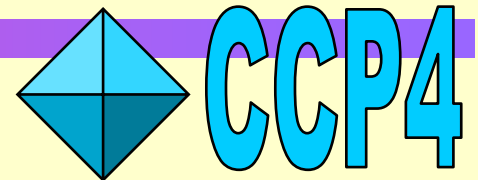

An Introduction to CCP4i

The CCP4 Graphical User Interface

Peter Briggs
CCP4

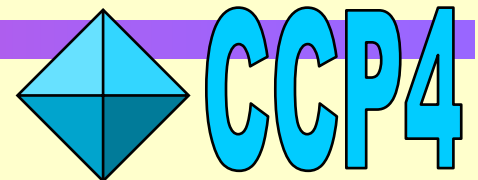


Introduction: Why use CCP4i?

- Offers user friendly interfaces to the programs
- Tools for file viewing & “project management”
- Integrated help system

How to get started

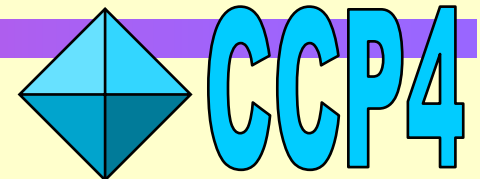
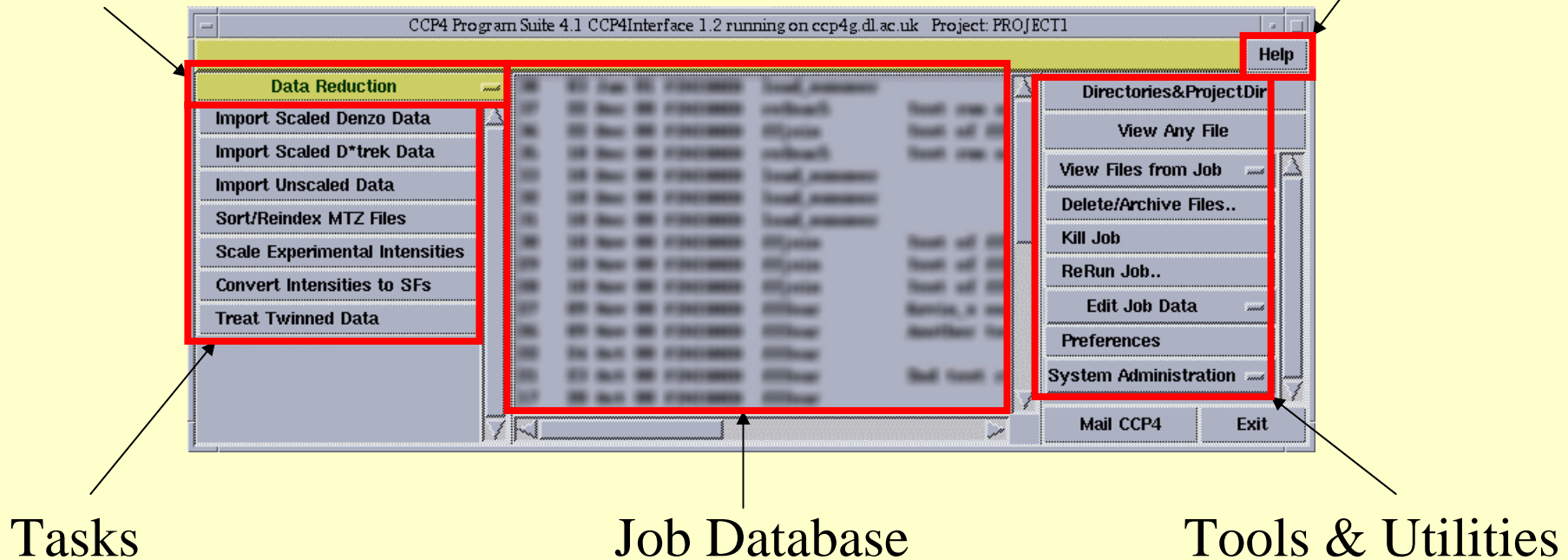
- (*Unix/Linux*) Type **ccp4i** at the command prompt
- (*Windows/NT*) Select **ccp4i** via the Start menu



Main CCP4i Window

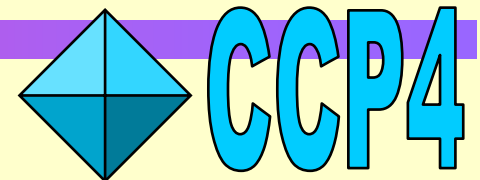
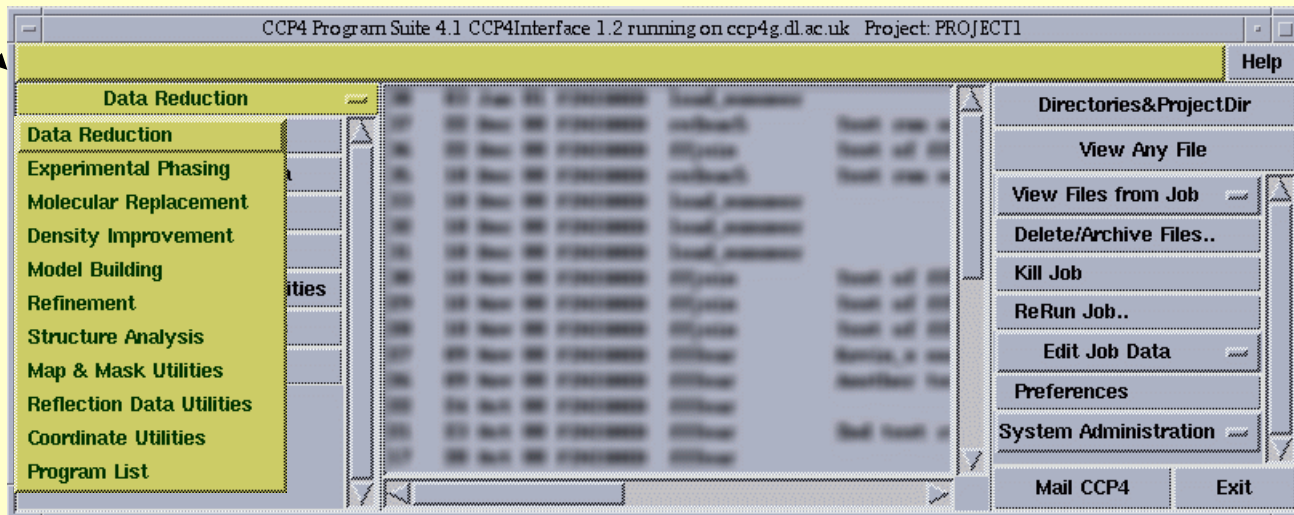
Modules

