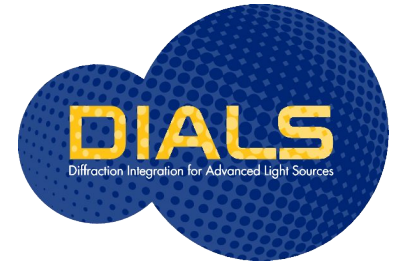
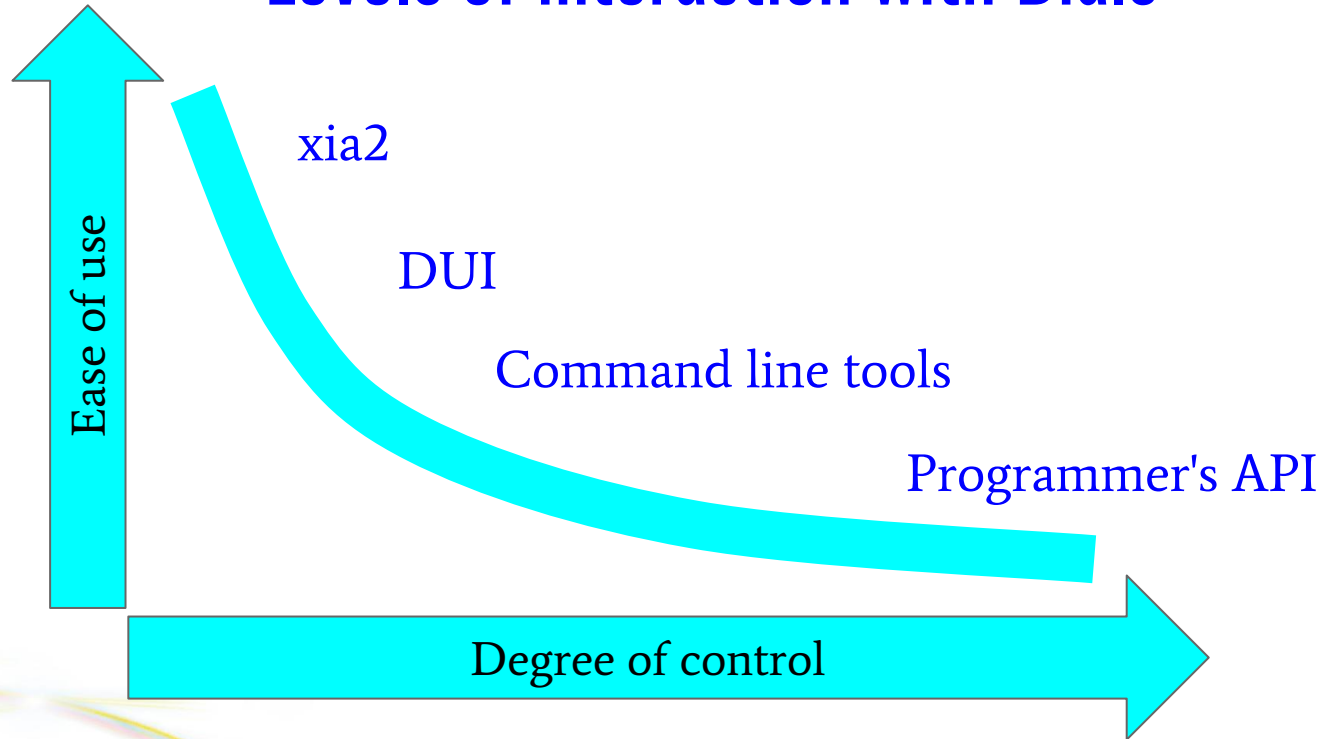


Data Integration with DUI:

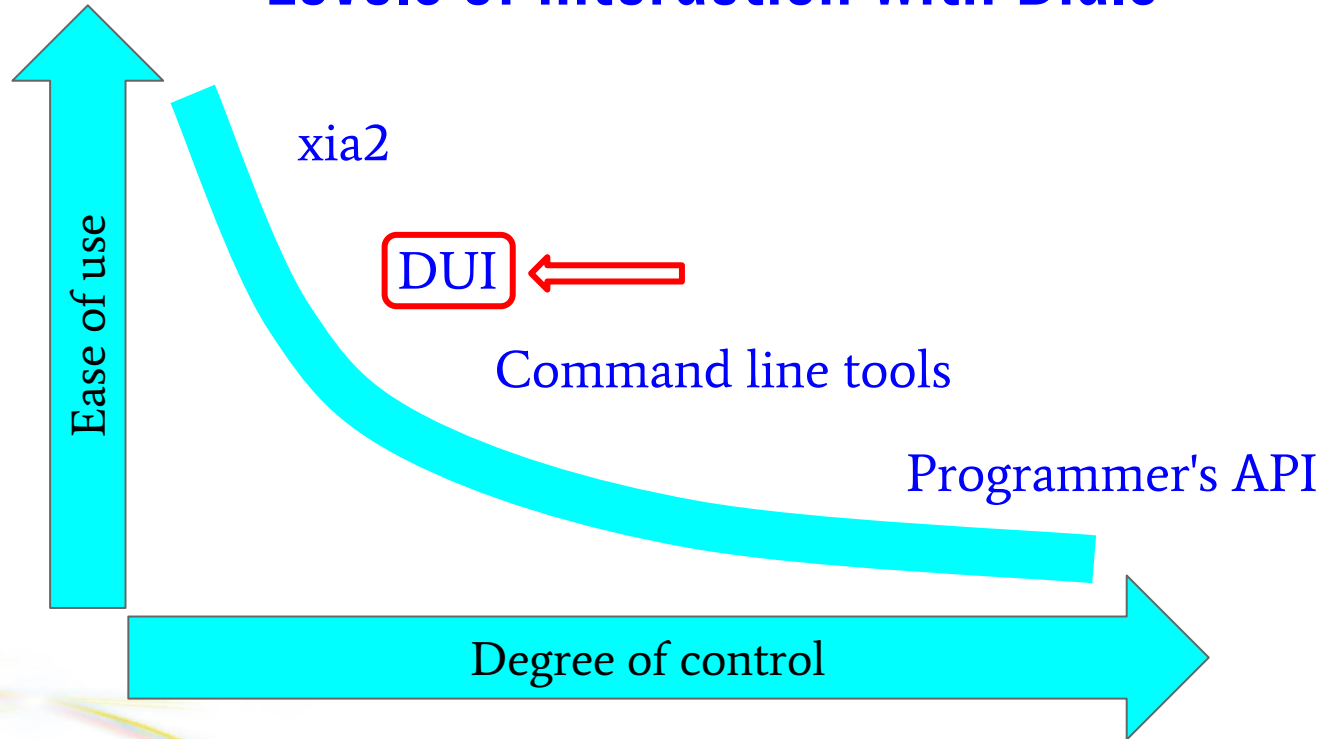
Dr. Luis Fuentes-Montero (Luiso)



Levels of interaction with Dials



Levels of interaction with Dials



What is DUI?



