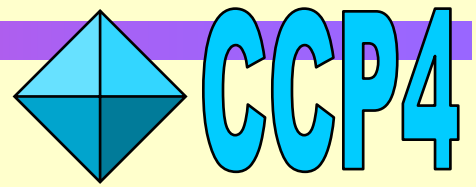
An Introduction to CCP4i

The CCP4 Graphical User Interface

Peter Briggs
CCP4

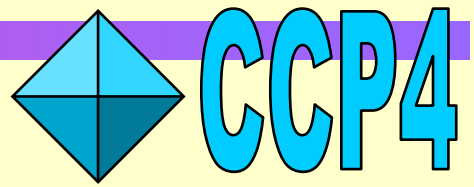


Introduction: Why use CCP4i?

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

How to get started

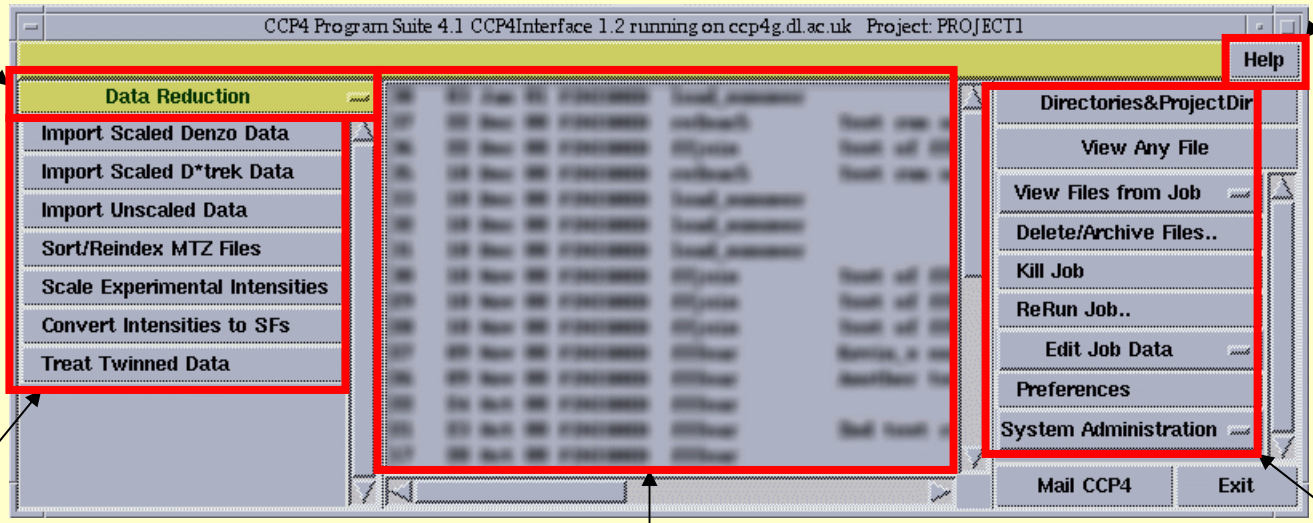
- *(Unix/Linux)* Type **`ccp4i`** at the command prompt
- *(Windows/NT)* Select **`ccp4i`** via the Start menu