On-line help



Modules

- Access the module list by clicking on the gold bar displaying the current module



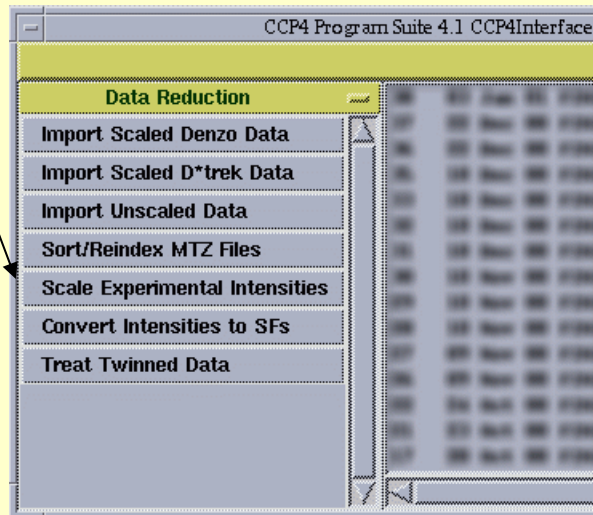
Modules

Data Reduction
Experimental Phasing
Molecular Replacement
Density Improvement
Model Building
Refinement
Structure Analysis
Map & Mask Utilities
Reflection Data Utilities
Coordinate Utilities
Program List

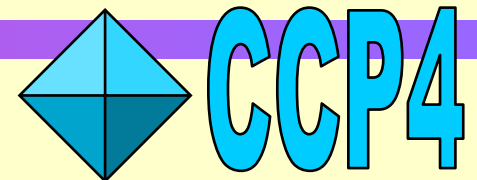
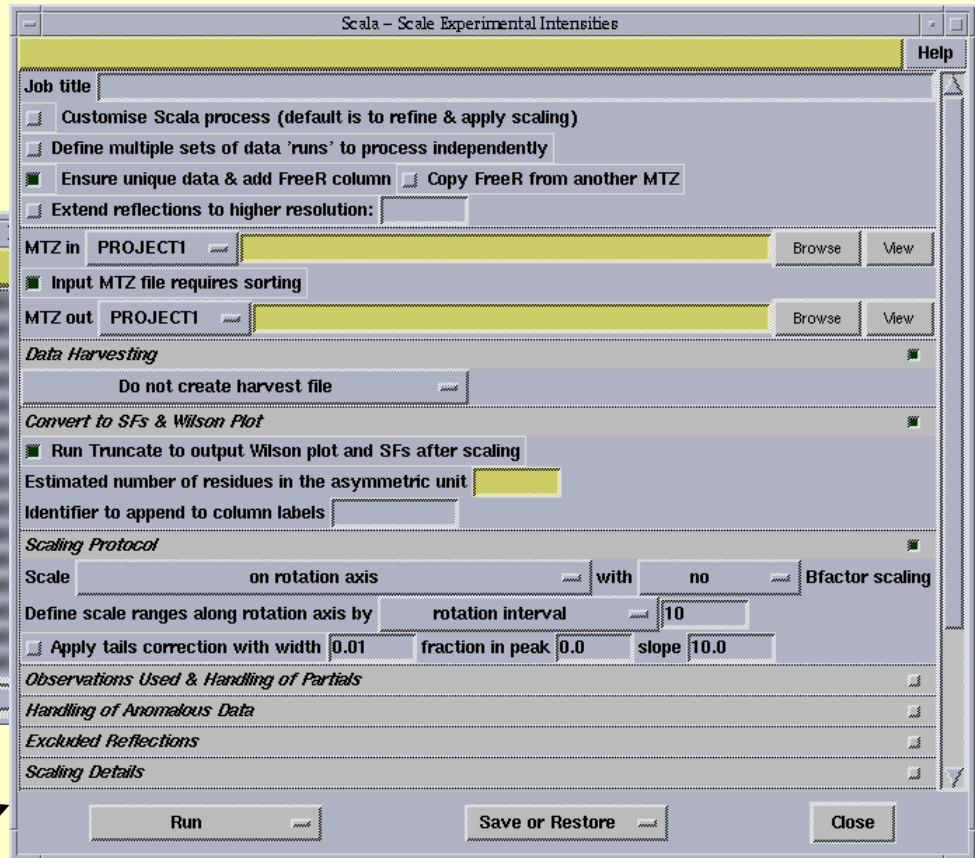
- Tasks used in a particular part of the structure determination process
- Utility tasks for manipulating different types of data
- Alphabetical list of programs/tasks

