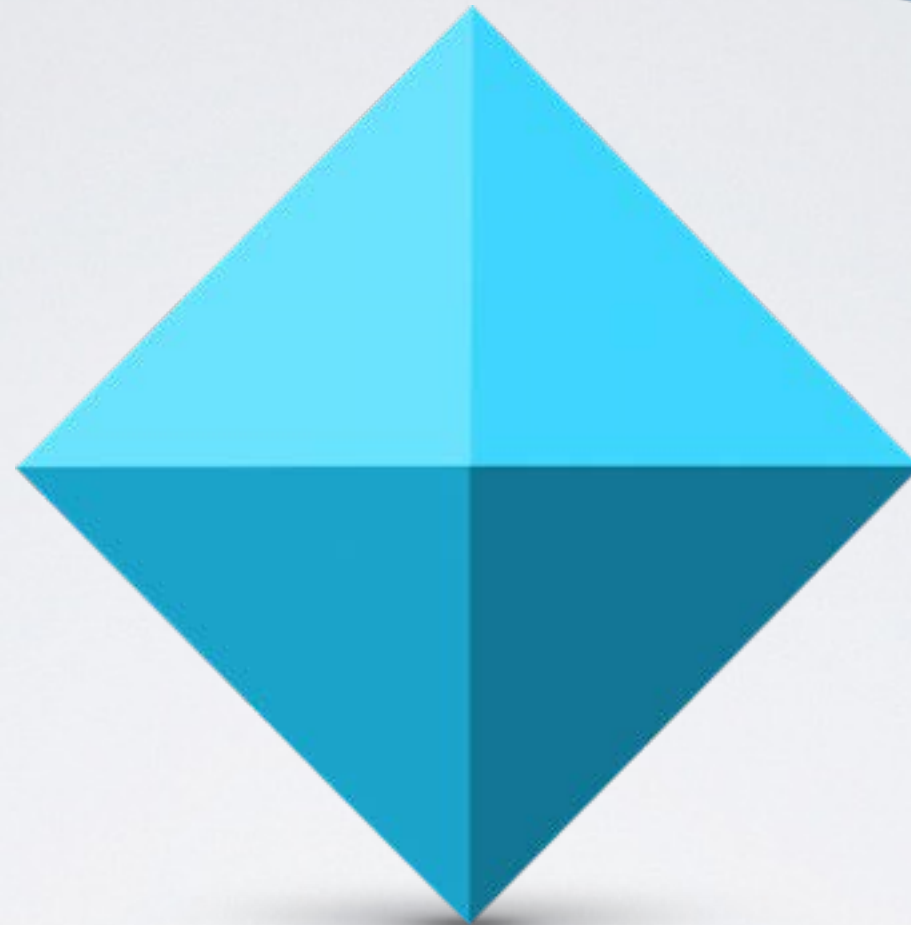




#asca2015
@alwaysonthejazz



CCP4 i2

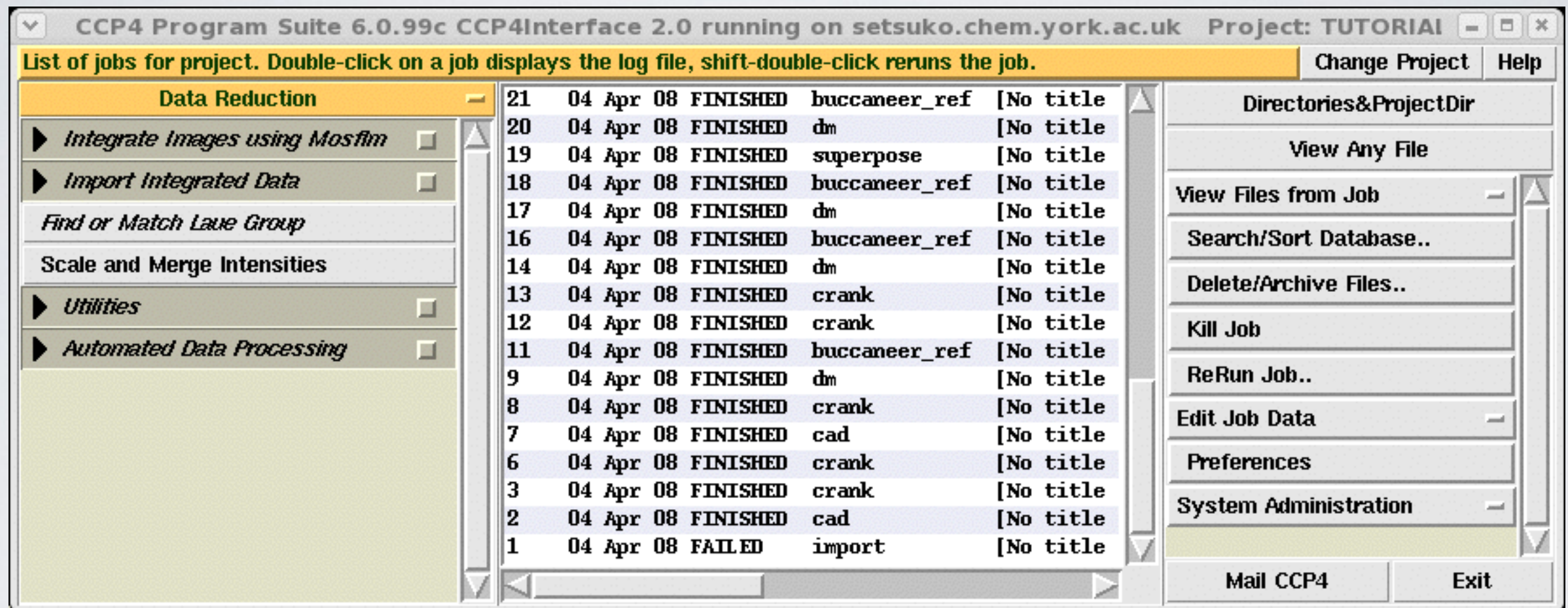
A new graphical interface for the CCP4 suite