Main CCP4i Window

Modules

On-line help



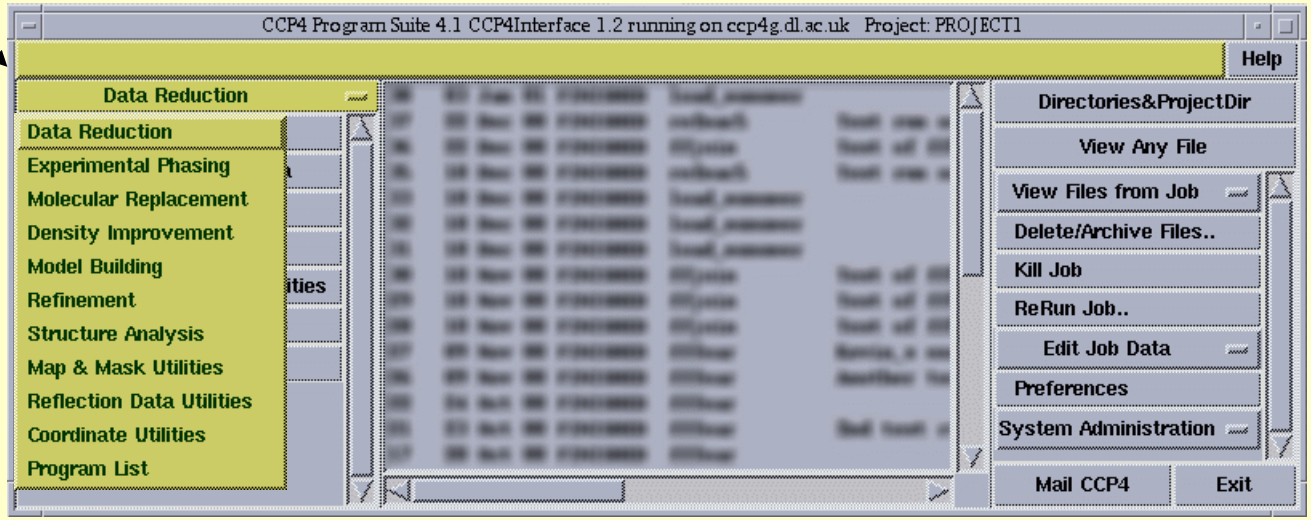
Tasks

Job Database

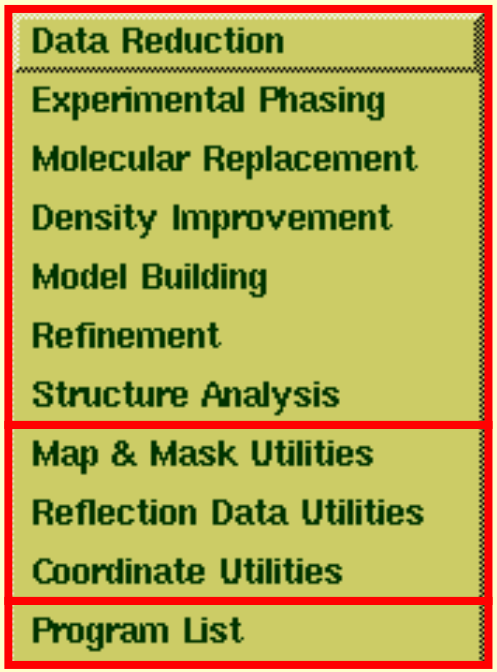
Tools & Utilities

Modules

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



Modules



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

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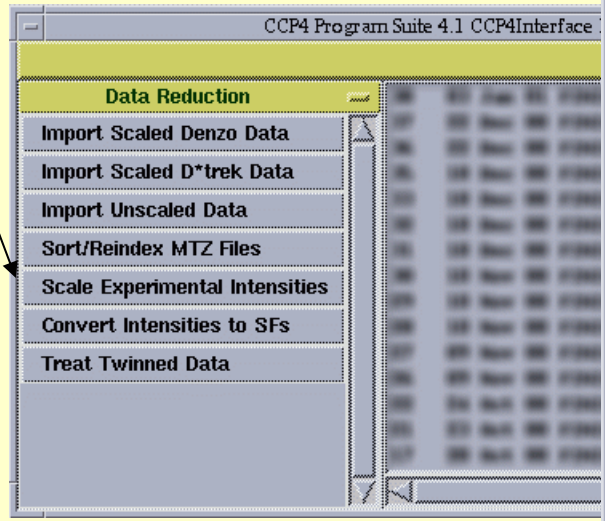
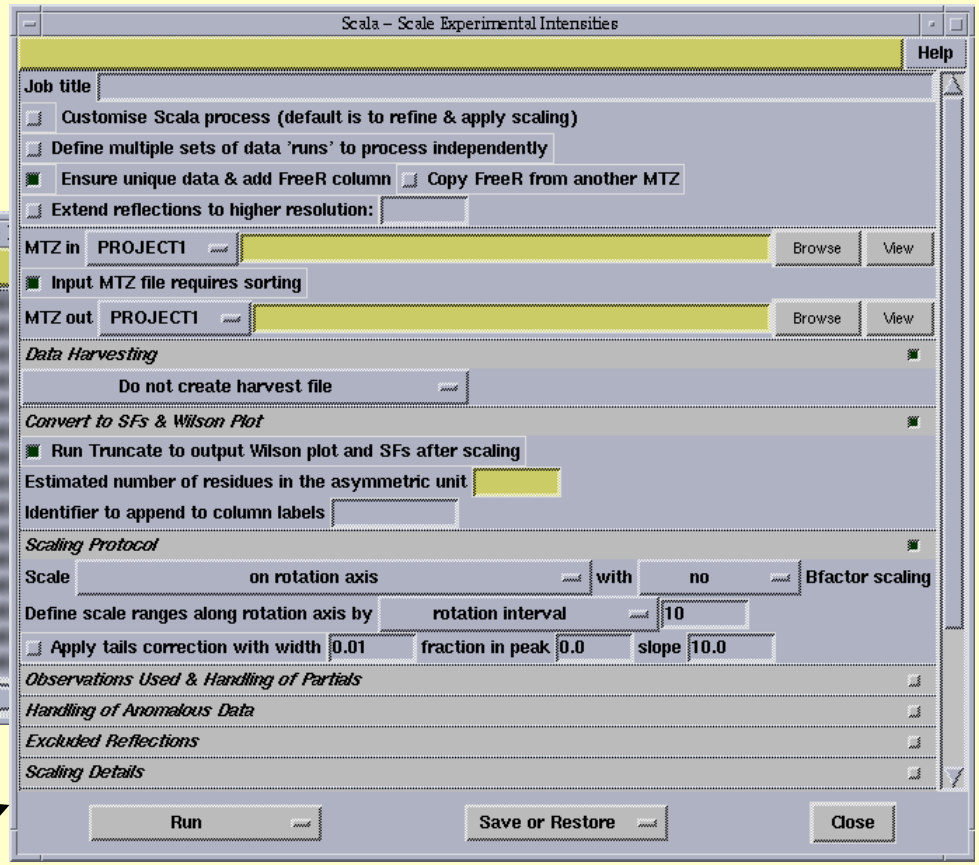
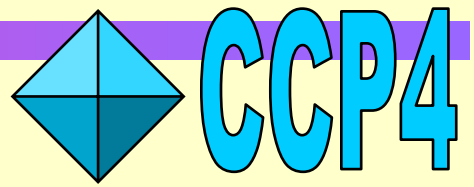
Tasks