Tasks

- Click on the appropriate button in the list to start a particular task



- This starts the interface for that task



Example Task Interface

WORK FROM THE TOP DOWN



Protocol folder

Make the key decisions

File folder

Set input and output file names

Open folders

Parameters that should be checked by the user before running
Highlights indicate compulsory input

Closed folders

Advanced/infrequently used options

Scala - Scale Experimental Intensities

Job title Always add a title to distinguish different runs of the same task

Customise Scala process (default is to refine & apply scaling)

Define multiple sets of data 'runs' to process independently

Ensure unique data & add FreeR column Copy FreeR from another MTZ

Extend reflections to higher resolution:

MTZ in PROJECT1 Browse View

Input MTZ file requires sorting

MTZ out PROJECT1 Browse View

Data Harvesting

Do not create harvest file

Convert to SFs & Wilson Plot

Run Truncate to output Wilson plot and SFs after scaling

Estimated number of residues in the asymmetric unit

Identifier to append to column labels

Scaling Protocol

Scale on rotation axis with no Bfactor scaling

Define scale ranges along rotation axis by rotation interval 10

Apply tails correction with width 0.01 fraction in peak 0.0 slope 10.0

Observations Used & Handling of Partials

Handling of Anomalous Data

Excluded Reflections

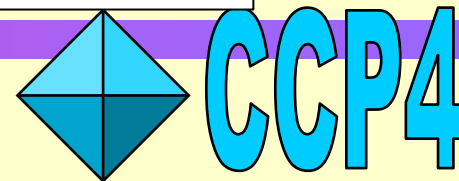
Scaling Details

Run Save or Restore Close

Run task

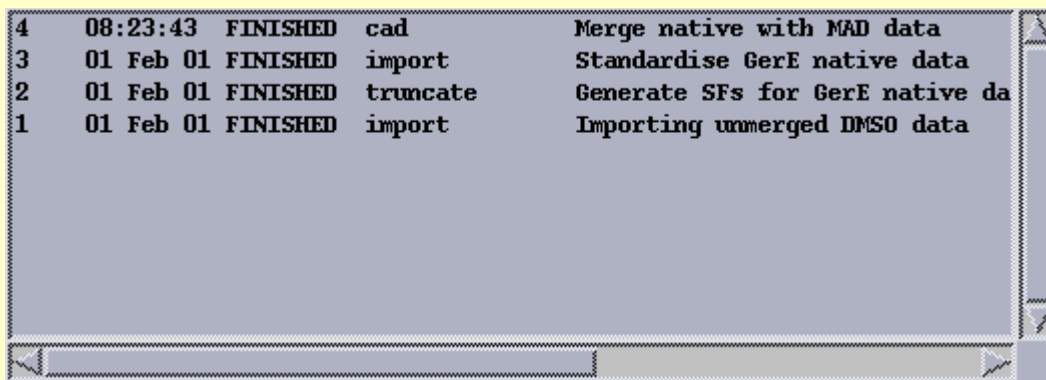
Save/restore parameters

Defaults - "If it's not visible then it's not important"



Running a task

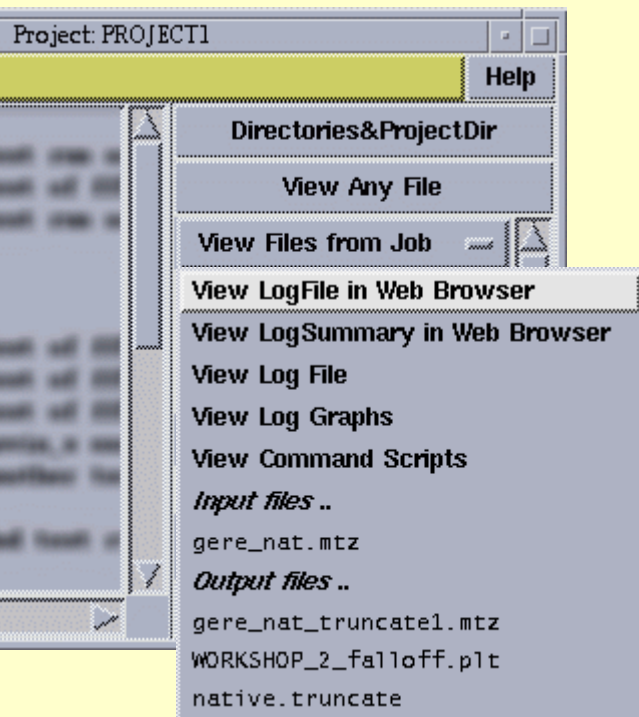
Watch the progress of the job in the Job Database window:



A screenshot of a 'Job Database' window. It contains a table with four columns: an index, a timestamp, a status, a task name, and a description. The table lists four tasks, all of which are 'FINISHED'. The window has a standard scroll bar on the right and a horizontal scroll bar at the bottom.

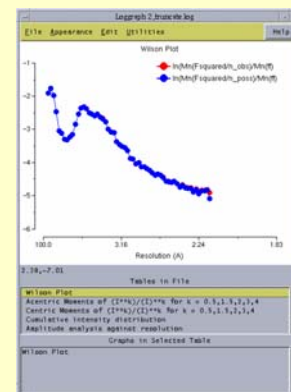
4	08:23:43	FINISHED	cad	Merge native with MAD data
3	01 Feb 01	FINISHED	import	Standardise GerE native data
2	01 Feb 01	FINISHED	truncate	Generate SFs for GerE native da
1	01 Feb 01	FINISHED	import	Importing unmerged DMSO data

