Project Name:
SHARP/autoSHARP

Name of pipeline:
autoSHARP

Author information:
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Current Status:
06/2000 – first beta release
01/2002 – first production release
02/2005 – SHARP 2.0.4, autoSHARP 3.2.3 (> 1000 sites)

Purpose

Extending the heavy atom refinement and phasing with **SHARP** both upstream (data analysis, heavy atom detection) and downstream (density modification, automatic building)

High Level Description

The pipeline is organised as a "information gathering" tool: from a minimal amount of user input data, each step/module tries to extract as much information as possible based on current knowledge. At various stages, feedback mechanisms are built in. The main steps are: **1.** data analysis (syntax checking, solvent content analysis, outlier detection, dataset scaling, self-rotation, native Patterson, data limiting for HA detection); **2**. HA detection (Harker section plotting, correlating initial direct methods solutions with Patterson, decision on number of sites); **3**. HA refinement and phasing (including automatic interpretation of LLG maps and phasing in inverted hand); **4**. density modification (SOLOMON, decision on correct hand, automatic optimisation of solvent content); **5**. automatic building (ARP/wARP, slightly altered to tie in with information coming from SHARP/SOLOMON)

Jiffies

A library of basic crystallographic tools (e.g. extracting information from MTZ, SCALEPACK or CCP4 MAP files; converting between different asymmetric unit conversions; switching hand, solvent content analysis etc); a peak picking program (PKMAPS) which can also read e.g. PDB files and perform boolean operations.

Decision Making

Each module inerits the information gathered at all previous steps. Based on this additional knowledge, better (or completely new) decisions can be taken. These can be either binary decisions (a calculation/step is either performed or skipped if some parameter is within pre-defined limits), more fuzzy (a parameter is only close to a predefined limit – but within certain boundaries – so that another step in the calculation is performed, for which now tighter restrictions are applied) or are resulting in an ordered succession of trials (sorted according to experience based highest success probablility)

Data Standards and Management

Database (information gathering process): simple flatfile that can either be read directly in Bourne shell or translated from its parameter=value format)
Coordinates: PDB or internal format for orthogonal coordinates; COORDCONV, *.hatom or internal format for fractional coordinates
Reflections: MTZ (but also SCALEPACK on user input)

Languages

autoSHARP is mainly written in standard Bourne-Shell (with some OS-dependent wrappers for portability), but some parts are written in Perl.
The GUI (Sushi) is written mainly in Perl, HTML/JavaScript and Bourne-Shell

External dependencies

OS: Bourne-Shell, Perl
Crystallographic tools: CCP4

Context/Audience/Environment

flexible installation scenarios (client/server design): single machine, network of several machines (queing mechanisms like LSF, DQS, PBS, ...or rsh/ssh submission), through the internet at any location.

Links to Supporting Documents

Home page: http://www.globalphasing.com/sharp/ (FAQ, Licence, Download, Support ...)
Manual: http://www.globalphasing.com/sharp/manual/index.html
Installation: http://www.globalphasing.com/sharp/installation/index.html

References

Generation, representation and flow of phase information in structure determination: recent developments in and around SHARP 2.0 (2003). G. Bricogne, C. Vonrhein, C. Flensburg, M. Schiltz & W. Paciorek. Acta D59, 2023-2030.