Data Management in CCP4(i)
Current Status and Future Plans

Peter Briggs
CCP4 Daresbury Laboratory

- Introduction/Overview

- Current status
  - Libraries/MTZ files
  - Data Harvesting
  - Automation in CCP4i
  - CCP4i Project History Database

- Ongoing developments & near-future plans
  - Database handler

- Further ahead
  - Expansion of database content
  - Project history visualisation

CCP4, Data Management and High Through-Put

- In this context HTP = automation
- Data management in automated procedures
  - Acquisition of necessary data on demand (both for running software components and for making decisions)
  - Capture as much information as possible at each step
  - Tracking required for review and diagnostics
  - Information required for validation and deposition
- Requirements are similar (if less formal) for human user
- Automatic transmission of data:
  - allows streamlining of procedures
  - cuts down on manual handling & transcription mistakes

Background: Quick Introduction to the CCP4 Suite

- Collaborative Computational Project No.4
  - software for macromolecular structure determination by X-ray crystallography

- Consists of a suite of ~150 programs plus a set of core software libraries
  - Scope: from data reduction to structure validation/analysis
  - Modular: each program covers small range of functionality
  - Data is transferred via files with standard formats
  - Core libraries used to provide a consistent user and developer environment

- CCP4i (graphical user interface)
  - Sits on top of programs
  - Adds extra functionality (project history database)

CCP4 Libraries: Moving Towards Improved Data Models

- Requirement to support legacy code while moving forward

- Currently: underlying libraries mix Fortran and C
  - "Data models" expressed in Fortran COMMON blocks

- New libraries based on C/C++
  - Data models expressed in C/C++ headers
  - Aim for consistency with community data models
  - Interfaces to Fortran, scripting languages (e.g. Python, Tcl)

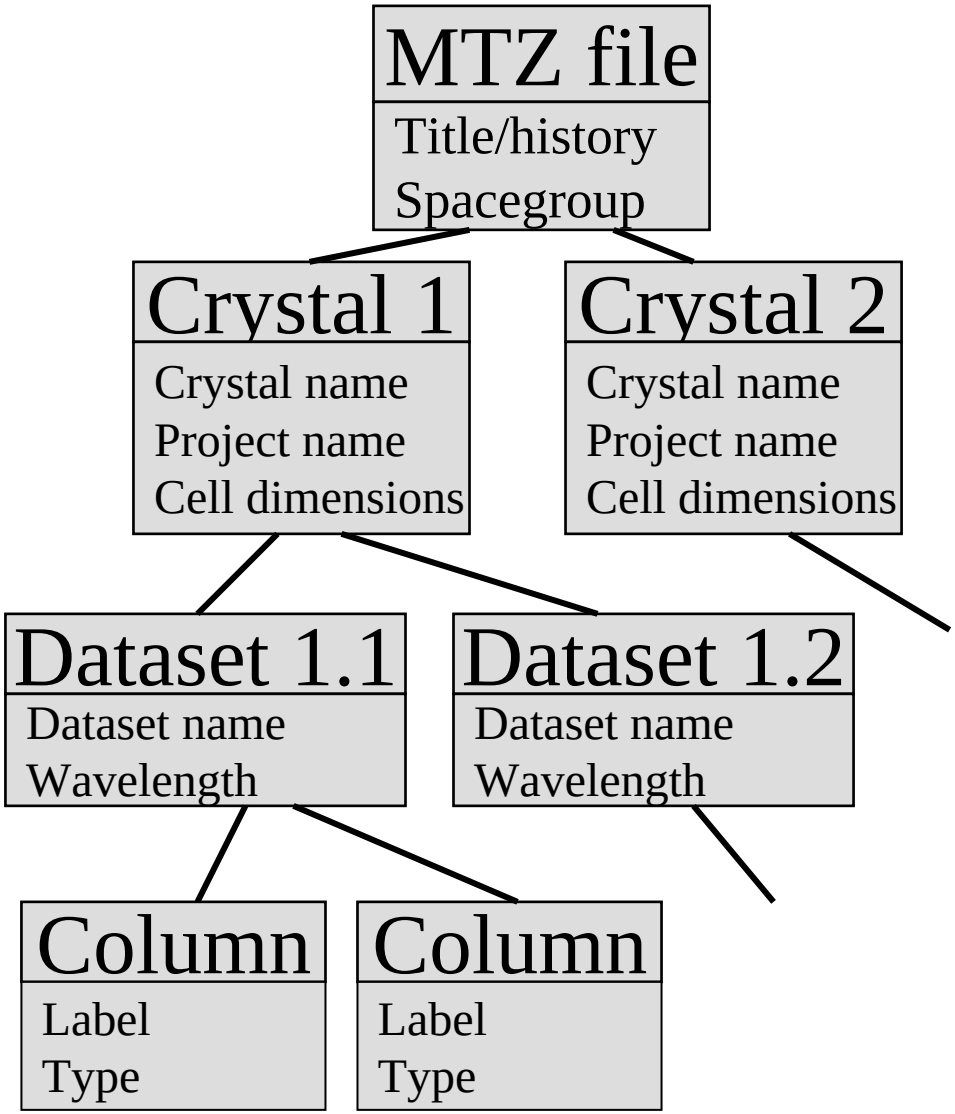
- Key components:
  - CMTZ: imposes formal structure on reflection data
  - MMDB: similar for co-ordinate data