View Output from Job

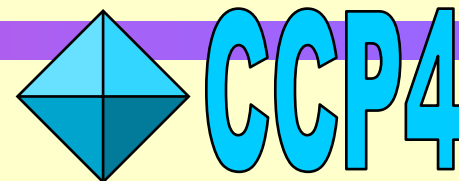


- View logfile in Netscape (if it contains HTML tags) and/or text browser

- View graphs in logfile using **loggraph**
 - also use `loggraph <filename>` at the command prompt

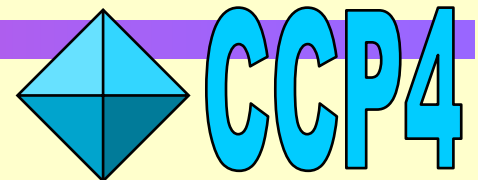


- View input and output files (.mtz, .pdb, CCP4 maps) using appropriate viewer
 - also use the View Any File option)
 - or `ccp4i -v <filename>` at the prompt



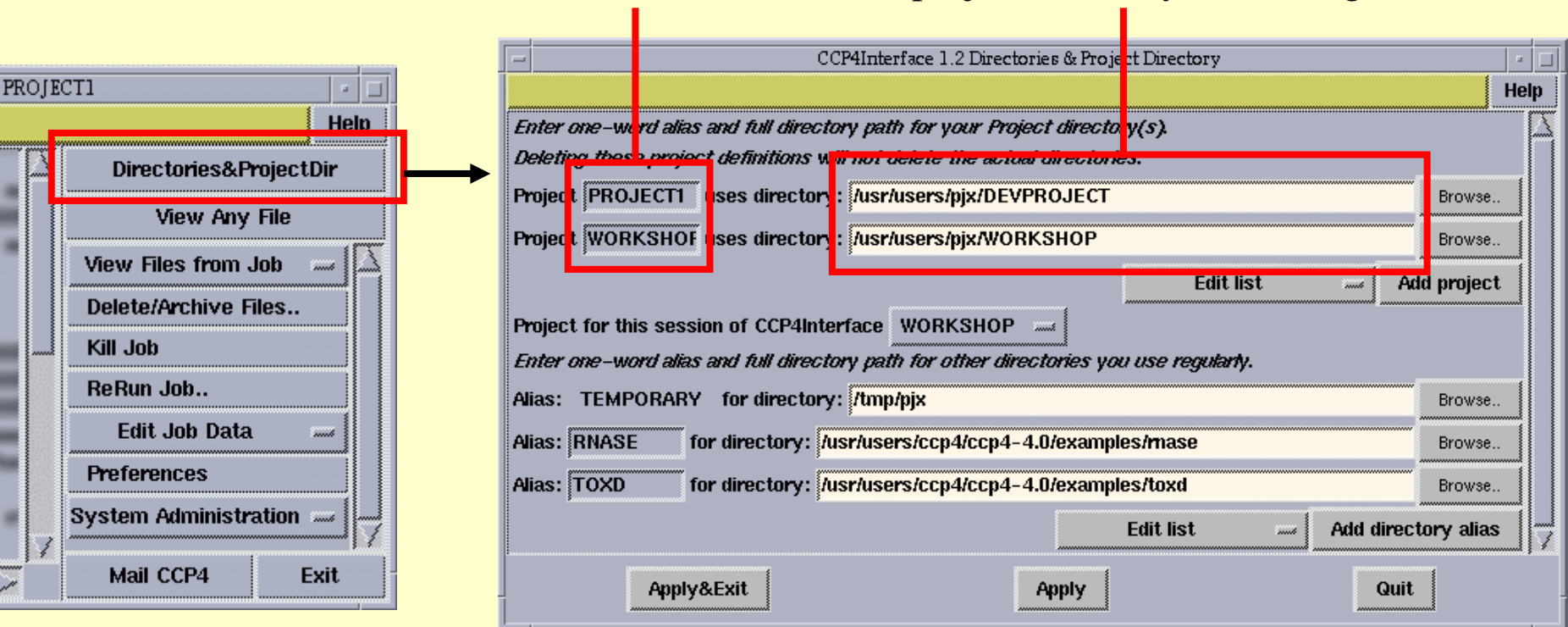
Project Management Using CCP4i

- Why bother?
- Benefits:
 - remind you what you did six months ago
 - keep track of multiple projects and associated data
 - facilitate “back-tracking”
 - make it easier to deposit your results/write your paper

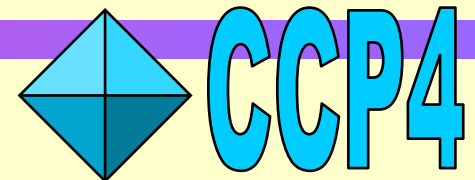


Project Directories

One word alias ... for project directory containing data files

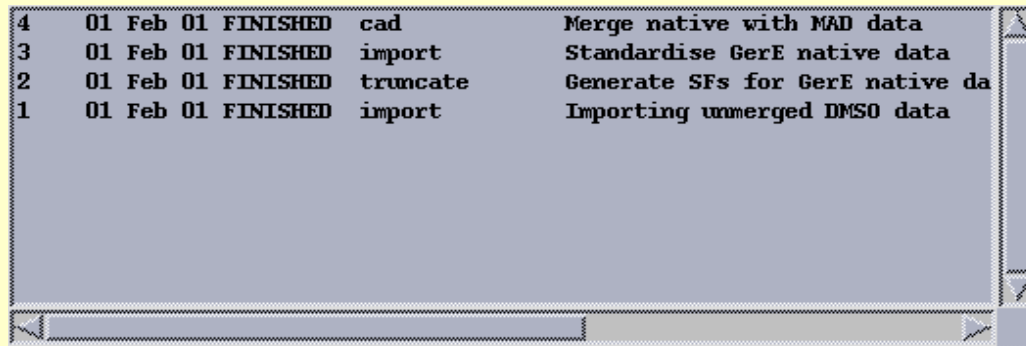


“All data files relating to one crystallographic project should be in a single project directory”