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





• This starts the interface for that task



Example Task Interface

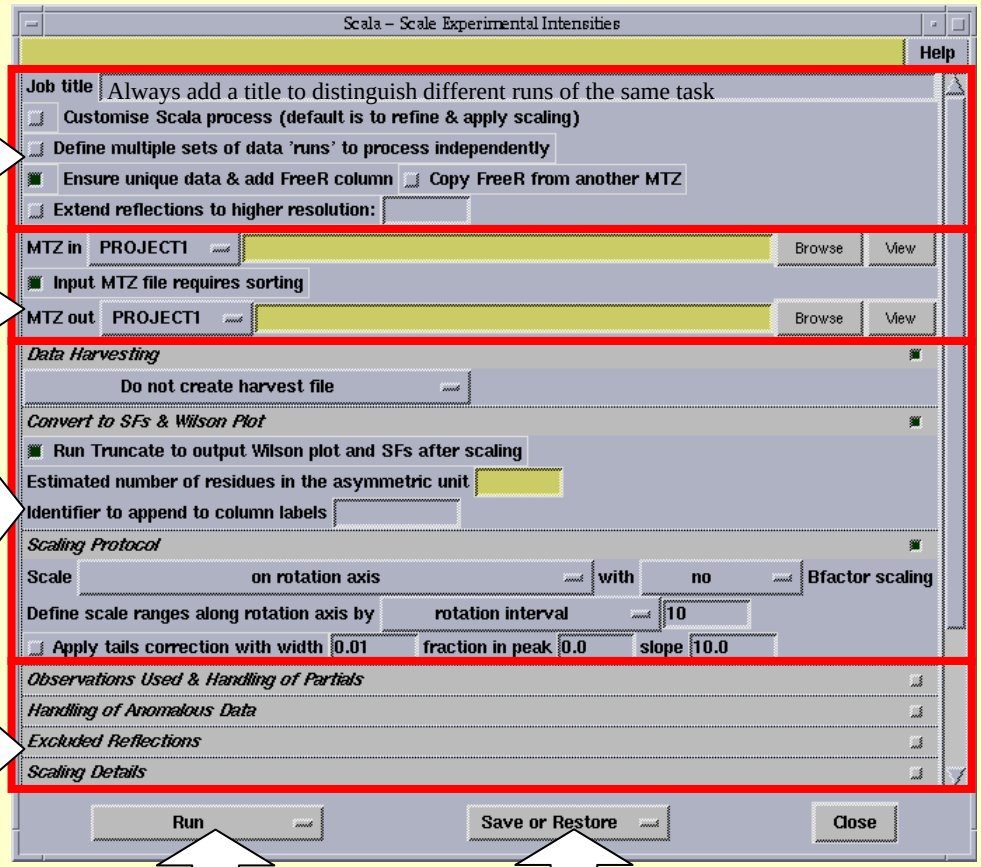
WORK FROM THE TOP DOWN

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



Run task

Save/restore parameters

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

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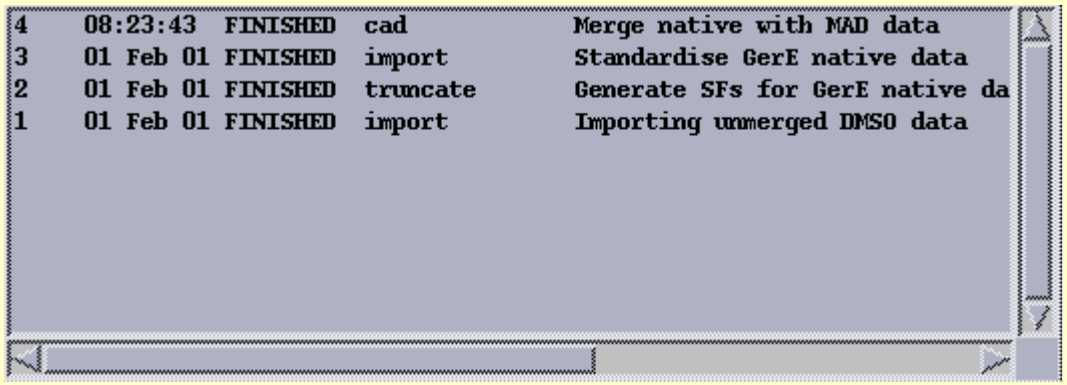
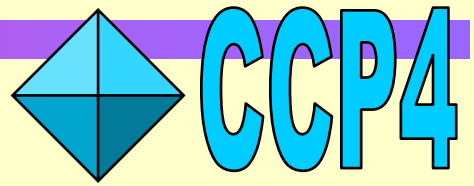
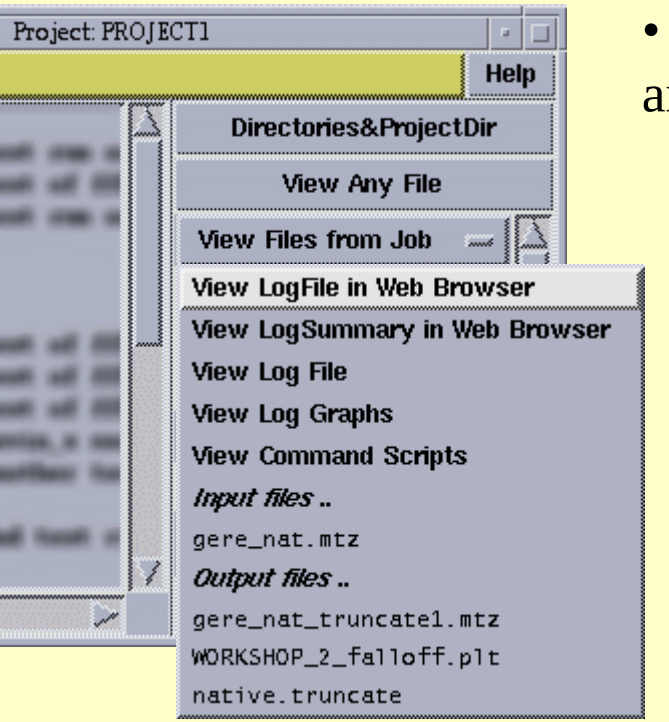
Running a task

