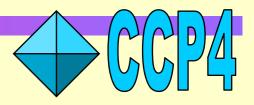
An Introduction to CCP4i The CCP4 Graphical User Interface

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

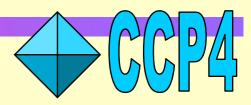
- (*Unix/Linux*) Type ccp4i at the command prompt
- (Windows/NT) Select ccp4i via the Start menu



Main CCP4i Window

Modules

CCP4 Program Suite 4.1 CCP4Interface 1.2 running on ccp4g.dl.ac.uk Project: PROJECT1 Help **Data Reduction** Directories&ProjectDir Import Scaled Denzo Data View Any File Import Scaled D*trek Data **View Files from Job Import Unscaled Data** Delete/Archive Files.. Sort/Reindex MTZ Files Kill Job Scale Experimental Intensities ReRun Job.. **Convert Intensities to SFs** Edit Job Data Treat Twinned Data Preferences System Administration 📟 Mail CCP4 Exit **Tools & Utilities** Tasks Job Database



On-line help

Modules

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

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Data Reduction									Directories&ProjectDir
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Density Improvement			1 844			boat, someoner			Delete/Archive Files
Model Building		: :				Stratt, someone	-		Kill Job
Refinement	ities					All parts	best of H		ReRun Job
Structure Analysis			-	-	-	Higherine	best of H		
Map & Mask Utilities						and the same	Barriss, a see		Edit Job Data 📖
Reflection Data Utilities			-	-		and the second s	And the second second		Preferences
Coordinate Utilities			-	-	-	dillinear .	Bad teast of		System Administration 🛲
Program List					-	(International Contraction of Contra		7	Mail CCP4 Exit



Modules

Data Reduction

- **Experimental Phasing**
- **Molecular Replacement**
- **Density Improvement**
- **Model Building**
- Refinement

Structure Analysis

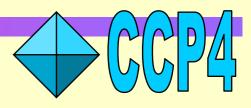
Map & Mask Utilities

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

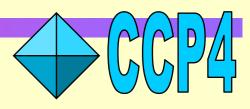
• Click on the appropriate button in the list to start a particular task

the list to start a particular task				Ensure unique data & add FreeR column 🛄 Copy FreeR from another MTZ		
				📰 Extend reflections to higher resolution:		
	CCP4 Program Suite 4.1 CCP4Interface			MTZ in PROJECT1 🛹 Brow	'se View	
\backslash				🗰 Input MTZ file requires sorting		
	Data Reduction		10 Jan 11 1946	MTZ out PROJECTI and Broy	se View	
\backslash	Import Scaled Denzo Data	A	II has its risk	Data Harvesting	<u> </u>	
\backslash	Import Scaled D*trek Data		18 Bac 18 194	Do not create harvest file		
\backslash	Import Unscaled Data		10 Nov 00 Film	Convert to SFs & Wilson Plot	*	
\ \	Sort/Reindex MTZ Files		18 Bas 18 1940	Run Truncate to output Wilson plot and SFs after scaling		
	Scale Experimental Intensities		10 Nov 00 1240	Estimated number of residues in the asymmetric unit		
	Convert Intensities to SFs		10 Nov 10 Film	Identifier to append to column labels Scaling Protocol		
	Treat Twinned Data		In tes in city		actor scaling	
				Define scale ranges along rotation axis by rotation interval 💷 10		
			23 Aut 48 1944	Apply tails correction with width 0.01 fraction in peak 0.0 slope 10.0		
				Observations Used & Handling of Partials		
		$\mathbb{N}\mathbb{N}$		Handling of Anomalous Data		
-				Excluded Reflections		
				Scaling Details	y L	
• This starts	the interface for	that	task	Run Save or Restore	Close	

Job title

Scala – Scale Experimental Intensities

Customise Scala process (default is to refine & apply scaling)
 Define multiple sets of data 'runs' to process independently



Help

Example Task Interface

WORK FROM THE TOP DOWN

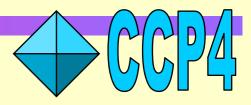
Protocol folder Make the key decisions File folder Set input and output file names **Open folders** Parameters that should be checked by the user before running *Highlights indicate compulsory input* **Closed folders** Advanced/infrequently used options, Defaults - "If it's not visible then it's not important"

x	ala – Scale Experimental Intensities	Help				
Customise Scala process (default is Define multiple sets of data 'runs' to	process independently Imn II Copy FreeR from another MTZ					
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Apply tails correction with width 0.01						
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Run	Save or Restore and Close					
Run task	Save/restore parameters					
	CCP	4				