MTZ files and Data Hierarchy

- MTZ files
  - **MTZ = M***cClaughlin* **T***erry and* **Z***elinka*
  - CCP4 reflection data format

- Next release introduces the concept of */crystal/dataset/column* hierarchy

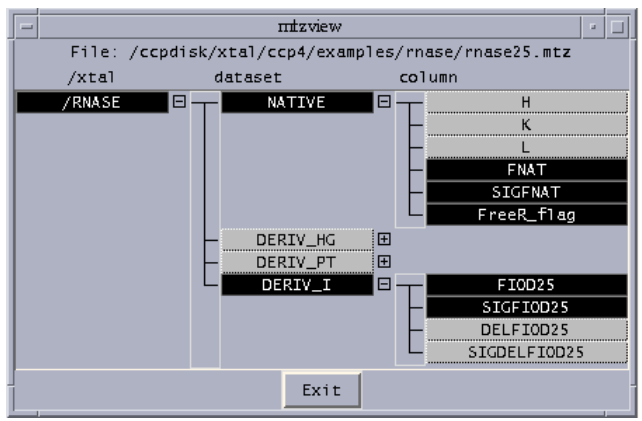
- Explicit relationships between column data enables basic automation:
  - e.g. automatic column selection for consistent scaling


MTZ file
Title/history
Spacegroup
Crystal 1
Crystal name
Project name
Cell dimensions
Crystal 2
Crystal name
Project name
Cell dimensions
Dataset 1.1
Dataset name
Wavelength
Dataset 1.2
Dataset name
Wavelength
Column
Label
Type
Column
Label
Type

MTZ Hierarchy - Other developments

- e-HTPX is developing XML Schema to describe HTP structure determination
  - XML schema based on CMTZ forms part of description of structure solution (Joel Fillon)
  - CCP4 libraries will be consistent with data model

- Viewer for hierarchical information
  - Selection
  - Editing



Data Harvesting

- Originally introduced into CCP4 in version 4.0 (2000)
  - Historically significant: introduced the concept of datasets into CCP4/MTZ files

- Key programs automatically capture data which are written to harvesting files:
  - MOSFLM, SCALA, TRUNCATE, MLPHARE, REFMAC
  - Harvest files written in mmCIF format
  - Use Project-Dataset name pairs in MTZ header
  - Can be uploaded to AutoDep and merged into current deposition