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





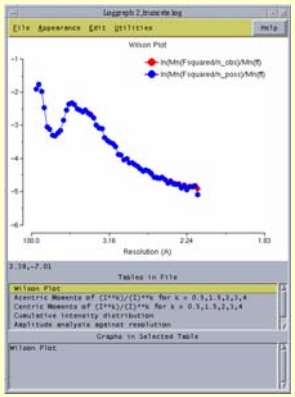
View Output from Job



• 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

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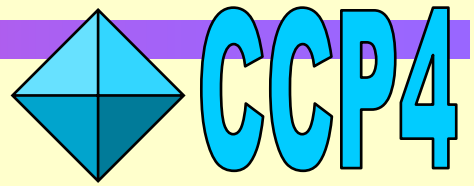
Project Management Using CCP4i

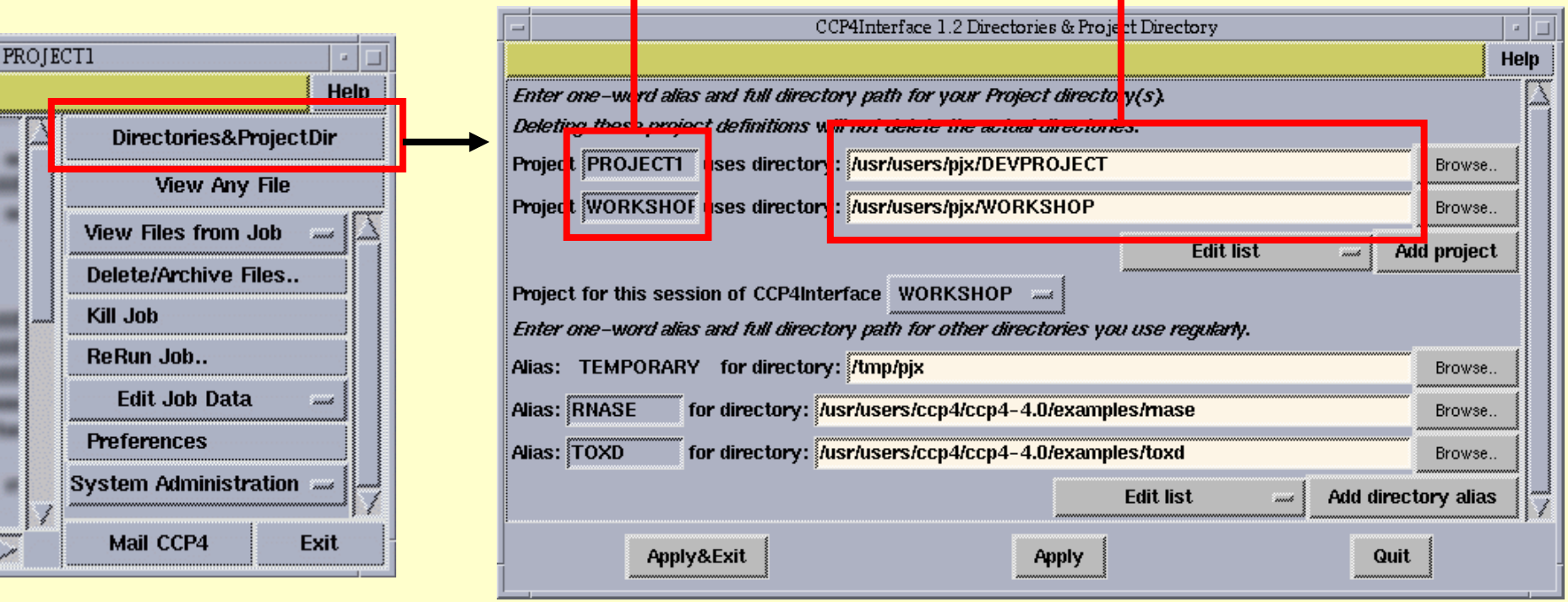
- Why bother?