Jon Agirre, University of York

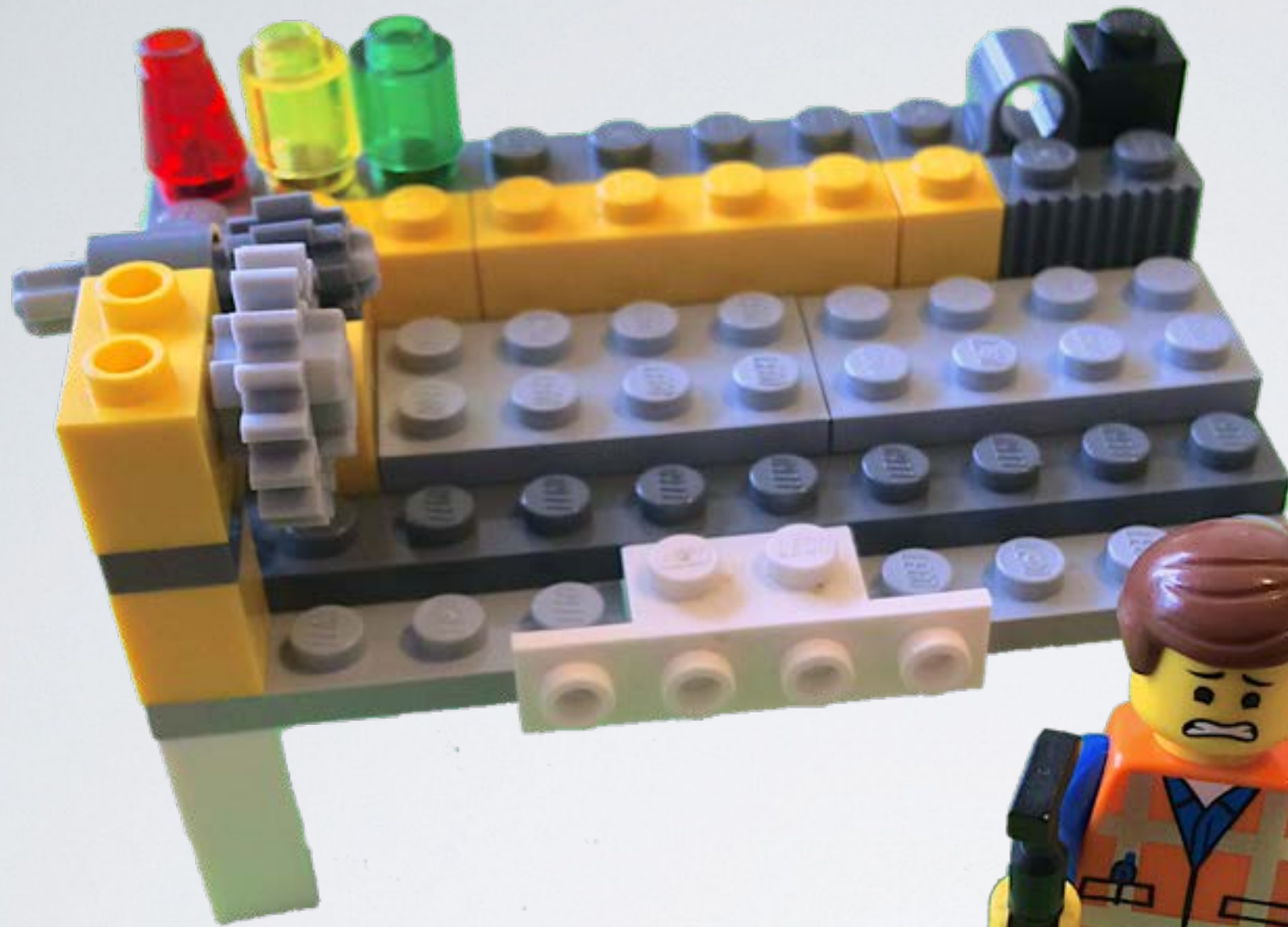
BRIEF OVERVIEW

- Why have we developed a new interface?
- Functionality and programs included
- Release plans

CCP4i



Designed in 1997, when GNU/Linux was taking off
Done in TCL/TK (not very popular nowadays)



CCP4i

- barebones interface
- little automation
- difficult for amateurs

? ?



feckless phaser
truncate stats
but caneer
stainless
approach war pad
CCP4i
aimol
stools
fall
pirate
sematch
more
ligand



CCP4i

uses bulky MTZ files

columns have cryptic labels

Which columns do I use?

*Has Refmac5 modified
my FP, SIGFP columns?*

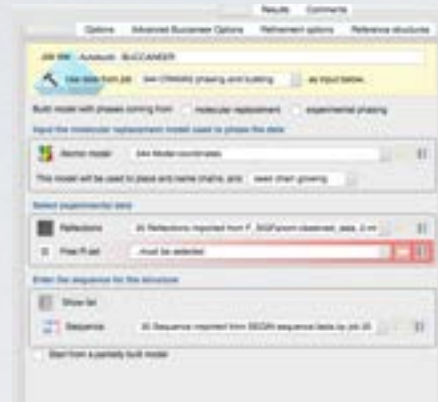
ON TOP OF THAT

- Barebones database, little tracking, almost no facilities for Research Data Management
- Limited pipelining capabilities
- No access to crystallographic libraries from TCL/TK