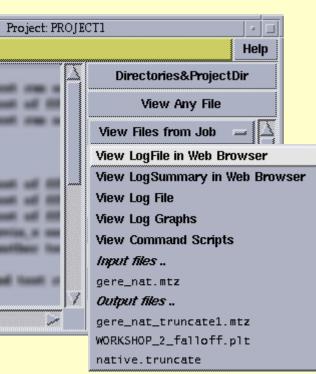
Running a task

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

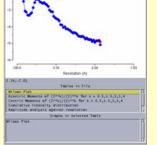
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2			truncate	Generate SFs for GerE native da
1	01 Feb 01	FINISHED	import	Importing unmerged DMSO data
				7
				······································



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



Figuared/h.posit)

- 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

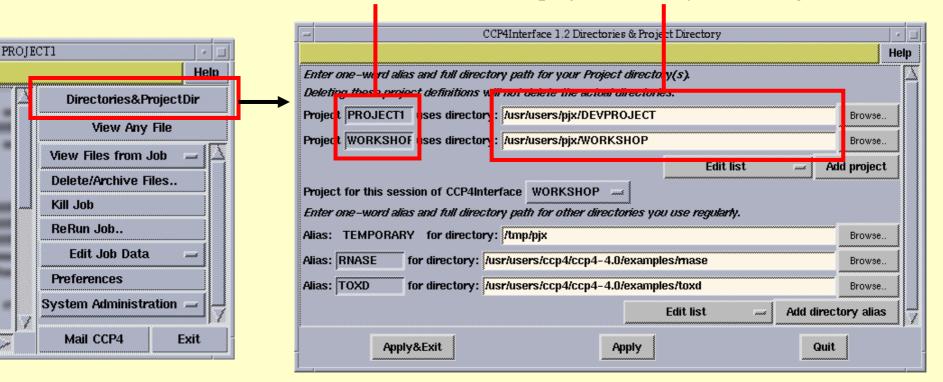
Project Management Using CCP4i

- 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:

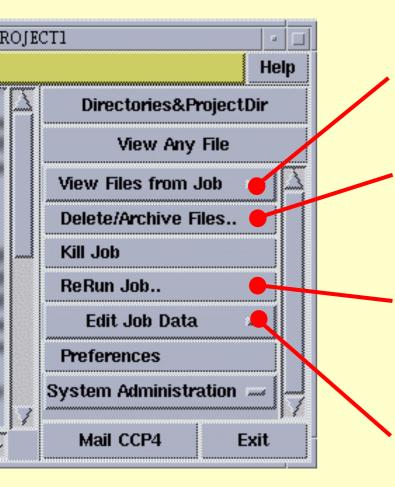
4 3 2 1	01 F 01 F	Feb 01 Feb 01	FINISHED FINISHED FINISHED FINISHED	cad import truncate import	Merge native with MAD data Standardise GerE native data Generate SFs for GerE native da Importing unmerged DMSO data
<u> []</u>					

• 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



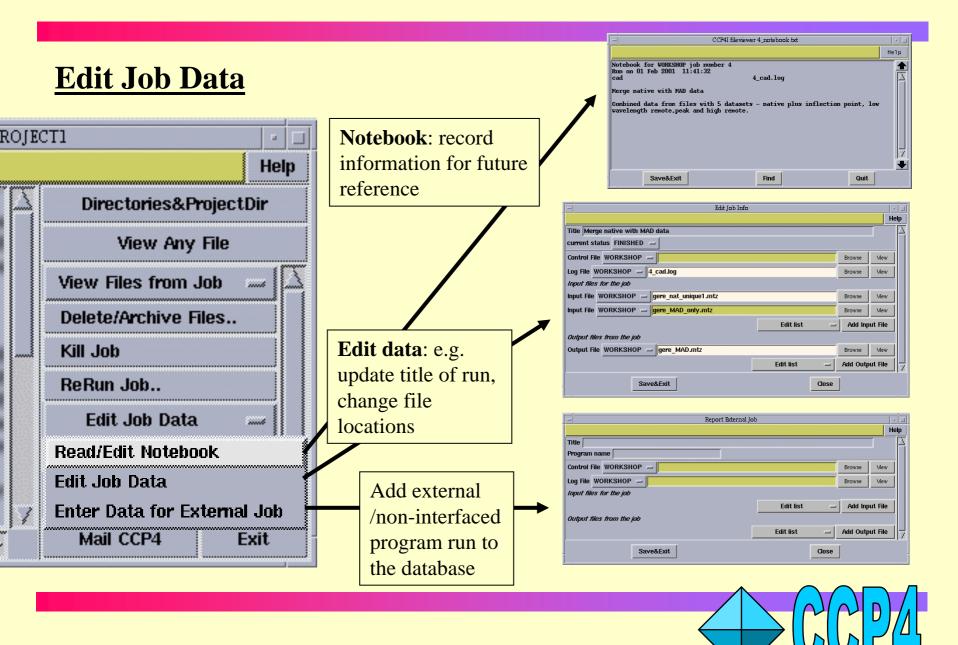
View files from any job in the database

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

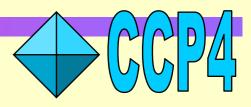
Keep the database up-to-date

• Add runs of "external" programs



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:

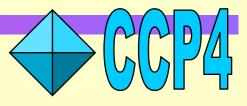
- in individual tasks e.g. SCALA, REFMAC, or

- set the harvesting defaults in the CCP4i Preferences window (RHS of the main window)

Data Harve	sting	
By default	Create harvest file in projec	-
🧾 Create h	narvest directories to be private	
	vidth of a row in the deposit file	

• Harvesting operates "invisibly"

- you don't need to think about it again until the end of the structure solution



			Netscape: CCP4 Interface Documen	ntation		
			File Edit View Go Communicator			
			👔 🌿 Bookmarks 🧔 Netsite: [http://www.dl.ac.uk/CCP/CCP4/d	ccp4/ccp4i/heli		
	On-line he	Brings up relevant documentation in browser	Back Forward Reload Home Search Netscape	Print Sec		
		help from	• · · · · · · · · · · · · · · · · · · ·			
	main w	indow	CCP4I:	: Graphical		
			CONTINUE IN FRAMES	CON		
t: PROJE	ECT1	Help for a particular task	Welcome to the CCP4 Task Interface			
			The Graphical User Interface for CCP4 simplifies running CCP4 programs and results. The advantages of the CCP4 Task Interface over other CCP4 interface	provides tools for re- es are:		
	Directories&Projec	tDir	 based on free, distributable software that runs on various systems; easy to port and maintain; 			
	View Any File	Scala – Scale Experimental Intensities	 possible for someone other than the original developer to modify and e: user not 'locked in' to using the Interface; simple interfaces, everything in one place and not too many windows; considerate to the needs of a novice user. 	xtend;		
	View Files from Job	Job title Customise Scala process (default is to refine & apply scaling)	The Interface is written in the scripting language Tel combined with the graphi Tel/Tk provides an easy to program, flexible graphical interface.	. Particularly useful is		
	Delete/Archive Files.	Define multiple sets of data 'runs' to process independently Ensure unique data & add FreeR column	can be made dynamic - their appearance being customised appr The Tcl scripting language is good for integrating multiple progr for accessing files and performing simple system level operation which provide simple and powerful graph drawing tools.	rams and provides ma		
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		Apply tails correction with width 0.01 fraction in peak 0.0 slope 10.0	over that option			
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		Handling of Anomalous Data				
		Excluded Reflections				
		Run				

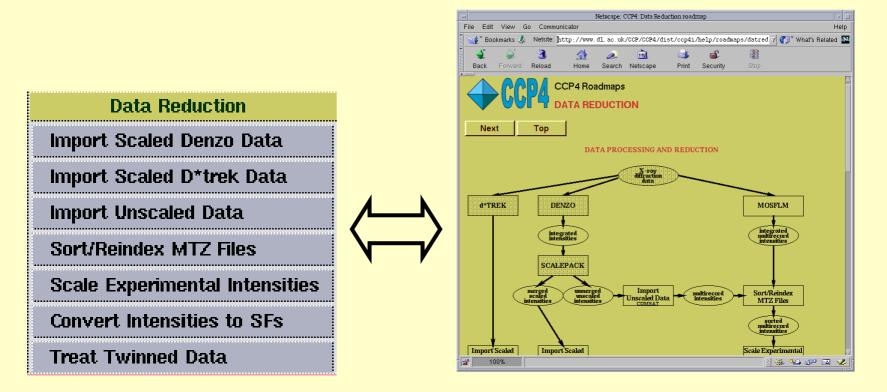
More help...

• Message line help

CCP4 Prog	Suite 4.1. CCP4Interface 1.2 running on cop4g dLac.ukProject: PRC	увста
One-line help message ap	ars in the bar at the top of the window	l <mark>l</mark> eip
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Import Scaled D*trek Data	It is not in concern others, but one a	View Files from Job 📟 🖾
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	at an and an exception entropy American to	Preferences
	It is not in concesso other. But test a	System Administration 🛲 💻
<u> </u>		Mail CCP4 Exit

• 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