- 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"

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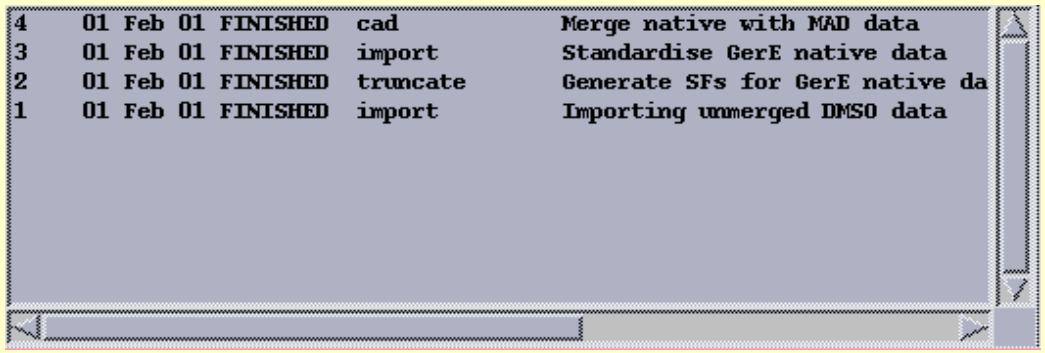
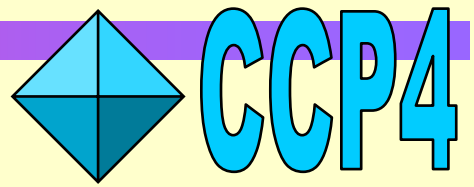
Job Database

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

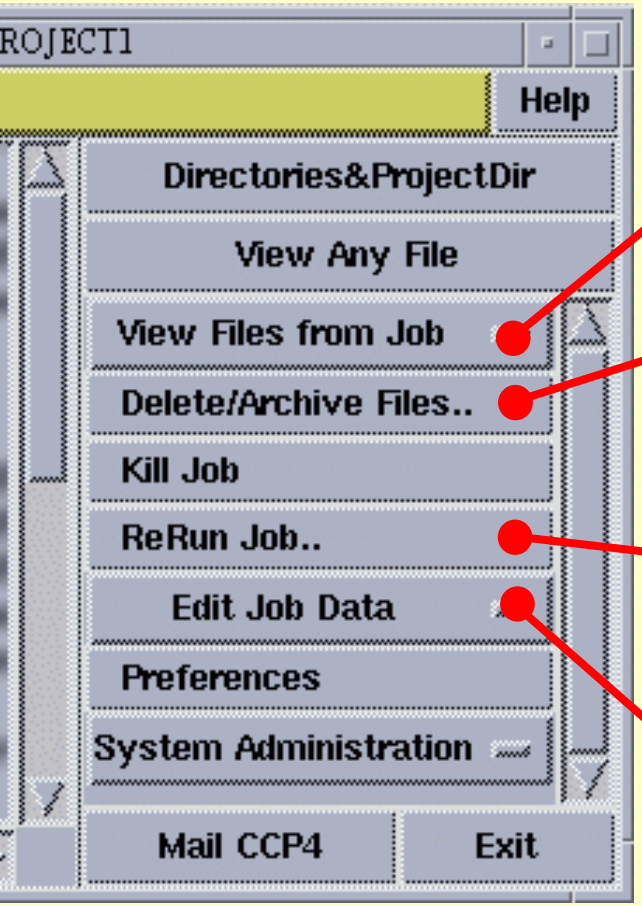


• This displays:
  - which tasks were run, and when
  - their status (`RUNNING`, `FINISHED`, `FAILED` etc)
  - the title entered by the user

• 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

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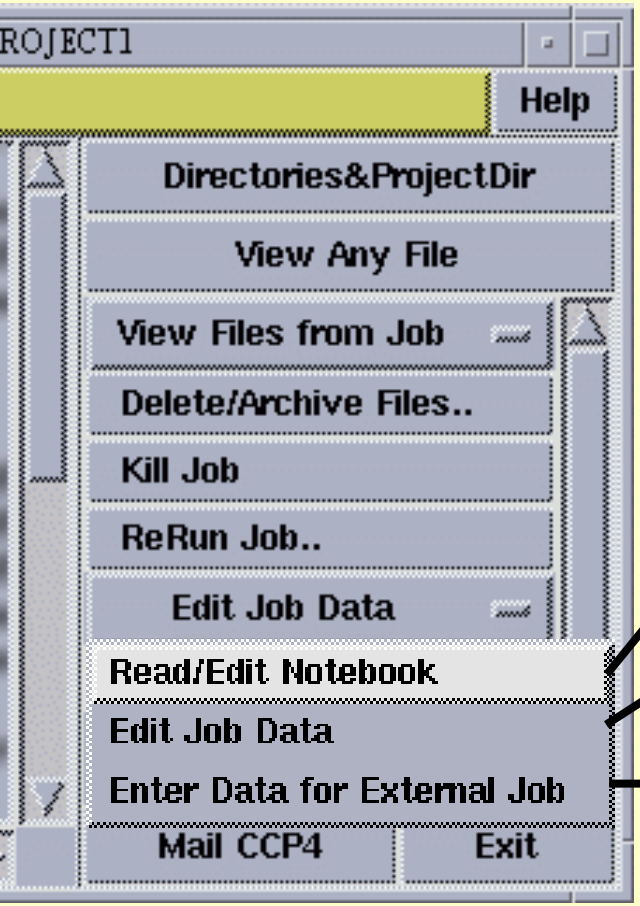
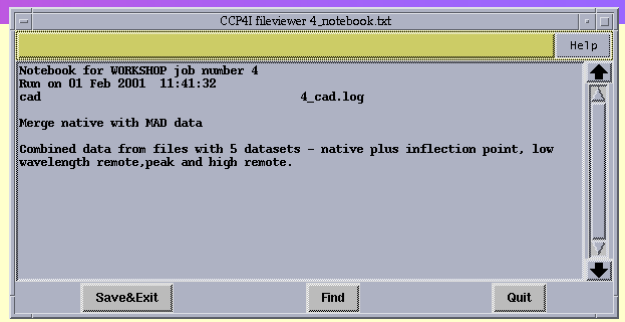
Edit Job Data