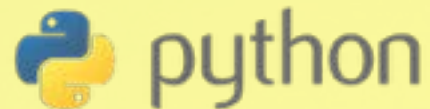
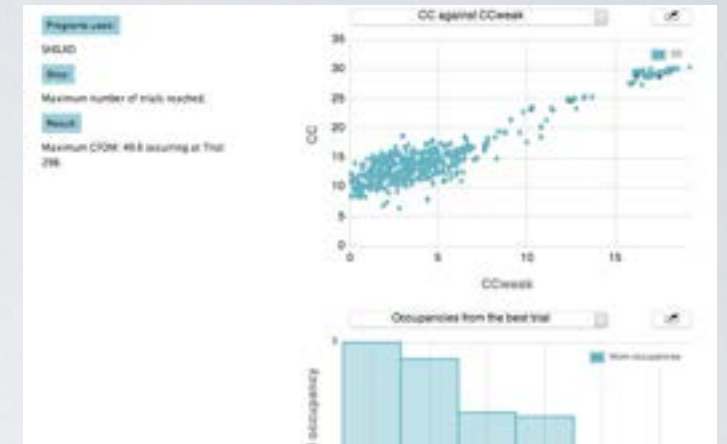
Time for a new interface!

CONCEPTS BEHIND CCP4i2

Interface



Reports



Engine



→ clipper-python

→ biopython

→ cctbx

Libraries



Database

New concept: data objects miniMTZ

Reflection data

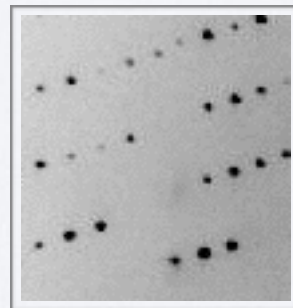
Column names and types are tied to the object type