Job Database

- Each project directory has an associated **job database** accessed through the central panel in the main window:

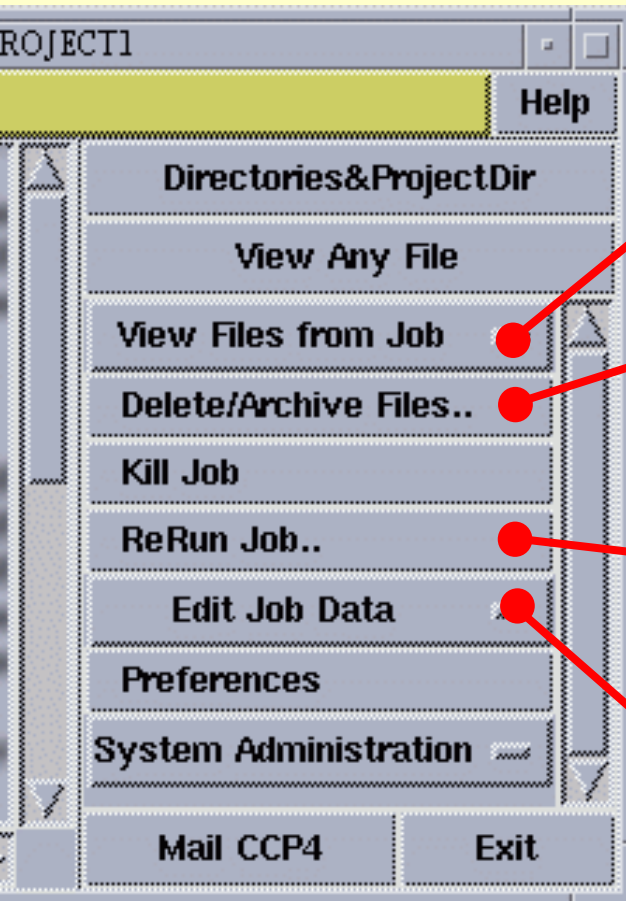


A screenshot of a job database window. It displays a list of four tasks, numbered 1 to 4 from bottom to top. Each task entry includes a number, a date and time, a status, a user, and a description. The status for all tasks is 'FINISHED'.

4	01 Feb 01	FINISHED	cad	Merge native with MAD data
3	01 Feb 01	FINISHED	import	Standardise GerE native data
2	01 Feb 01	FINISHED	truncate	Generate SFs for GerE native da
1	01 Feb 01	FINISHED	import	Importing unmerged DMSO data

- This displays:
 - which tasks were run, and when
 - their status (RUNNING, FINISHED, FAILED etc)
 - the title entered by the user
- The database also keeps a record of:
 - the parameters used to run the task
 - the input, output and log files associated with the task

Job Database Utilities



View files from *any* job in the database

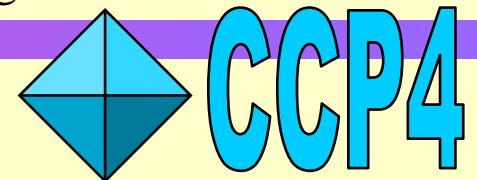
Remove failed/unwanted jobs from the database and archive important data

Rerun *any* job in the database (with the option of changing the parameters first)

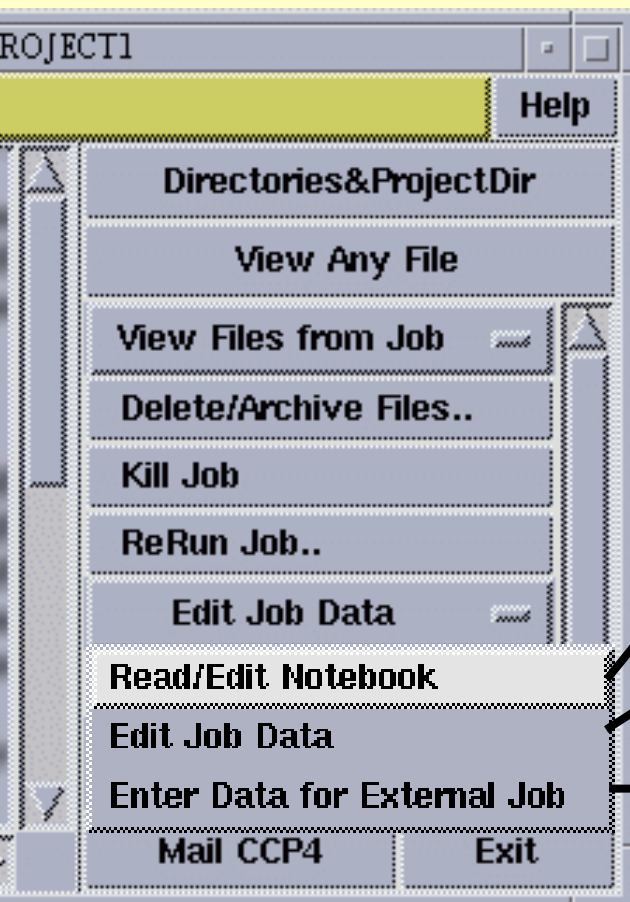
- Use this to review parameters used in an earlier run