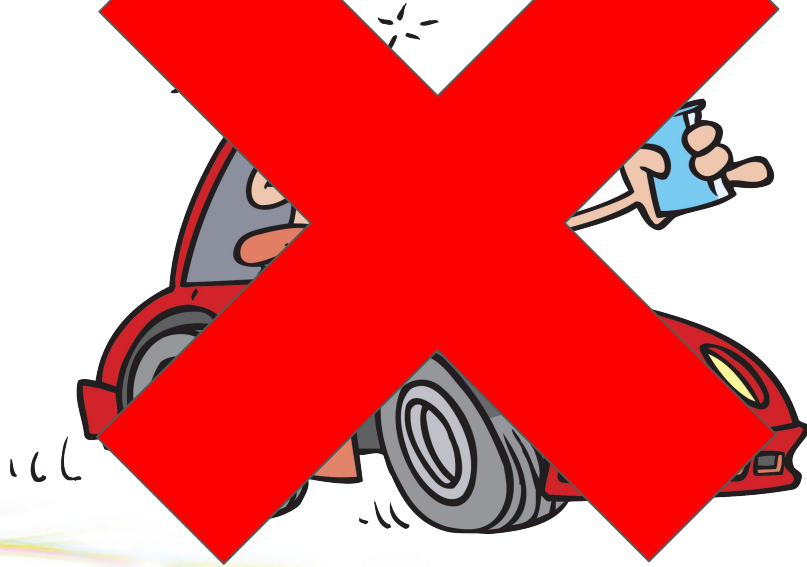
What is DUI?

Drive Under Influence



What is DUI?

Drive Under Influence



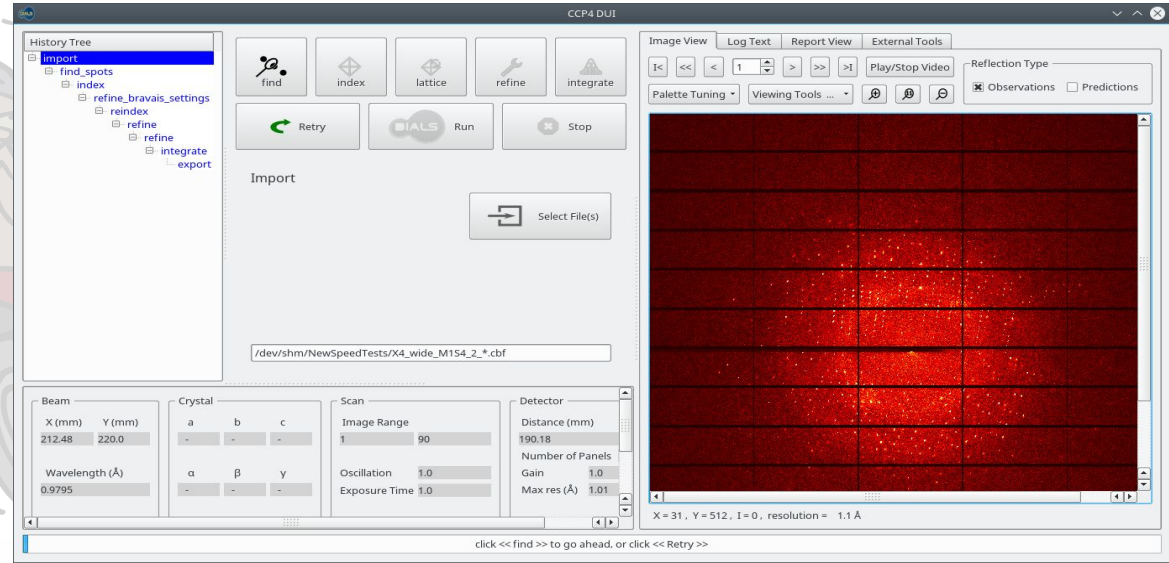
What is DUI?

Dials User Interface



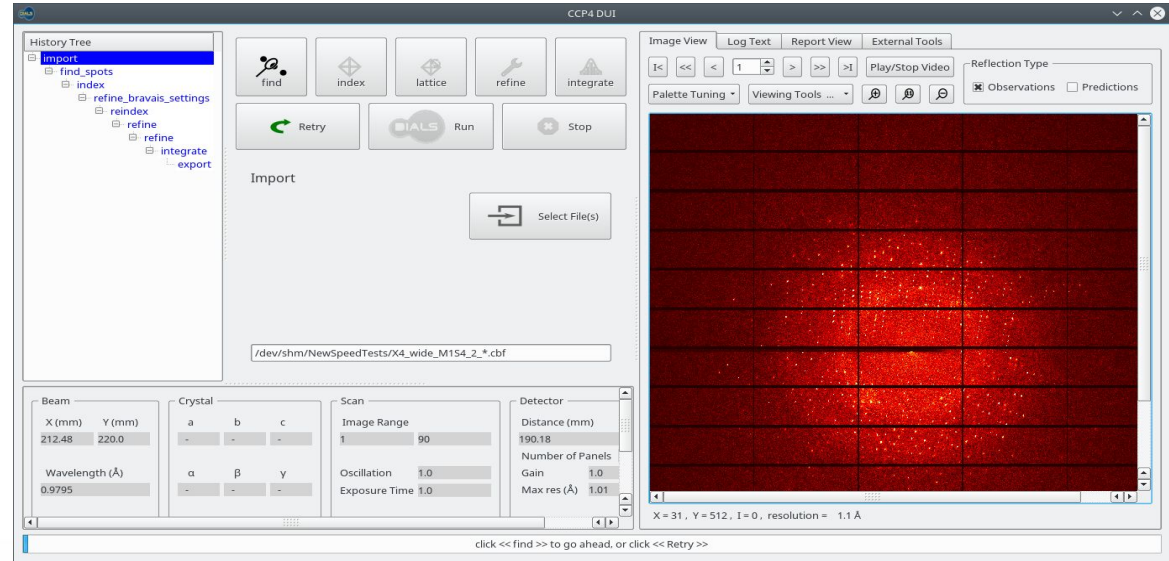
What is DUI?

Dials User Interface



What is DUI?