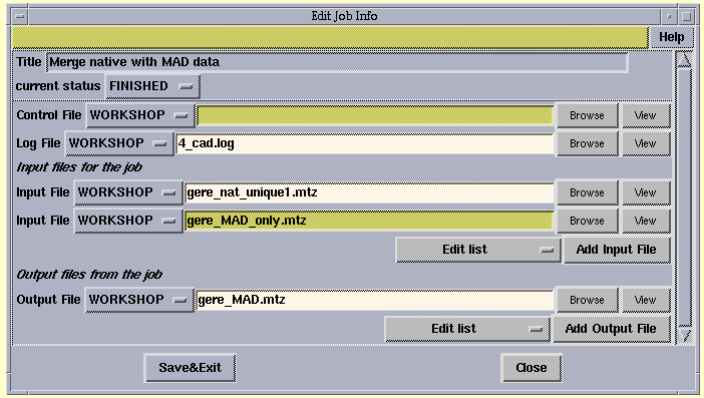


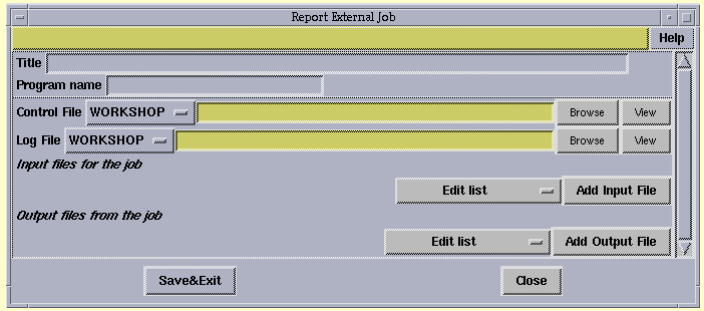
Notebook: record information for future reference

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

Add external /non-interfaced program run to the database







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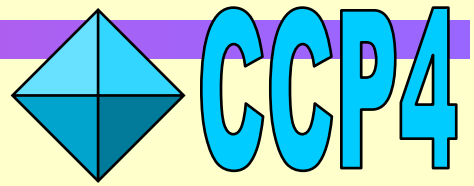
Data Harvesting

• 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

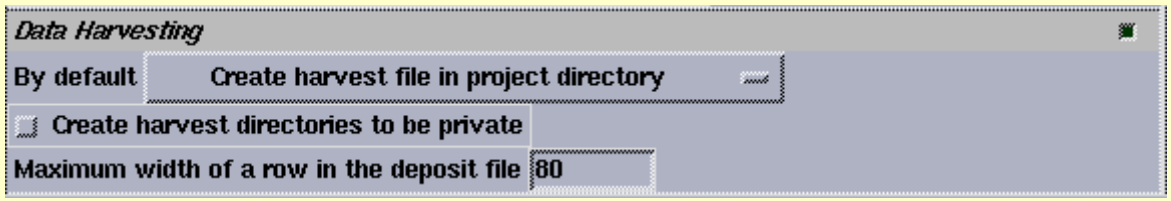
• Harvest files can be sent directly to the deposition site, avoiding much manual processing