H, K, L

F

=

SIGF



New concept: miniMTZ

Map coefficients

Column names and types are tied to the object type

H, K, L

F

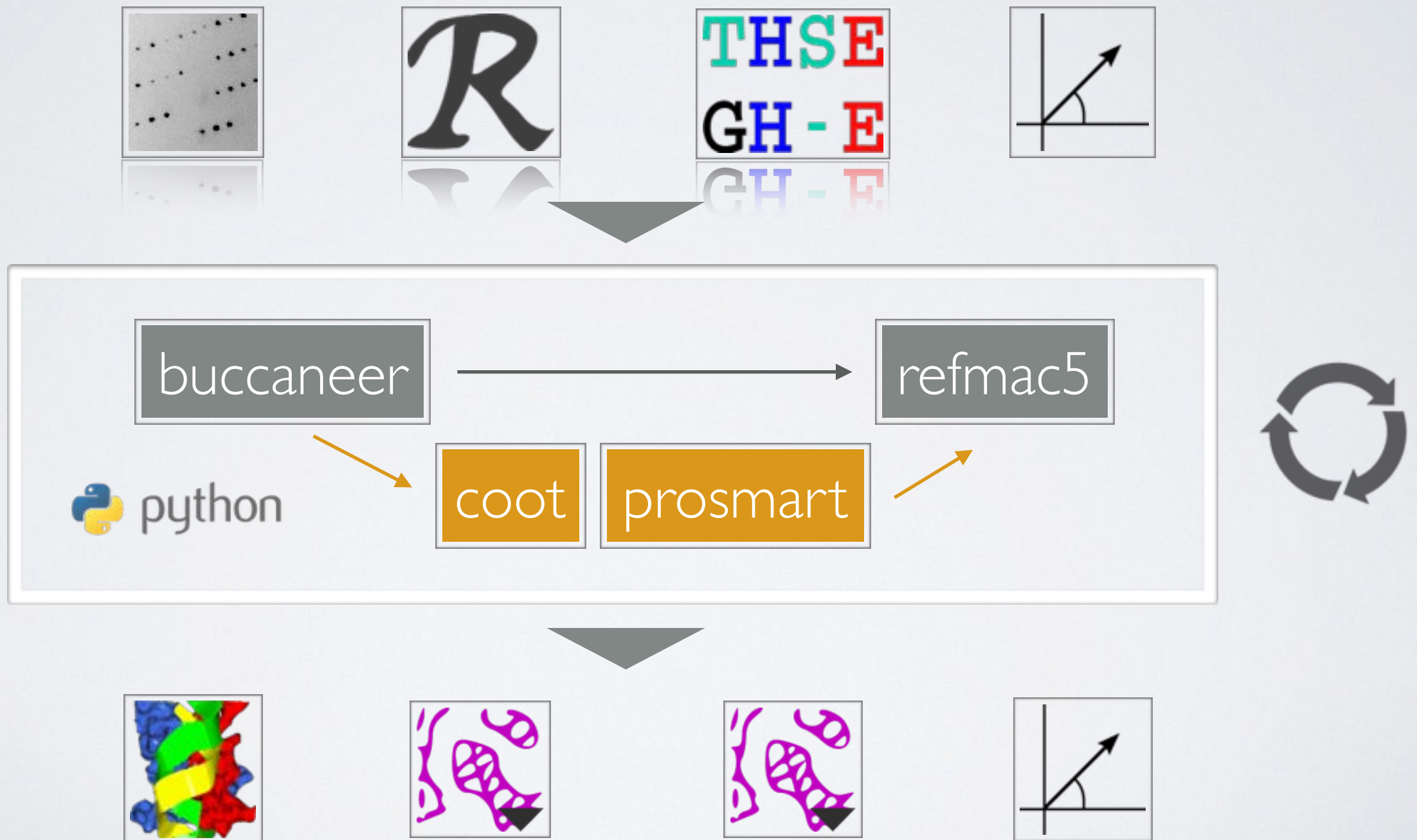
PHI

=



input and output

Pipelines



FUNCTIONALITY AND PROGRAMS INCLUDED



CCP4i2

Welcome

New to CCP4i2?

Try the ten minute [Quickstart](#) introduction.

View any file

Use this window as a web browser – select **Open file** from the **File** pull-down menu.

Open an existing project

Use the **Project** pull-down menu

[Start a new crystallography project](#)

Create a project. [More about CCP4i2 projects.](#)

[Work in a 'General' project](#)

A 'General' project will be created automatically and all your work will be saved under that project name. Then click the **Task menu** button to choose the program or pipeline to run. [More about CCP4i2 projects.](#)

[CCP4i2 Tutorial](#)

[Example data](#)

[CCP4i2 Programmers Documentation](#)

[CCP4 Main Page](#)

[Known issues with current release](#)

[Test page](#)

Creating a new project

The screenshot shows the CCP4i2 web interface. The main content area has a 'New to CCP4i2?' section with a link 'Start a new crystallography project' circled in red. Below this is a 'Work in a 'General' project' section. At the bottom, a 'Create a New Project' dialog box is open, showing the project name 'MyNewProject' and buttons for 'Help', 'Select directory', 'Cancel', and 'Create project'.