Keep the database up-to-date

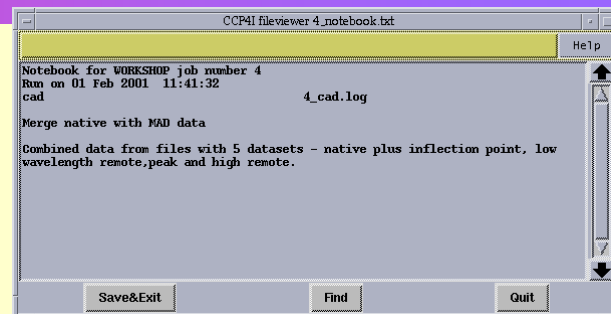
- Add runs of “external” programs



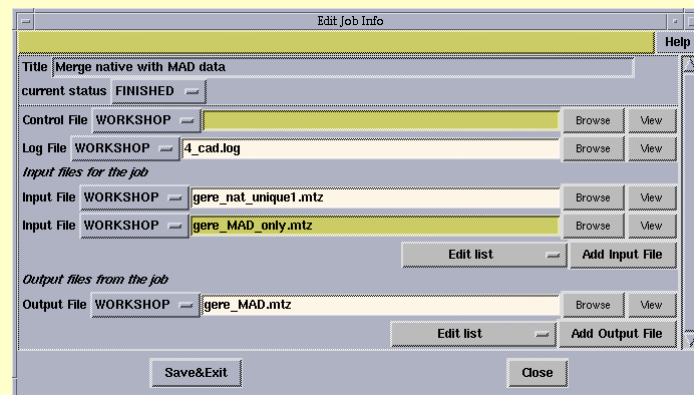
Edit Job Data



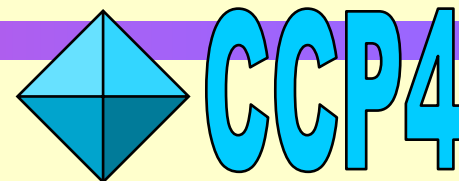
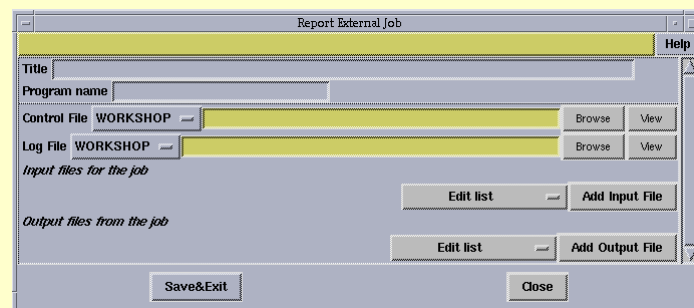
Notebook: record information for future reference



Edit data: e.g. update title of run, change file locations

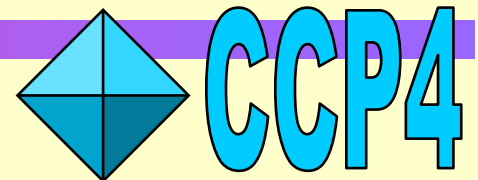


Add external /non-interfaced program run to the database



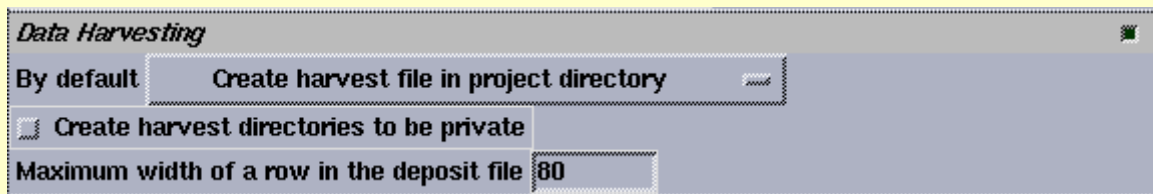
Data Harvesting

- Key programs in the structure solution procedure write out **harvest files**
 - in CCP4 these are SCALA, TRUNCATE, MLPHARE, REFMAC and RESTRAIN
- Each file records details of the **method** used and the **results** obtained (e.g. heavy atom sites used in phasing)
- At deposition time these files represent an accurate record of how the final model was obtained
- Harvest files can be sent directly to the deposition site, avoiding much manual processing

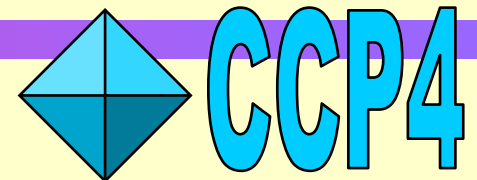


Data Harvesting in CCP4i

- Harvesting requires MTZ files contain **Project** and **Dataset** names:
 - add these when data is first imported into CCP4 (**Import Unscaled Data** or **Convert to MTZ & Standardise** tasks in **Data Reduction Module**), *or*
 - edit Project name or Dataset name using **Edit MTZ Project&Dataset** (in the **Reflection Data Utilities** module)
- Switch on the harvesting options:
 - in individual tasks e.g. **SCALA**, **REFMAC**, *or*
 - set the harvesting defaults in the CCP4i Preferences window (RHS of the main window)



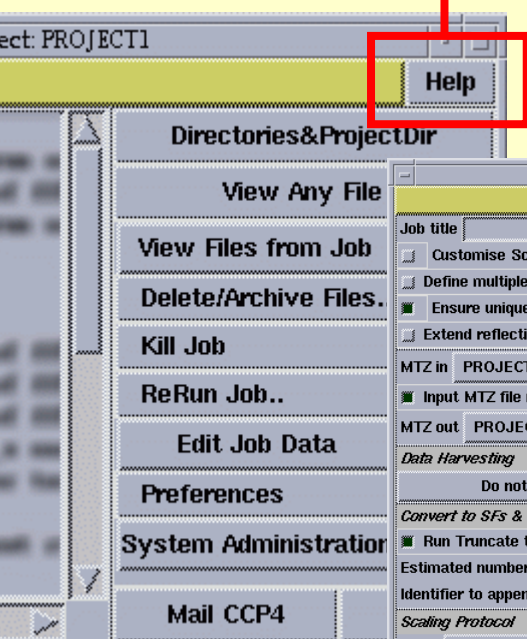
- Harvesting operates “invisibly”
 - you don’t need to think about it again until the end of the structure solution