Dials User Interface



DUI Running DIALS



DUI Running DIALS

The screenshot displays the CCP4 DUI (Data User Interface) software running the DIALS workflow. The interface is divided into several sections:

- History Tree:** Shows the sequence of actions performed, including 'import', 'find_spots', 'index', 'refine_bravais_settings', 'reindex', 'refine', 'integrate', and 'export'. The 'refine' step is currently selected.
- Workflow Buttons:** A row of buttons for 'find', 'index', 'lattice', 'refine', and 'integrate'. Below them are 'Retry', 'DIALS Run', and 'Stop' buttons.
- Refine Panel:** Contains a 'Simple' and 'Advanced' tab. The 'Advanced' tab is active, showing a dropdown menu for 'refinement.parameterisation.scan_varying' set to 'True'. A 'Reset to Default' button is located below.
- Beam, Crystal, Scan, Detector Parameters:** A table at the bottom left provides experimental parameters:

Beam		Crystal			Scan		Detector
X (mm)	Y (mm)	a	b	c	Image Range	Distance (mm)	
218.58	209.18	40.55	40.56	69.29	1 720	169.08	
- Log View:** The right-hand pane shows the output of the DIALS workflow. It includes a table of image statistics, a message 'RMSD no longer decreasing', 'RMSDs by experiment' table, and the 'Final refined crystal model' details.

Image View	Log Text	Report View	External Tools	
6	90581	0.04069	0.036367	0.099104
7	90581	0.040693	0.036349	0.099105
8	90581	0.040692	0.036345	0.099104
9	90581	0.040691	0.036344	0.099105

RMSD no longer decreasing

RMSDs by experiment:

Exp id	Nref (px)	RMSD_X (px)	RMSD_Y (px)	RMSD_Z (images)
0	90581	0.23658	0.2113	0.19821

Final refined crystal model:

Crystal:
Unit cell: (40.5519(3), 40.5585(3), 69.2944(5), 92.0191(2), 91.9744(2), 98.0733(2))
Space group: P 1
U matrix: {{ 0.8429, 0.5342, 0.0638}, {-0.1841, 0.1749, 0.9672}, {0.5955, -0.8270, 0.2458}}
B matrix: {{ 0.0247, 0.0000, 0.0000}, {0.0035, 0.0249, 0.0000}, {0.0018, 0.0010, 0.0145}}
A = UB: {{ 0.0227, 0.0134, 0.0009}, {-0.0030, 0.0053, 0.0140}, {0.0098, -0.0203, 0.0036}}
A sampled at 721 scan points

Saving refined experiments to /memdisk/dui_files/11_experiments.json
Updating predictions for indexed reflections
Saving reflections with updated predictions to /memdisk/dui_files/11_reflections.pickle
Total time taken: 79.76s
- Status Bar:** A message at the bottom reads 'click <<integrate>> to go ahead, or click <<Retry>>'.



DUI Running DIALS

```
File Edit View Bookmarks Settings Help
update_pbar_msg = click << integrate>> to go ahead, or click <<
self.load_finished(ok) = True

status
|  lin num
|  |  command
|  |  |
-----
S  0  \_Root
S  1  |  \_import
S  2  |  |  \_find_spots
S  3  |  |  |  \_index
S  4  |  |  |  |  \_refine_braavais_settings
S  5  |  |  |  |  |  \_reindex
S  6  |  |  |  |  |  |  \_refine
S  7  |  |  |  |  |  |  |  \_refine
S  8  |  |  |  |  |  |  |  |  \_integrate
S  9  |  |  |  |  |  |  |  |  |  \_export
S 10  |  |  |  |  |  |  |  |  |  |  \_refine
S 11  |  |  |  |  |  |  |  |  |  |  |  \_refine

-----
turning log fonts to GREEN
turning log fonts to BLUE
path_to_log = /memdisk/dui_files/11_refine.log
```

The screenshot shows the CCP4 DUI interface. On the left is a History Tree with a tree view of the workflow: find_spots, index, refine_braavais_settings, reindex, refine, integrate, and export. The 'refine' step is currently selected. In the center are control buttons for 'find', 'index', 'lattice', 'refine', and 'integrate', along with 'Retry', 'Run', and 'Stop' buttons. Below these are 'Simple' and 'Advanced' tabs for the 'refine' step, with a dropdown menu set to 'refinement.parameterisation.scan_varying True' and a 'Reset to Default' button. At the bottom are input fields for 'Beam', 'Crystal', 'Scan', and 'Detector'.

On the right is a log window with tabs for 'Image View', 'Log Text', 'Report View', and 'External Tools'. The 'Log Text' tab is active, showing a table of RMSDs by experiment:

Exp id	Nref	RMSD_X (px)	RMSD_Y (px)	RMSD_Z
6	90581	0.04069	0.036367	0.099104
7	90581	0.040693	0.036349	0.099105
8	90581	0.040692	0.036345	0.099104
9	90581	0.040691	0.036344	0.099105

Below the table, it states 'RMSD no longer decreasing'. Further down, it shows 'Final refined crystal model:' with the following data:

Crystal:
Unit cell: (40.5519(3), 40.5505(3), 69.2944(5), 92.0191(2), 91.9744(2), 98.0733(2))
Space group: P 1
U matrix: {{ 0.8429, 0.5342, 0.0630}, {-0.1841, 0.1749, 0.9672}, {0.5955, -0.8270, 0.2450}}
B matrix: {{ 0.0247, 0.0000, 0.0000}, {0.0035, 0.0249, 0.0000}, {0.0010, 0.0010, 0.0145}}
A = UB: {{ 0.0227, 0.0134, 0.0000}, {0.0030, 0.0053, 0.0140}, {0.0098, -0.0203, 0.0036}}
A sampled at 721 scan points

At the bottom of the log window, it says 'Saving refined experiments to /memdisk/dui_files/11_experiments.json', 'Updating predictions for indexed reflections', 'Saving reflections with updated predictions to /memdisk/dui_files/11_reflections.pickle', and 'Total time taken: 79.76s'.



DUI Running DIALS

```
memdisk : python2.7 — Konsole
File Edit View Bookmarks Settings Help
update_pbar_msg = click << integrate>> to go ahead, or click << Retry >>
self.load_finished(ok) = True

status
|  lin num
|  |  command
|  |  |
|  |  |-----
S  0  \__Root
S  1  \__  \__import
S  2  \__  \__  \__find_spots
S  3  \__  \__  \__  \__index
S  4  \__  \__  \__  \__refine_bravais_settings
S  5  \__  \__  \__  \__  \__reindex
S  6  \__  \__  \__  \__  \__  \__refine
S  7  \__  \__  \__  \__  \__  \__  \__refine
S  8  \__  \__  \__  \__  \__  \__  \__  \__integrate
S  9  \__  \__  \__  \__  \__  \__  \__  \__  \__export
S 10  \__  \__  \__  \__  \__  \__  \__  \__  \__refine
S 11  \__  \__  \__  \__  \__  \__  \__  \__  \__refine

<<< here

-----
turning log fonts to GREEN
turning log fonts to BLUE
path_to_log = /memdisk/dui_files/11_refine.log
```