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

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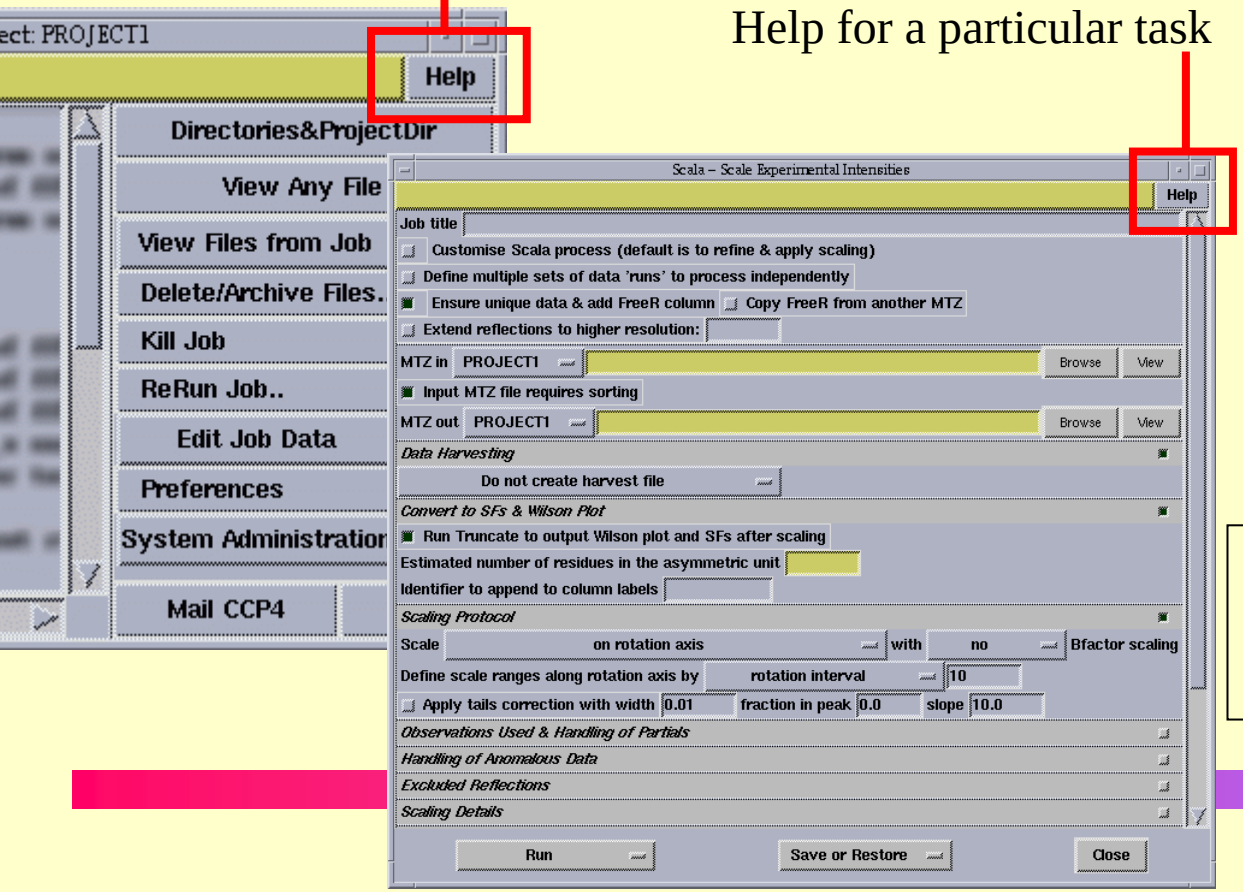
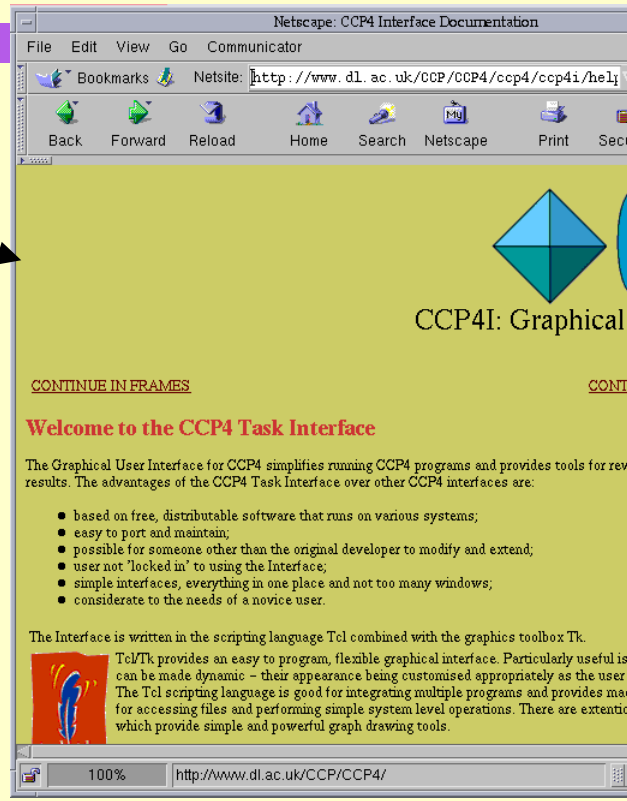
On-line help