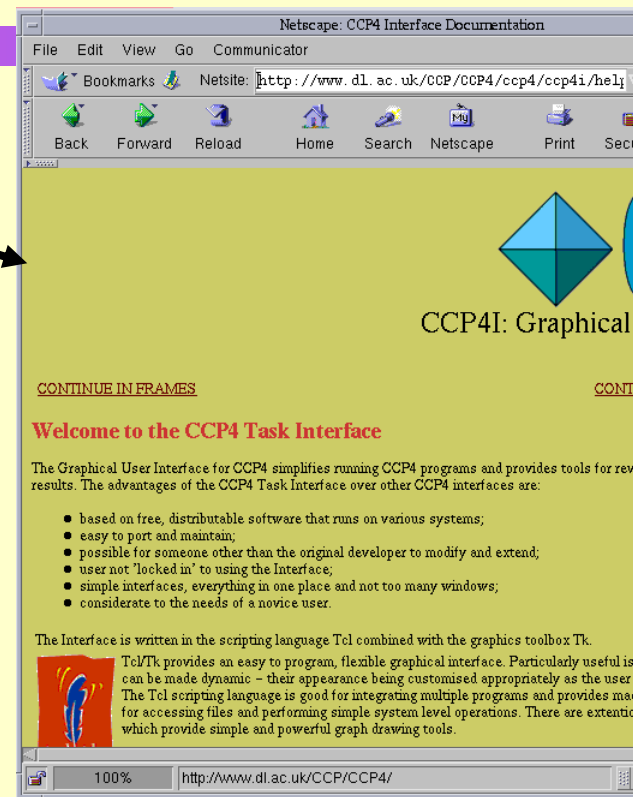
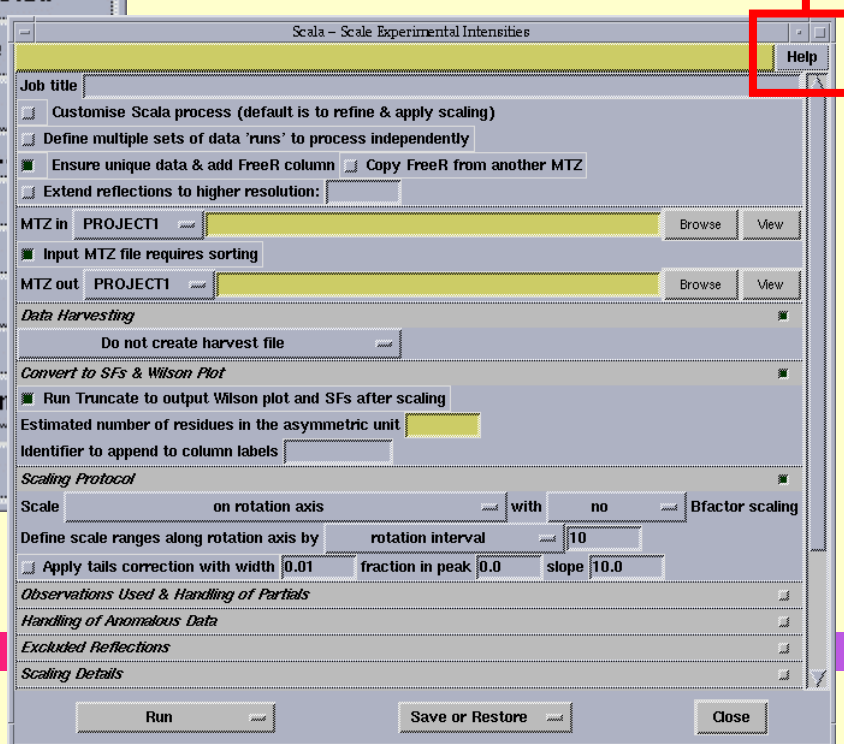
On-line help

