Project Name: Crank

Name of pipeline: Crank

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Current Status: beta release

Purpose

To automatically take measured structure factor amplitudes and, using a wide variety of crystallographic programs, perform the various steps of crystal structure determination including: determine an anomalously diffracting or heavy atom substructure, refine and phase this substructure, perform density modification on these phases and build a protein model. Crank currently works with SAD and SIRAS data, with other experiment types currently being added.

High Level Description

Crank is a pipeline that has a CCP4i GUI and runs a variety of crystallographic programs including:

CRUNCH2
BP3
SOLOMON
SHELX[C/D/E]
DM
Various CCP4 programs and utilities

Crank provides for a simple way to setup jobs via the well known CCP4i interface and run them through a variety of different programs. For instance, once you have setup the CCP4i interface to find a substructure with CRUNCH2, you can easily change to run SHELXD instead by selecting SHELXD from a pulldown menu.

Crank uses the XML eXtensible Markup Language for all communications between programs. XML is currently being used by various crystallographic projects, including the DNA project and PDBml. This standard language has received much development in the computing community, and using it allows to take advantage of these existing development efforts.

Jiffies

Crank is composed of a small main "crank" script helped by many custom jiffy and utility programs that peform many functions, including converting XML to program input, converting program output to XML and extracting various pieces of information from reflection files.

For example, to convert the output of Crunch2 to a format suitable to BP3, one would run the programs:
crunch2trial2xmlcoords.tcl => Converts Crunch2 trial to XML
xml2bp3com.tcl => Converts XML to a BP3 command file

The full listing of Crank jiffy programs can be found on the Crank website.

Decision Making

Decision making in Crank is to be external to the Crank programs, and is to be encoded in XML.

Data Standards and Management

Data is stored and transferred primarily in XML. Reflection data is currently stored in MTZ files. There are a few different types of Crank XML data, including coordinate data, dataset information and program control information. These files are produced by Crank and can be converted to be of use with other packages with jiffies within the Crank suite.

Languages

The main Crank program is written in a variety of languages, including Tcl, C, C++, sh, csh, FORTRAN, and Python. However, Crank is written primarily in Tcl for ease of communication with the CCP4i suite.

External dependencies

Crank has only the CCP4i package as its single dependency. Internally, it contains programs to find a substructure (CRUNCH2), refine and phase this substructure (BP3) and perform density modification (SOLOMON.

However, Crank also interfaces with external crystallographic programs, including, amongst others SHELX[C/D/E] and the cctbx suite. To fully utilize Crank, these programs should also be obtained.

Context/Audience/Environment

Crank is designed to both enable experts as well as helping to teach crystallography to beginning students. By using a simple GUI, beginners can easily setup their jobs in CCP4i. Crank creates run directories for each crystallographic program, setting up a standard .com command file in each one, running this .com file, and outputting the log file information. In this way, beginning users can then look at the input and output to these various crystallographic programs, learning about their use. Finally, Crank enables experts by decoupling the CCP4i interface from the Crank engine, allowing the user to either directly modify the input to Crank, or alternatively, to run the various Crank jiffy programs by hand.

Links to Supporting Documents

http://www.bfsc.leidenuniv.nl/software/crank

References

Crank: New methods for automated macromolecular crystal structure solution Steven R. Ness, Rudolf A.G. de Graaff, Jan Pieter Abrahams, and Navraj S. Pannu Structure Vol 12, 1753-1761, October 2004