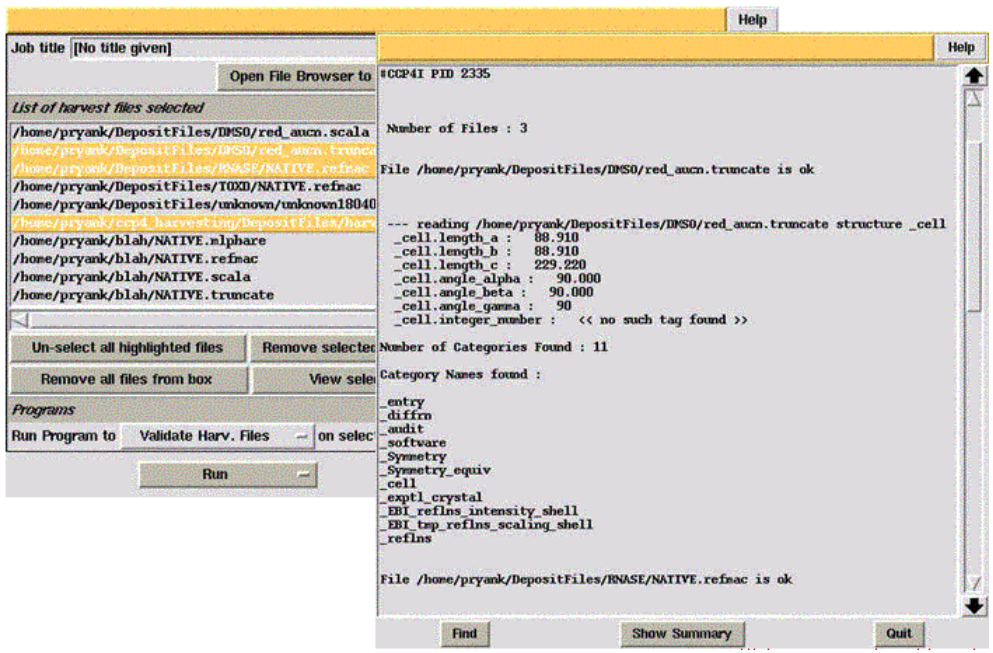
- Harvesting integrated into CCP4i
  - Turned on by default

Data Harvesting: Harvesting Management Tool (Pryank Patel)

- Raise profile of harvesting within user community
- Graphical tool to assist users in managing harvest files prior to uploading at deposition site

Functions:

- Select and view harvest files
- (Cross) validate files
- Convert mmCIF to XML



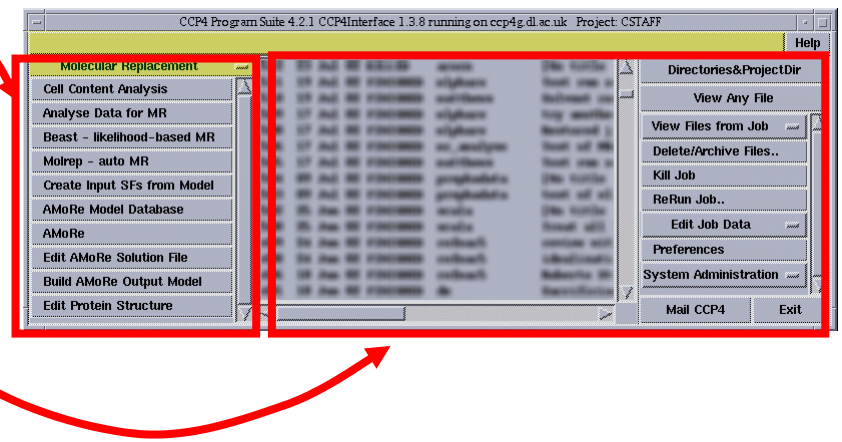
CCP4i - CCP4 graphical user interface

• Development started 1997; public release 1999; part of main CCP4 suite 2000.

• Introduced an integrated environment for running CCP4 programs, particularly suitable for novice users

• Easier to run programs

• Data management features:
  • Basic file management
  • Job database
  • Electronic notebook
  • Retrieval of parameters



CCP4i: Automating Tasks

CCP4i build around interfaces to **tasks**

- Task = script running one or more programs

Two approaches to automation piloted within CCP4i:

- Add automated procedures within existing tasks
- Automated transfer of data between tasks

Use XML files as transport mechanism for data

CCP4i Automated Parameter Passing within Tasks

- Example 1: CAD Auto-reindexing
  - CAD is program for merging two or more reflection files
  - Merging files which are inconsistently indexed can be disastrous
  - Can be checked and corrected automatically
  - CAD task runs ALMN program:
    - performs pair-wise comparison of MTZ files
    - generates XML file with reindexing instructions
    - file is parsed by CAD script
    - runs REINDEX with appropriate parameters if necessary
  - *Automation of a "trivial" but convoluted operation*