Brings up relevant documentation
in browser

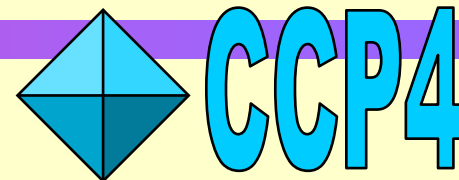
General help from
main window



Help for a particular task

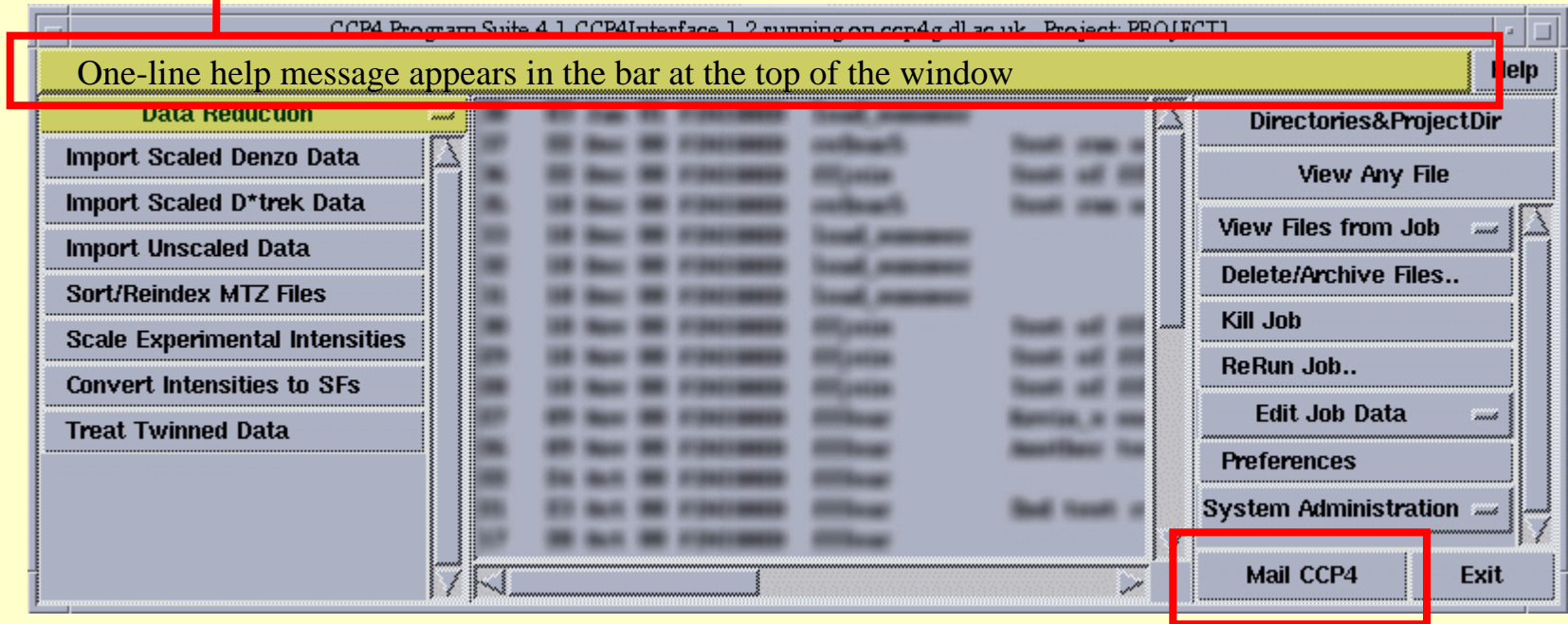


*Help with a particular option -
Right hand mouse button click
over that option*

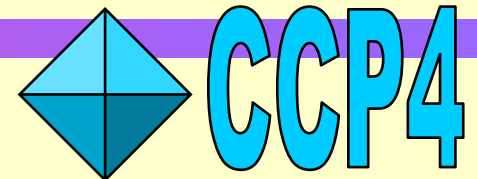


More help...

- Message line help



- Send e-mail to directly to CCP4
(please send as much information as possible!)



Navigating Modules

Data Reduction

Import Scaled Denzo Data

Import Scaled D*trek Data

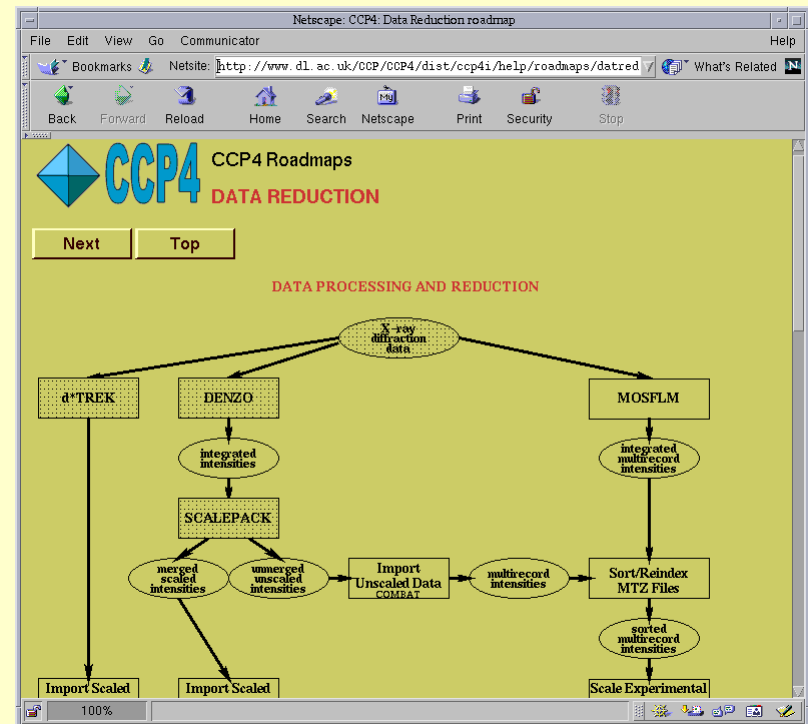
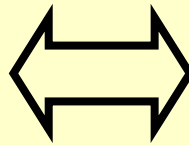
Import Unscaled Data

Sort/Reindex MTZ Files

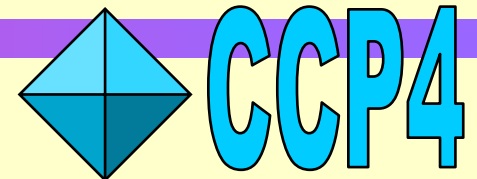
Scale Experimental Intensities

Convert Intensities to SFs

Treat Twinned Data



- CCP4 Roadmaps - accessed via program index (under **General**)
- CCP4 Tutorial2000 - also from the program index



CCP4i Help: Summary

- On-line help:
 - **help** button on main window for general info
 - **help** button on task interfaces for help with individual tasks
 - right-hand mouse button click over part of the window for help on that option or feature.
- Roadmaps through the structure determination process:
 - `$CCP4/ccp4i/help/roadmaps/index.html`
- Tutorial material
 - `$CCP4/examples/tutorial2000/html/index.html`
- E-mail CCP4
 - `ccp4@ccp4.ac.uk`