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

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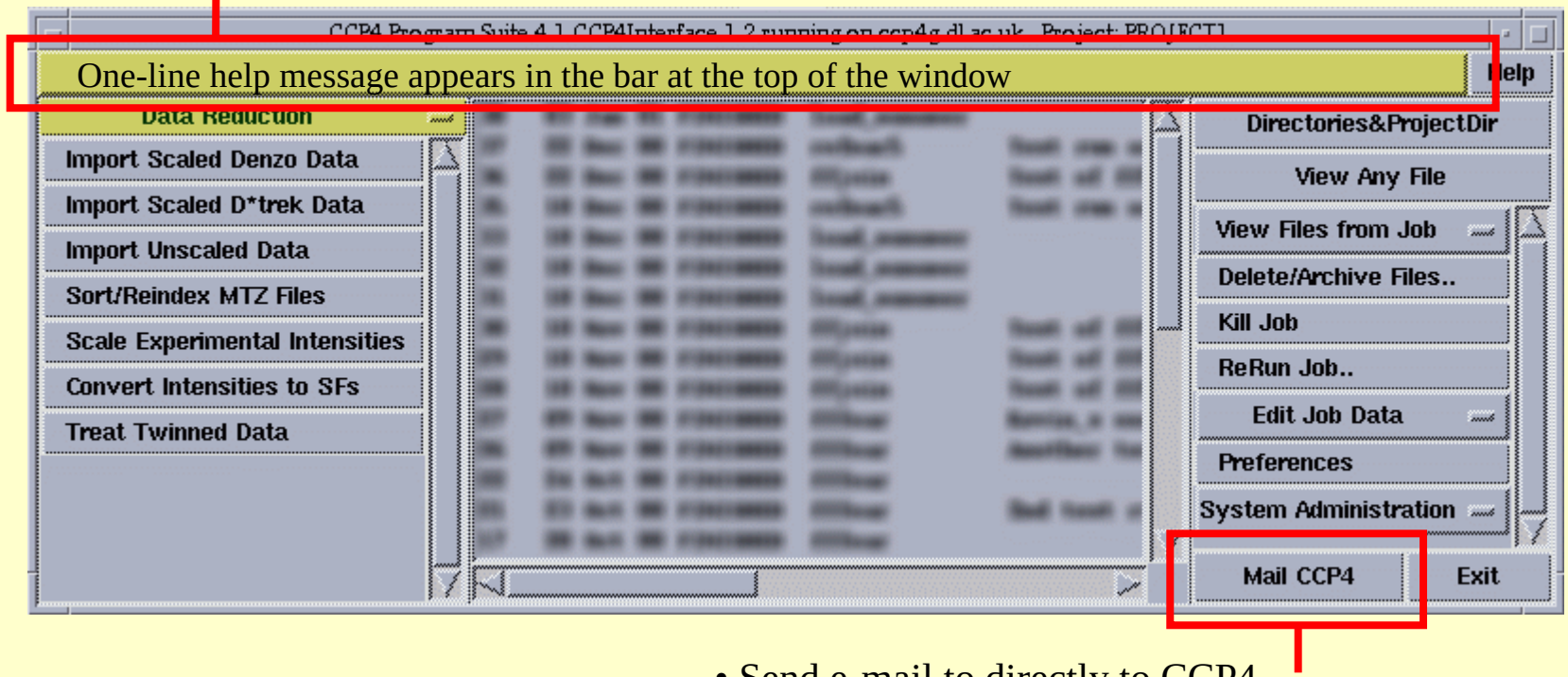
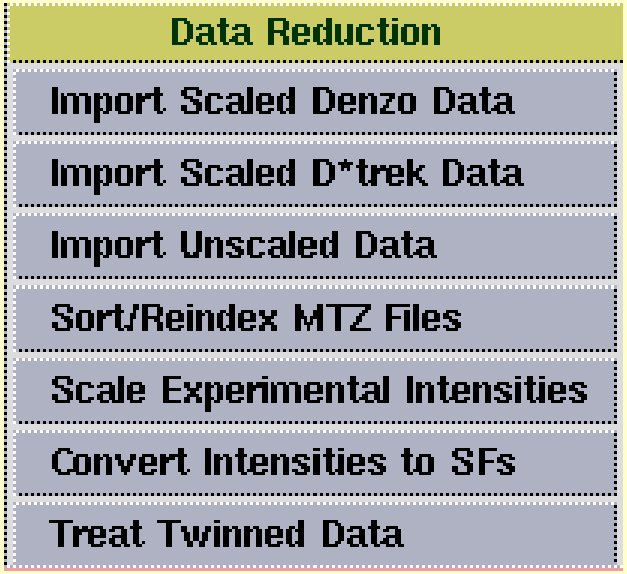
More help...

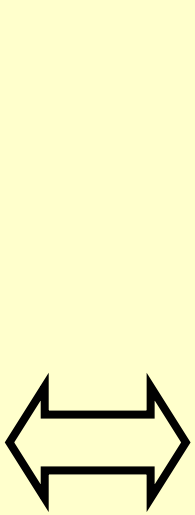
- Message line help

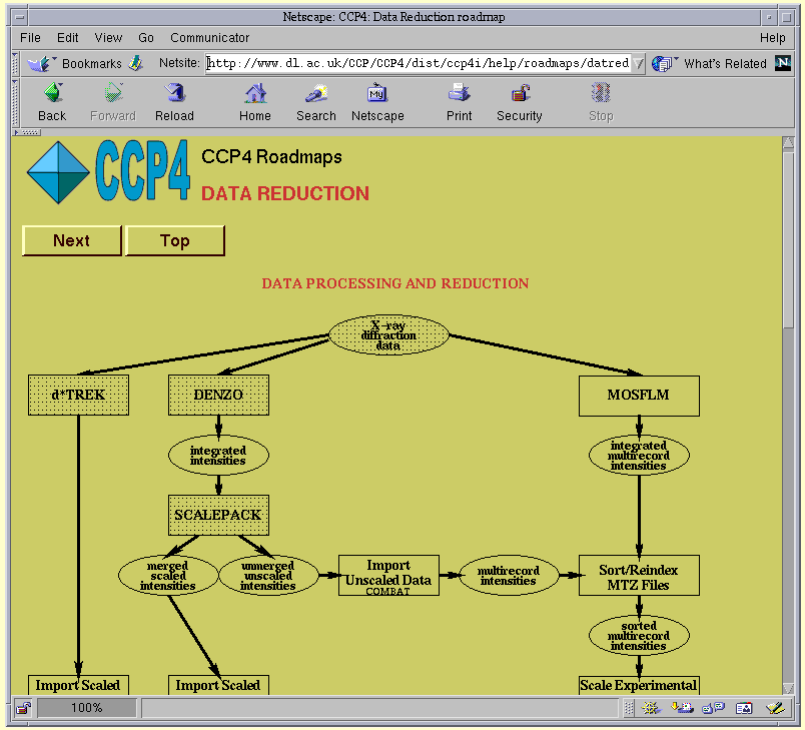


- Send e-mail to directly to CCP4
(please send as much information as possible!)

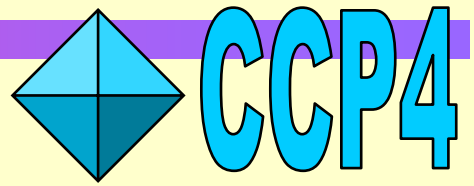
Navigating Modules







- **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**