CCP4i Automated Parameter Passing between Tasks

- Example 2: Molecular Replacement
  - "Cell content" and "MR Analyse" tasks are be run prior to "Molrep"
    - "Cell content" calculates # of monomers in asu
    - "MR Analyse" identifies pseudo translations from Patterson
  - User must transfer data manually to input of "Molrep"

  - Instead: programs write information to XML files:
    - MATTHEWS_COEF for "Cell content"
    - PEAKMAX for "Analyse MR"
  - "Molrep" task parses XML files on startup and reads in data automatically

  - *Reduce manual handling by users*

Example XML Parameter File Fragment

- MR_ANALYSE.xml (output from PEAKMAX)

```
<?xml version="1.0"?>
 <peakmax_run>
  <PEAKMAX ccp4_version="4.2" date=" 7/17/02" />
  <peakmax_keyword>
  </peakmax_keyword>
  <peakmax_result
    order_number="           1"
    site_number="           1"
    height_over_rms="   38.66371"
    peak_frac_x="  0.5000000"
    peak_frac_y="  0.5000000"
    peak_frac_z="  0.0000000E+00"
   />
  ...
```

CCP4i XML Parsing

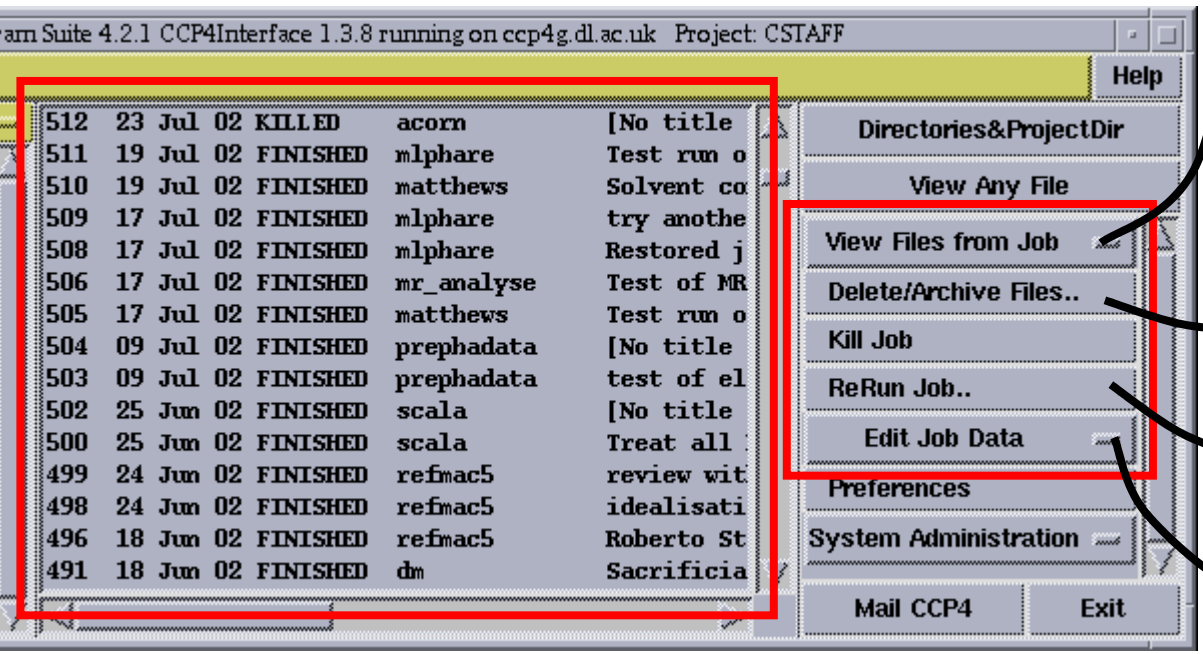
- Programs:
  - Use PXXML library to generate XML files
- CCP4i: use xml.tcl/sgml.tcl
  - Write custom code based on xml.tcl to parse XML files
  - Currently need to write specific code for each file
- Generally: XML is not defined in a global context
  - i.e there is no ccp4.xml schema defining the tags
  - would be useful to standardise output from programs
  - should be consistent with schema being developed by e-HTPX