CCP4i2
Welcome

New to CCP4i2?

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Open an existing project

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[CCP4i2 Tutorial](#)
[Example data](#)
[CCP4 Main Page](#)

Create a New Project

Name of project/folder

By default all projects go in the 'CCP4i2_PROJECTS' directory in your home area - click 'Select directory' to choose an alternative.

Hint to organise your projects: in the 'Manage projects' window you can use a project as a folder and drag other projects into it

The 'Manage projects' window displays a table of projects and their locations. A red arrow points from the 'New project' button in the 'Projects' menu to this window.

Name	Directory
AmphNT	/Users/pre/Projects/AmphNT/CCP4i2
Brp	/Users/pre/Projects/Brp
DCop	/Users/pre/Projects/DCop/l2
DRpipelineTestjobs	/Users/pre/CCP4i2_PROJECTS/DRpipelineTestjobs
FCH	/Users/pre/CCP4i2_PROJECTS/FCH
Gamma	/Users/pre/Projects/Xtal/Gamma
I2demo	/Users/pre/Projects/Xtal/I2demo
Johanna	/Users/pre/Projects/MuC/Johanna
MyNewProject	/Users/pre/CCP4i2_PROJECTS/MyNewProject
V7D	/Users/pre/CCP4i2_PROJECTS/V7D
Wrobel	/Users/pre/Projects/Wrobel

Buttons: Open, Add project or folder, Rename project, Move directory, Delete, Export, Import, Cleanup tmp files, Rerun test project