DUI Running DIALS

```
File Edit View Bookmarks Settings Help
update_pbar_msg = click << integrate>
self.load_finished(ok) = True

status
|  lin num
|  |  command
|  |  |
|  |  |-----
S  0  \__ Root
S  1  |  |  |  |  |
S  2  |  |  |  |  |  |  |
S  3  |  |  |  |  |  |  |  |
S  4  |  |  |  |  |  |  |  |  |
S  5  |  |  |  |  |  |  |  |  |
S  6  |  |  |  |  |  |  |  |  |
S  7  |  |  |  |  |  |  |  |  |
S  8  |  |  |  |  |  |  |  |  |
S  9  |  |  |  |  |  |  |  |  |
S 10  |  |  |  |  |  |  |  |  |
S 11  |  |  |  |  |  |  |  |  |
-----
turning log fonts to GREEN
turning log fonts to BLUE
path_to_log = /memdisk/dui_files/11_refine.log
```

```
memdisk : python2.7 — Konsole
File Edit View Bookmarks Settings Help
failed to << check_gray_outs() >>
update_pbar_msg = click dials icon to run refine
found val, v= True
run_clicked
..currentWidget(ref) = <mini_idials_w_GUI.custom_widgets.ParamWidget object at 0x7fef23dc6b98>
cmd_tmp = ['refine', 'refinement.parameterisation.scan_varying=True']
starting motion
cmd_lst_to_run = ['dials.refine', 'refinement.parameterisation.scan_varying=True', 'input.experiments
=/memdisk/dui_files/10_experiments.json', 'input.reflections=/memdisk/dui_files/10_reflections.pickle
', 'output.experiments=/memdisk/dui_files/11_experiments.json', 'output.reflections=/memdisk/dui_file
s/11_reflections.pickle', 'output.log=/memdisk/dui_files/11_refine.log', 'output.debug_log=/memdisk/d
ui_files/11_refine.debug.log']

[[ running >>

dials.refine
refinement.parameterisation.scan_varying=True
input.experiments=/memdisk/dui_files/10_experiments.json
input.reflections=/memdisk/dui_files/10_reflections.pickle
output.experiments=/memdisk/dui_files/11_experiments.json
output.reflections=/memdisk/dui_files/11_reflections.pickle
output.log=/memdisk/dui_files/11_refine.log
output.debug_log=/memdisk/dui_files/11_refine.debug.log

: bash memdisk : python2.7
refine
\__ refine <<< here
```

DUI Running DIALS

```
memdisk: python2.7 — Konsole
File Edit View Bookmarks Settings Help
failed to << check_gray_outs() >>
update_pbar_msg = click_dials_icon to run refine
found val, v= True
run_clicked
..currentWidget(ref) = <mini_idials_w_GUI.custom_widgets.ParamWidget object at 0x7fef23dc6b98>
cmd_tmp = ['refine', 'refinement.parameterisation.scan_varying=True']
starting motion
cmd_lst_to_run = ['dials.refine', 'refinement.parameterisation.scan_varying=True', 'input.experiments
=/memdisk/dui_files/10_experiments.json', 'input.reflections=/memdisk/dui_files/10_reflections.pickle
', 'output.experiments=/memdisk/dui_files/11_experiments.json', 'output.reflections=/memdisk/dui_file
s/11_reflections.pickle', 'output.log=/memdisk/dui_files/11_refine.log', 'output.debug_log=/memdisk/d
ui_files/11_refine.debug.log']

[[ running >>

dials.refine
refinement.parameterisation.scan_varying=True
input.experiments=/memdisk/dui_files/10_experiments.json
input.reflections=/memdisk/dui_files/10_reflections.pickle
output.experiments=/memdisk/dui_files/11_experiments.json
output.reflections=/memdisk/dui_files/11_reflections.pickle
output.log=/memdisk/dui_files/11_refine.log
output.debug_log=/memdisk/dui_files/11_refine.debug.log

: bash
```



DUI Running DIALS

```
memdisk: python2.7 — Konsole
File Edit View Bookmarks Settings Help
failed to << check_gray_outs() >>
update_pbar_msg = click_dials_icon to run refine
found val, v= True
run_clicked
..currentWidget(ref) = <mini_idials_w_GUI.custom_widgets.ParamWidget object at 0x7fef23dc6b98>
cmd_tmp = ['refine', 'refinement.parameterisation.scan_varying=True']
starting motion
cmd_lst_to_run = ['dials.refine', 'refinement.parameterisation.scan_varying=True', 'input.experiments
=/memdisk/dui_files/10_experiments.json', 'input.reflections=/memdisk/dui_files/10_reflections.pickle
', 'output.experiments=/memdisk/dui_files/11_experiments.json', 'output.reflections=/memdisk/dui_file
s/11_reflections.pickle', 'output.log=/memdisk/dui_files/11_refine.log', 'output.debug_log=/memdisk/d
ui_files/11_refine.debug.log']

[[ running >>

dials.refine
refinement.parameterisation.scan_varying=True
input.experiments=/memdisk/dui_files/10_experiments.json
input.reflections=/memdisk/dui_files/10_reflections.pickle
output.experiments=/memdisk/dui_files/11_experiments.json
output.reflections=/memdisk/dui_files/11_reflections.pickle
output.log=/memdisk/dui_files/11_refine.log
output.debug_log=/memdisk/dui_files/11_refine.debug.log

: bash memdisk: python2.7
```


DUI Running DIALS

```
dials.refine
refinement.parameterisation.scan_varying=True
input.experiments=/memdisk/dui_files/10_experiments.json
input.reflections=/memdisk/dui_files/10_reflections.pickle
output.experiments=/memdisk/dui_files/11_experiments.json
output.reflections=/memdisk/dui_files/11_reflections.pickle
output.log=/memdisk/dui_files/11_refine.log
output.debug_log=/memdisk/dui_files/11_refine.debug.log
```

```
dials.refine
refinement.parameterisation.scan_varying=True
input.experiments=/memdisk/dui_files/10_experiments.json
input.reflections=/memdisk/dui_files/10_reflections.pickle
output.experiments=/memdisk/dui_files/11_experiments.json
output.reflections=/memdisk/dui_files/11_reflections.pickle
output.log=/memdisk/dui_files/11_refine.log
output.debug_log=/memdisk/dui_files/11_refine.debug.log
```

: bash

memdisk: python2.7



Embedded image viewer



Embedded image viewer

The screenshot shows the CCP4 GUI with the following components:

- History Tree:** A tree view on the left showing the workflow: `limport` (selected), `find_spots`, `index`, `refine_bravais_settings`, `reindex`, `refine`, `integrate`, and `export`.
- Control Panel:** A set of buttons for `find`, `index`, `lattice`, `refine`, `integrate`, `Retry`, `Run` (with the DIALS logo), and `Stop`.
- Import Section:** Labeled "Import" with a "Select File(s)" button and a text input field containing `/dev/shm/NewSpeedTests/X4_wide_M1S4_2_*.cbf`.
- Parameter Panels:** Four panels at the bottom left:
 - Beam:** X (mm) 212.48, Y (mm) 220.0, Wavelength (Å) 0.9795.
 - Crystal:** a, b, c, α , β , γ .
 - Scan:** Image Range 1 to 90, Oscillation 1.0, Exposure Time 1.0.
 - Detector:** Distance (mm) 190.18, Number of Panels, Gain 1.0, Max res (Å) 1.01.
- Image View:** The main window on the right, titled "Image View", showing a grid of diffraction images. It includes navigation controls (I, <<, <, 1, >, >>, >I), a "Play/Stop Video" button, and checkboxes for "Reflection Type", "Observations", and "Predictions".
- Status Bar:** At the bottom, it displays `X = 31, Y = 512, I = 0, resolution = 1.1 Å` and a message: "click << find >> to go ahead, or click << Retry >>".

Embedded image viewer

History Tree

- limport
 - find_spots
 - index
 - refine_bravais_settings
 - reindex
 - refine
 - refine
 - integrate
 - export

find index lattice refine integrate

Retry Run Stop

Import

Select File(s)

/dev/shm/NewSpeedTests/X4_wide_M1S4_2_*.cbf

Beam		Crystal			Scan		Detector	
X (mm)	Y (mm)	a	b	c	Image Range	Distance (mm)	Number of Panels	
212.48	220.0	-	-	-	1 90	190.18	Gain 1.0	
Wavelength (Å)		α	β	γ	Oscillation 1.0		Max res (Å) 1.01	
0.9795		-	-	-	Exposure Time 1.0			

X = 1289, Y = 1019, I = 7, resolution = 4.2 Å

click << find >> to go ahead, or click << Retry >>

Adjustable
Image Palette

Embedded image viewer

The screenshot displays the CCP4 GUI with the 'find_spots' workflow selected in the History Tree. The main interface includes a toolbar with icons for 'find', 'index', 'lattice', 'refine', and 'integrate', along with 'Retry', 'Run', and 'Stop' buttons. The 'find_spots' configuration panel shows the following parameters:

Parameter	Value
spotfinder.threshold.dispersion.gain	0.00
spotfinder.threshold.dispersion.sigma_background	6.00
spotfinder.threshold.dispersion.sigma_strong	3.00
spotfinder.threshold.dispersion.global_threshold	0.00
spotfinder.mp.nproc	12

The 'Image View' window shows a diffraction image with several spots highlighted by red and green boxes. The status bar at the bottom of the image viewer indicates: X = 1300, Y = 1085, I = 6, resolution = 5.4 Å.

At the bottom of the CCP4 GUI, there are sections for 'Beam', 'Crystal', 'Scan', and 'Detector' parameters:

Beam		Crystal			Scan		Detector	
X (mm)	Y (mm)	a	b	c	Image Range	Distance (mm)	Number of Panels	
212.48	220.0	-	-	-	1 90	190.18	Gain	
Wavelength (Å)		α	β	γ	Oscillation	1.0	1.0	
0.9795		-	-	-	Exposure Time	1.0	Max res (Å)	
							1.01	

click <<index>> to go ahead, or click <<Retry>>

Updates
With
Processing
Steps

Embedded image viewer

The screenshot shows the CCP4 GUI with an embedded image viewer window. The image viewer displays a diffraction pattern with several spots indexed with Miller indices. The indices shown are: (9, -1, -1), (9, -2, -3), (8, -1, -1), (8, -2, -3), (7, -1, -1), (7, -2, -3), (6, -1, -1), (6, -2, -3), (5, -1, -1), (5, -2, -3), and (5, -3, -3). The image viewer also shows a status bar at the bottom with the text: X = 1282, Y = 1095, I = 7, resolution = 5.9 Å.

History Tree

- limport
 - find_spots
 - index
 - refine_bravais_settings
 - reindex
 - refine
 - refine
 - refine
 - integrate
 - export

index

Simple | Advanced

indexing.method: ff3d

Reset to Default

Beam

X (mm)	Y (mm)
212.64	219.87

Crystal

a	b	c
39.73	42.32	42.41

Scan

Image Range	Oscillation	Exposure Time
1 - 90	1.0	1.0

Detector

Distance (mm)	Number of Panels	Gain	Max res (Å)
192.04	1.0	1.0	1.01

click << reindex >> to go ahead, or click << Retry >>

Updates
With
Processing
Steps

Embedded image viewer

The screenshot displays the CCP4 DUI (Data User Interface) software. The main window is titled "CCP4 DUI". On the left, a "History Tree" shows a sequence of actions: limport, find_spots, index, refine_bravais_settings, reindex, refine, integrate, and export. The "reindex" step is currently selected. Below the tree is a toolbar with icons for find, index, lattice, refine, and integrate, along with buttons for Retry, Run (with the DIALS logo), and Stop. A section titled "refine_bravais_settings" contains a "Simple" tab and an "Advanced" tab, with a dropdown menu for "refinement.parameterisation.scan_varying" set to "False" and a "Reset to Default" button. At the bottom left, a summary table provides experimental parameters:

Beam		Crystal			Scan		Detector	
X (mm)	Y (mm)	a	b	c	Image Range	Distance (mm)		
212.63	219.87	42.38	42.38	39.74	1 90	192.08		
Wavelength (Å)		α	β	γ	Oscillation	Number of Panels	Gain	
0.9795		90.0	90.0	90.0	1.0	1.0	1.0	
					Exposure Time	Max res (Å)		
					1.0	1.01		

The main "Image View" window shows a diffraction pattern with several spots highlighted in green and labeled with Miller indices: (-1, -1, -9), (-2, -3, -9), (-1, -1, -8), (-2, -3, -8), (-1, -1, -7), (-2, -3, -7), (-1, -1, -6), (-2, -3, -6), (-1, -1, -5), (-2, -3, -5), and (-3, -5, -5). The status bar at the bottom of the image viewer shows "X = 1266, Y = 1084, I = 13, resolution = 5.6 Å". At the very bottom of the software window, a message reads "click <<refine >> to go ahead, or click <<Retry >>".

Updates
With
Processing
Steps

Embedded image viewer

The screenshot shows the CCP4 GUI with an embedded image viewer window. The image viewer displays a diffraction pattern with several spots indexed with Miller indices. The indices shown are: (-1, 0, -9), (-1, -1, -9), (-2, -2, -9), (-2, -3, -9), (-3, -4, -9), (-1, 0, -8), (-1, -1, -8), (-2, -2, -8), (-3, -4, -8), (-1, 0, -7), (-2, -2, -7), (-3, -4, -7), (-2, -2, -6), (-3, -4, -6), and (-2, -2, -5). The status bar at the bottom of the image viewer window reads: X = 1338, Y = 1045, I = -1, resolution = 4.4 Å.

