designed therefore to work at the back end of Mosflm: (*i.e.* Auto-Mosflm would process the (typically) MAD data: write a simple parameter file (describing the derivative, number of residues, file locations *etc.*) and then spawns a process to run CHART).

2 Current Coding Efforts

I am adding an Acorn interface. This is the major issue to be resolved before the next release. Currently, I am sorting out the calculation of E's from the Anomalous (I amuse myself with the idea of using Clipper to do this).

3 Portability of scsh

Binaries for WindowsXX, SGI, "Linux" exist and are distributable. The spanner in the works is (64 bit) Alphas. However, I am working on a solution to that using **guile** (which truth to tell, is not completely working yet).

4 CCP4i Task

...on its way - I hope that it's in the next CHART release.

5 CHART and Python

I am not currently a Python user (I intend to be a routine Python programmer). I am not opposed to re-writing CHART in Python and don't want to make a decision about it now - I will come back to it.

I estimate 4-6 months to convert - maybe this is a conservative.

Also, CHART re-written in Python will have an attractively amusing name.

[1]because it incorporates ARP/wARP