Manage all projects

By default projects are created in \$HOME/CCP4i2_PROJECTS but you can put them anywhere

Avoid spaces in project names (and other names)

THE TASK MENU

- ▶  Import merged data, sequences, alignments or coordinates
- ▶  Integrate X-ray images
- ▶  X-ray data reduction and analysis
- ▶  Experimental phasing
- ▶  Bioinformatics and model preparation for Molecular Replacement
- ▶  Molecular Replacement
- ▶  Model building and Graphics
- ▶  Refinement
- ▶  Ligands
- ▶  Validation and analysis
- ▶  Export and Deposition
- ▶  Reflection data tools
- ▶  Coordinate data tools
- ▶  Developer tools

Set input

CCP4i2 alpha-4496 Project Viewer: I2demo

Bibliography Clone job **Run**

Job 25: Data reduction - AIMLESS The job is Pending

Input Results Comments

Input Data Important Options Additional Options

Job title Data reduction

Use data from job 23 Data reduction gere Se from EJD as input below..

Show list Select unmerged data files

/Users/pre/Projects/Xtal/I2demo/CCP4_IMPORTED_FILES/gamma_Xe_mosflr

Crystal name **dataset name**

Batches in file: 1 - 100

Exclude batches from calculations and output

Resolution range (Å) to Maximum resolution in files 1.78Å

☐ use explicit resolution range in symmetry determination as well as in scaling

Options for symmetry determination Determine Laue group and space group

Optional input data

1. Reference data to resolve indexing ambiguity and space group

☐ use reference data in analysis against Batch after scaling

Reference data are Reflection list and is optionally defined in next line

Reflections ..is not used

2. Optional existing FreeR set, define to copy or extend if necessary

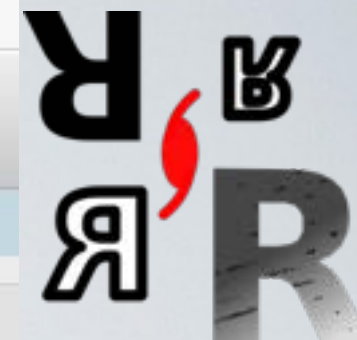
Free R set 23 FreeR - Spg:C 1 2 1;ResIn:2.72Å;Cell:108.7,61.7,71.7,90.0,9

then click "Run"

Extra options

Choose input data

Compulsory (red)
crystal and dataset
names, used to identify
data object
Short, no spaces!



Reports

Some tasks give live updates (though not this one yet)
More will in future



CCP4i2 alpha-0 Project Viewer: exp_phasing_test

Task menu View in Coot View in CCP4mg Export MTZ Help Bibliography Clone job Run

Job 1: Data reduction - AIMLESS **The job is Finished**

Input Results Comments

Headline Summary SpaceGroupDetails MergingGraphs MergingDetails Istats Biblio Run

12:23 25-Nov-2015

▼ Key summary

Selecting space group P 21 21 21
as there is a single space group with the highest score

Solution probability: 0.701, Confidence 0.626 (high resolution limit for symmetry testing 1.781Å)

Key statistics for Dataset: exp_phasing_test/Xe/Xenon

Unit cell: 34.150 54.810 68.000 90.000 90.000 90.000
Resolution of input data: 1.78Å, resolution estimate: beyond 1.78Å
R_{meas}: overall 0.048, inner bin 0.069
In outer bin: Mean(I/sdI) 3.9 CC(1/2) 0.876
Anomalous CC(1/2) in inner bin 0.653
Significant anomalous signal extends to a resolution of 1.94Å (above C_{canom} threshold 0.15)

No evidence of twinning

No evidence of possible translational non-crystallographic symmetry

Some anisotropy detected. This may have an effect on statistics.

Completeness test shows good data.

No ice rings found.