Below the image viewer, the main CCP4 GUI is visible, showing a History Tree on the left, a central control panel with buttons for find, index, lattice, refine, and integrate, and a bottom panel with parameters for Beam, Crystal, Scan, and Detector.

Beam		Crystal			Scan		Detector	
X (mm)	Y (mm)	a	b	c	Image Range	Distance (mm)	Number of Panels	
212.62	219.89	42.36	42.36	39.71	1 90	191.77	Gain	
Wavelength (Å)		α	β	γ	Oscillation		Max res (Å)	
0.9795		90.0	90.0	90.0	1.0		1.01	
					Exposure Time			
					1.0			

Updates
With
Processing
Steps

Embedded image viewer

The screenshot displays the CCP4 DUI (Data User Interface) software. The interface is divided into several sections:

- History Tree:** A tree view on the left showing the workflow steps: import, find_spots, index, refine_bravais_settings, reindex, refine, integrate, and export. The 'integrate' step is currently selected.
- Control Buttons:** A row of icons for 'find', 'index', 'lattice', 'refine', and 'integrate'. Below them are 'Retry', 'Run' (with the DIALS logo), and 'Stop' buttons.
- Integrate Settings:** A panel with 'Simple' and 'Advanced' tabs. Under 'Advanced', there are dropdown menus for 'integration.profile.fitting' (set to 'True'), 'integration.background.algorithm' (set to 'glm'), and 'integration.mp.nproc' (set to '6'). There is a text field for 'mtz output name:' containing 'hkl_out.mtz' and a 'Reset to Default' button.
- Parameter Tables:**

Beam		Crystal			Scan		Detector		
X (mm)	Y (mm)	a	b	c	Image Range	Distance (mm)			
212.62	219.89	42.36	42.36	39.71	1 90	191.77			
Wavelength (Å)				Oscillation	1.0	Number of Panels			
0.9795				Exposure Time	1.0	Gain	1.0		
		α	β	γ			Max res (Å)	1.01	
		90.0	90.0	90.0					
- Image View:** A large window showing a dark red diffraction pattern with several bright spots. Each spot is enclosed in a green rectangular box, and its Miller indices are printed in green above it. The visible indices include (-1, -1, 9), (-2, -3, 9), (-3, -4, 8), (-1, -1, 8), (-2, -3, 8), (-3, -4, 7), (-1, -1, 7), (-2, -3, 7), (-3, -4, 6), (-1, -1, 6), (-2, -3, 5), (-3, -4, 5), (-1, -1, 5), and (-3, -5, 5). At the bottom of the image view, it reads: 'X = 1276, Y = 1032, I = 10, resolution = 4.5 Å'.
- Footer:** A status bar at the bottom of the window contains the text: 'click << Retry >> or navigate elsewhere in the tree'.

Updates
With
Processing
Steps



Running Dials visualisation “*commands*”



Running Dials visualisation “commands”

The screenshot displays the CCP4 GUI with the DIALS Run interface. The main window is titled "CCP4 DUI" and contains several panels:

- History Tree:** A tree view on the left showing the workflow: import > find_spots > index > refine_bravais_settings > reindex > refine > integrate > export. The "find_spots" node is highlighted.
- Command Buttons:** A row of icons for "find", "index", "lattice", "refine", and "integrate". Below them are "Retry", "DIALS Run", and "Stop" buttons.
- find_spots Panel:** A configuration panel for the "find_spots" command. It has "Simple" and "Advanced" tabs. The "Advanced" tab is active, showing five spinners:
 - spotfinder.threshold.dispersion.gain: 0.00
 - spotfinder.threshold.dispersion.sigma_background: 6.00
 - spotfinder.threshold.dispersion.sigma_strong: 3.00
 - spotfinder.threshold.dispersion.global_threshold: 0.00
 - spotfinder.mp.nproc: 12A "Reset to Default" button is at the bottom.
- Parameter Panels:** Four panels at the bottom left:
 - Beam:** X (mm) 212.48, Y (mm) 220.0, Wavelength (Å) 0.9795.
 - Crystal:** a, b, c, α, β, γ.
 - Scan:** Image Range 1 to 90, Oscillation 1.0, Exposure Time 1.0.
 - Detector:** Distance (mm) 190.18, Number of Panels, Gain 1.0, Max res (Å) 1.01.
- Main View Area:** A large area on the right with tabs for "Image View", "Log Text", "Report View", and "External Tools". It contains two large buttons: "Open Reciprocal Lattice Viewer" and "Open Image Viewer".
- Status Bar:** At the bottom, it says "click dials icon to run find_spots".

Running Dials visualisation “commands”

The screenshot shows the CCP4 DIALS GUI with the following components:

- History Tree:** A tree view on the left showing the command sequence: import, find_spots, index, refine_bravais_settings, reindex, refine, integrate, export. The 'find_spots' command is highlighted.
- Command Buttons:** A row of icons for 'find', 'index', 'lattice', 'refine', and 'integrate'. Below them are 'Retry', 'DIALS Run', and 'Stop' buttons.
- find_spots Configuration:** A panel with 'Simple' and 'Advanced' tabs. Under 'Advanced', there are five spinners:
 - spotfinder.threshold.dispersion.gain: 0.00
 - spotfinder.threshold.dispersion.sigma_background: 6.00
 - spotfinder.threshold.dispersion.sigma_strong: 3.00
 - spotfinder.threshold.dispersion.global_threshold: 0.00
 - spotfinder.mp.nproc: 12A 'Reset to Default' button is at the bottom.
- Beam, Crystal, Scan, Detector Parameters:** A grid of input fields at the bottom left.

Beam		Crystal			Scan		Detector	
X (mm)	Y (mm)	a	b	c	Image Range	Distance (mm)	Number of Panels	
212.48	220.0	-	-	-	1 90	190.18	Gain	
Wavelength (Å)		α	β	γ	Oscillation		Max res (Å)	
0.9795		-	-	-	1.0		1.01	
					Exposure Time			
					1.0			
- Main View:** A large area on the right with tabs for 'Image View', 'Log Text', 'Report View', and 'External Tools'. It contains two buttons: 'Open Reciprocal Lattice Viewer' and 'Open Image Viewer'. A red arrow points to the 'Open Image Viewer' button.
- Status Bar:** A message at the bottom reads 'click dials icon to run find_spots'.