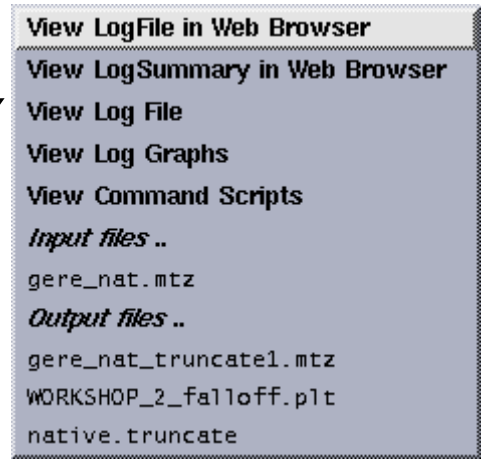
CCP4i Project History Database

- CCP4i uses the concept of Projects and Project Directories
  - CCP4i creates a database subdirectory in the Project directory which stores database file and job parameter files
  - Definition of a Project is left up to the user
  - One Project per Project Directory

- Job Database (Project History Database)
  - Keeps record of each instance of a task (=job) run in Project

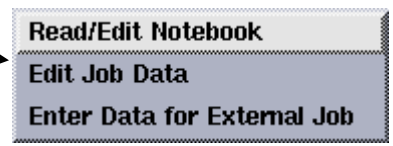
CCP4i Project History Database





Perform clean up

Review parameters



Job Database

Utilities

CCP4i Project History Database - technical details

- Flat file storage
  - CCP4i .def file format
  - Indexed parameter-value pairs
  - Associated parameter files (.def files) are identified via standard naming scheme

- Example entry:

```
STATUS,55                  FINISHED
DATE,55                   985023073
LOGFILE,55                55_superpose.log
TASKNAME,55               superpose
TITLE,55                  "overlaying reduced on oxidised wdmsor"
INPUT_FILES,55            "/dl/sr/homes/px/slj/1e18.pdb ...
INPUT_FILES_DIR,55        "FULL_PATH FULL_PATH"
INPUT_FILES_STATUS,55     ""
OUTPUT_FILES,55           "overlaid_1.pdb overlaid_2.pdb ...
OUTPUT_FILES_DIR,55       "PROJECT PROJECT PROJECT PROJECT ...
OUTPUT_FILES_STATUS,55    ""
```

CCP4i Database: Limitations

Technical:

- Tcl API to interact with the database embedded in core CCP4i
- Not accessible from outside of CCP4i
- Ambiguous status for many-user access
- Flat file format doesn’t scale well

Content:

- Relationships between jobs can only be inferred from file names
- Focused on history content

CCP4i Database: Database Handler (dbCCP4i)

- Server process running independently of main CCP4i
- Current prototype version:
  - Uses Tcl sockets (allow many processes/users to connect across network boundaries)
  - Need to define communication protocol (request/response)
  - Issues with security/authentication/authorisation

- Manages interactions with Project Database
  - Hides database implementation details
  - Easier to migrate database backend e.g. mySQL

- Alpha version of CCP4i using dbCCP4i available summer 03
  - See **`http://www.ccp4.ac.uk/peter/dbhandler_specification.html`**

CCP4i Database: Expanding Scope/Content

- Improving project tracking facilities
  - Capture more information about each job:
    - Logical flow
    - Data flow
  - Fill in gaps from other dbs?

- Expand scope of Project Database
  - e.g. sequence information, MR trial models, HA derivative preparation
  - Could be obtained from external databases e.g. LIMS

- Use community standards (XML schema) to facilitate Data Exchange (both ways)

- Requires redesign/re-implementation of the database

Future Plans: Project History Visualisation Tools

- Currently in CCP4i: just a list

- Investigate other ways of presenting history to emphasise particular aspects:
  - Flow of data - where data comes from
  - Logical flow
  - Paths (“How did I get here?”)
  - Searching/Querying

- Facilitate understanding of the structure solution
  - Increasingly important for reviewing automated procedures
  - Trend towards data-driven interfaces?

Acknowledgements

CCP4 Daresbury

Core developers: Martyn Winn, Alun Ashton, Charles Ballard, Peter Briggs
TEMBLOR/Data Harvesting: Pryank Patel

CCP4 University of York

Liz Potterton

e-HTPX (EBI)

Joel Fillon

… and countless other contributors to the CCP4 Project

The End.