▼ Overall summary

Space group determination	Data internal consistency statistics
Selecting space group P 21 21 21 as there is a single space group with the highest score	Summary of merging statistics for dataset

Molecular Replacement and refinement - PHASER Molecular Replacement and refinement- MOLREP CRANK2 phasing and building

ShelxCd

More details later

Follow-on

Next job suggestions, with main inputs filled in automatically



Molecular Replacement and refinement - PHASER

Molecular Replacement and refinement- MOLREP

CRANK2 phasing and building

ShelxCD

From Data Reduction
Solve structure by Molecular
replacement or
Experimental phasing

▼ Elements and scores of current solution

Current best solution has spacegroup P 21 21 21

Ensemble name	Rot Func Z-score	Trans Func Z-score	Refined TFZ-equiv	Packing clashes	Log likelihood gain	Overall LLG
Ensemble_1	5.2	9.1	56.3	0	111	5028

▼ Comparison of solutions

Unique solution found :-)

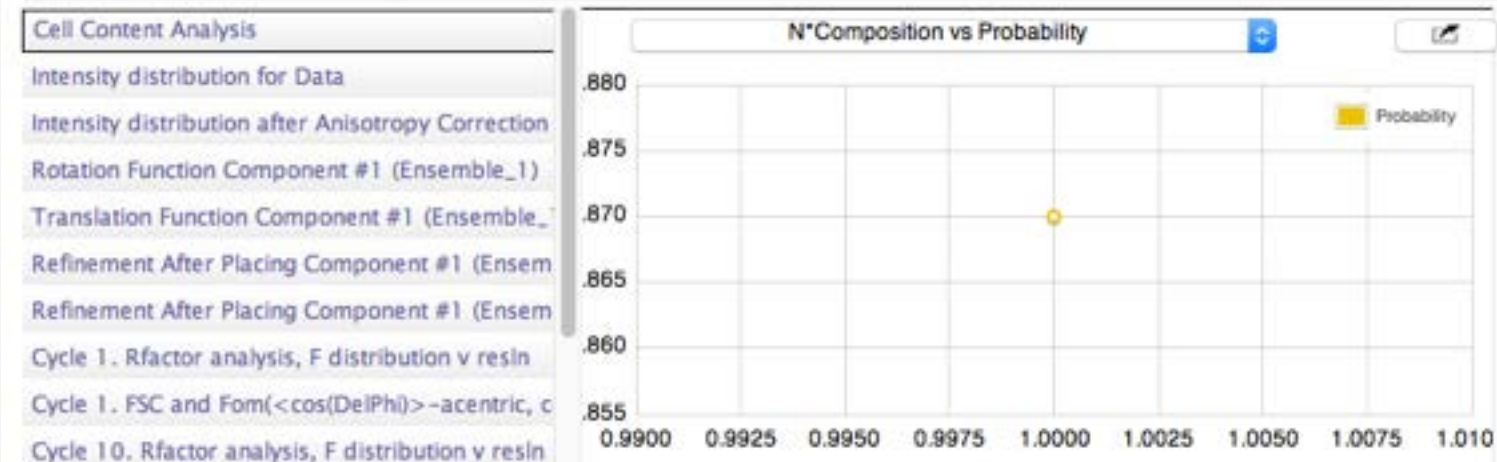
Space group	Trans. Z-score	Refined Trans. Z-score	Initial LLG	Refined LLG	Initial Rfactor	Refined Rfactor	Clashes
P 21 21 21	56.30	56.30	3241.37	3241.37	32.31	30.69	0.00

► Analysis of composition and data

► COM file for this run

► Search strategy employed by PHASER

▼ Plots from PHASER output



Refinement - REFMAC5

Autobuild - BUCCANEER

Manual model building - COOT

From Molecular
Replacement
Refine, Model build or
Manual building

RELEASE PLANS

- First version to roll out with CCP4 7.0 in late December
- Updates will incorporate new programs. Next: Arcimboldo, ACORN
- Alpha-test version available now. Contact me if you want to test it: jon.agirre@york.ac.uk

To start ccp4i2

Usually type “ccp4i2”

BUT here type “locali2”

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Johan Turkenburg

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