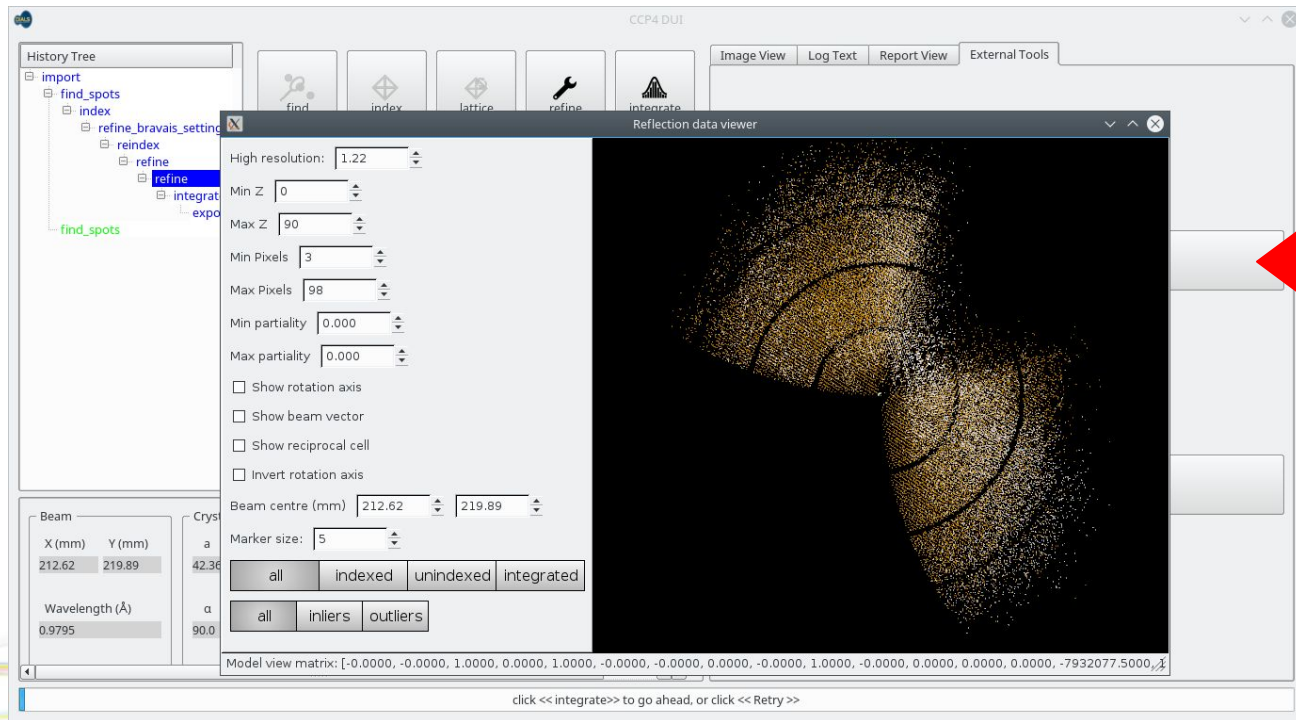
Click Here



Running Dials visualisation “commands”

The screenshot displays the DIALS software interface. On the left, a History Tree shows a sequence of operations: import, find_spots, index, refine_bravais_settings, reindex, refine, and integrate. Below this, the Beam parameters are listed: X (mm) 212.48, Y (mm) 220.0, and Wavelength (Å) 0.9795. The main window shows a grid of diffraction images with a settings panel on the right. The settings panel includes options for Zoom level (25%), Color scheme (grayscale), Brightness (100), and various checkboxes for visualization options like 'Show resolution rings', 'Mark beam center', 'Spot max pixels', 'Draw reflection shoebox', 'Basis vectors', 'Integrating only', 'Show ice rings', 'Mark centers of mass', 'Spot all pixels', 'Show predictions', 'Show hkl', 'Show mask', and 'Indexed only'. The 'find_spots.phil' file is loaded, and the 'Save' button is visible. At the bottom, a status bar reads: 'Picture: slow=1494.160 / fast=407.500 pixels. Readout: slow=1494.160 / fast=407.500 pixels. I=2.0000 resolution: 1.515'.

Running Dials visualisation “commands”



The screenshot displays the CCP4 GUI with the Dials reflection data viewer window open. The viewer shows a 3D visualization of a crystal lattice with a red arrow pointing to it. The interface includes a History Tree on the left, a top toolbar with icons for find, index, lattice, refine, and integrate, and a main control panel with various settings.

Reflection data viewer settings:

- High resolution: 1.22
- Min Z: 0
- Max Z: 90
- Min Pixels: 3
- Max Pixels: 98
- Min partiality: 0.000
- Max partiality: 0.000
- Show rotation axis
- Show beam vector
- Show reciprocal cell
- Invert rotation axis
- Beam centre (mm): 212.62, 219.89
- Marker size: 5
- Buttons: all, indexed, unindexed, integrated
- Buttons: all, inliers, outliers

Beam and Crystal parameters:

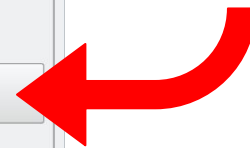
Beam		Crys a
X (mm)	Y (mm)	
212.62	219.89	42.36

Wavelength (Å)		α
0.9795		
		90.0

Model view matrix: [-0.0000, -0.0000, 1.0000, 1.0000, -0.0000, -0.0000, 0.0000, -0.0000, 1.0000, -0.0000, 0.0000, 0.0000, 0.0000, -7932077.5000, 3]

click << integrate >> to go ahead, or click << Retry >>

Or Click
Here



Log Text



Log Text

The screenshot shows the CCP4 GUI with the 'Log Text' window open. The 'Log Text' window displays the following output:

```
Found 4357 strong pixels on image 76
Found 4221 strong pixels on image 77
Found 4338 strong pixels on image 78
Found 4286 strong pixels on image 79
Found 4419 strong pixels on image 80
Found 4349 strong pixels on image 81
Found 4420 strong pixels on image 82
Found 4496 strong pixels on image 83
Found 4417 strong pixels on image 84
Found 4497 strong pixels on image 85
Found 4453 strong pixels on image 86
Found 4232 strong pixels on image 87
Found 4493 strong pixels on image 88
Found 4268 strong pixels on image 89
Found 4397 strong pixels on image 90

Extracted 64736 spots
Removed 31976 spots with size < 3 pixels
Removed 31 spots with size > 100 pixels
Calculated 32729 spot centroids
Calculated 32729 spot intensities
Filtered 31840 of 32729 spots by peak-centroid distance

Histogram of per-image spot count for imageset 0:
31840 spots found on 90 images (max 987 / bin)
```

The GUI also shows a 'find_spots' panel with the following settings:

- spotfinder.threshold.dispersion.gain: 0.00
- spotfinder.threshold.dispersion.sigma_background: 6.00
- spotfinder.threshold.dispersion.sigma_strong: 3.00
- spotfinder.threshold.dispersion.global_threshold: 0.00
- spotfinder.mp.nproc: 12

At the bottom of the GUI, the following parameters are displayed:

Beam		Crystal			Scan		Detector	
X (mm)	Y (mm)	a	b	c	Image Range	Distance (mm)	Number of Panels	
212.48	220.0	-	-	-	1 90	190.18	Gain 1.0	
Wavelength (Å)		α	β	γ	Oscillation	Max res (Å)		
0.9795		-	-	-	1.0	1.01		
					Exposure Time			
					1.0			

Shows
output
of
Processing
Commands

HTML report view



HTML report view

The screenshot displays the CCP4 GUI interface. On the left, a History Tree shows the workflow: import, find_spots, index, refine_bravais_settings, reindex, refine, integrate, and export. The main panel is titled "find_spots" and includes a "Simple" / "Advanced" toggle and several input fields for spotfinder parameters: dispersion.gain (0.00), dispersion.sigma_background (6.00), dispersion.sigma_strong (3.00), dispersion.global_threshold (0.00), and mp.nproc (12). A "Reset to Default" button is located below these fields. The bottom section of the GUI contains metadata for the Beam, Crystal, Scan, and Detector. The Scan section shows an Image Range of 1 to 90, Oscillation of 1.0, and Exposure Time of 1.0. The Detector section shows a Distance of 190.18 mm, Number of Panels, Gain of 1.0, and Max res of 1.01 Å. On the right, the "Report View" tab is active, displaying "DIALS analysis plots" for "Analysis of strong reflections". The plot, titled "Spot count per image", shows a line graph of Spot count (0 to 500) versus Image (0 to 80). The spot count starts around 300 and generally increases to about 450 over the 80 images. A blue arrow points to the plot area.

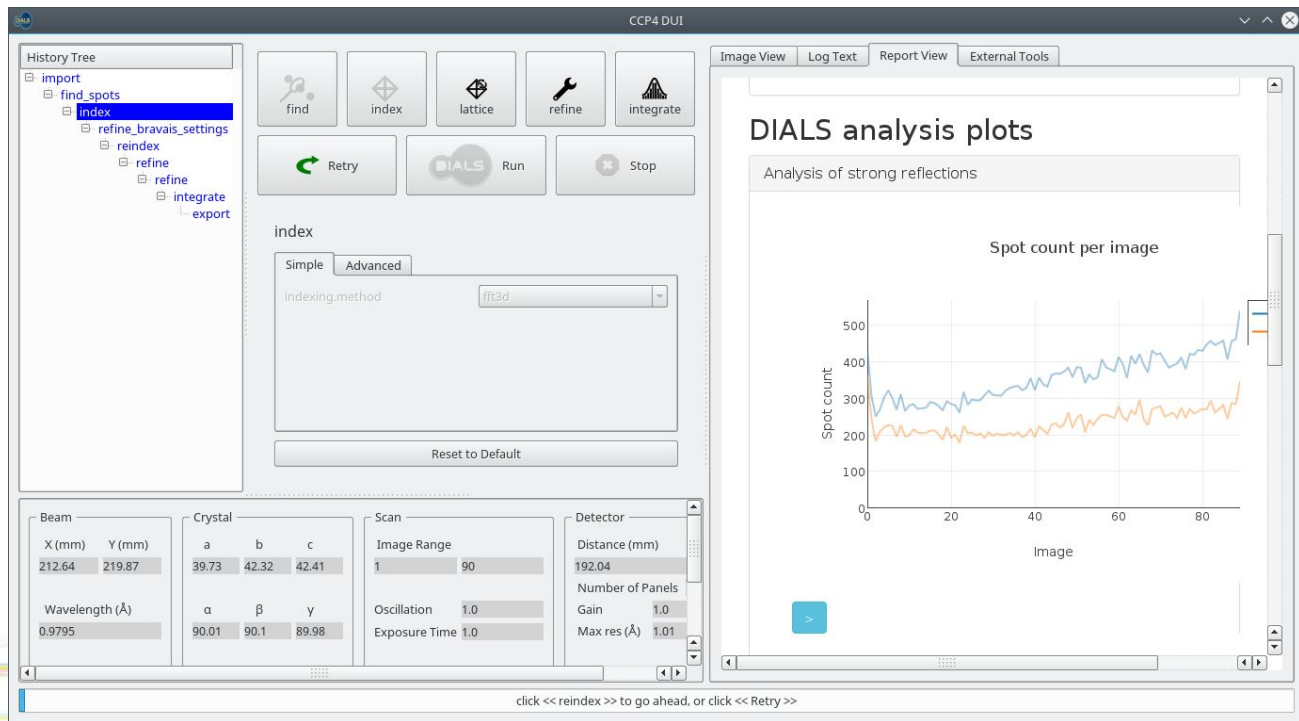
Beam	Crystal	Scan	Detector
X (mm): 212.48 Y (mm): 220.0 Wavelength (Å): 0.9795	a: - b: - c: - α: - β: - γ: -	Image Range: 1 to 90 Oscillation: 1.0 Exposure Time: 1.0	Distance (mm): 190.18 Number of Panels: Gain: 1.0 Max res (Å): 1.01

runs:

dials.report

automatically

HTML report view



runs:

dials.report

automatically

HTML report view

History Tree

- import
 - find_spots
 - index
 - refine_bravais_settings
 - reindex
 - refine
 - refine
 - integrate
 - export

find index lattice refine integrate

Retry Run Stop

index

Simple Advanced

indexing.method ff3d

Reset to Default

Beam

X (mm)	Y (mm)
212.64	219.87

Crystal

a	b	c
39.73	42.32	42.41

Scan

Image Range	Oscillation	Exposure Time
1 90	1.0	1.0

Detector

Distance (mm)	Number of Panels	Gain	Max res (Å)
192.04	1.0	1.0	1.01

Centroid residuals in Z and Y

Centroid residuals in X and Z

click << reindex >> to go ahead, or click << Retry >>

runs:

dials.report

automatically

HTML report view

History Tree

- import
 - find_spots
 - index
 - refine_bravais_settings
 - reindex
 - refine
 - refine
 - integrate
 - export

find index lattice refine integrate

Retry Run Stop

refine

Simple Advanced

refinement.parameterisation.scan_varying True

Reset to Default

Beam

X (mm)	Y (mm)
212.62	219.89

Crystal

a	b	c
42.36	42.36	39.71

Scan

Image Range	Oscillation	Exposure Time
1 90	1.0	1.0

Detector

Distance (mm)	Number of Panels	Gain	Max res (Å)
191.77	1.0	1.0	1.01

Centroid residuals in Z and Y

Centroid residuals in X and Z

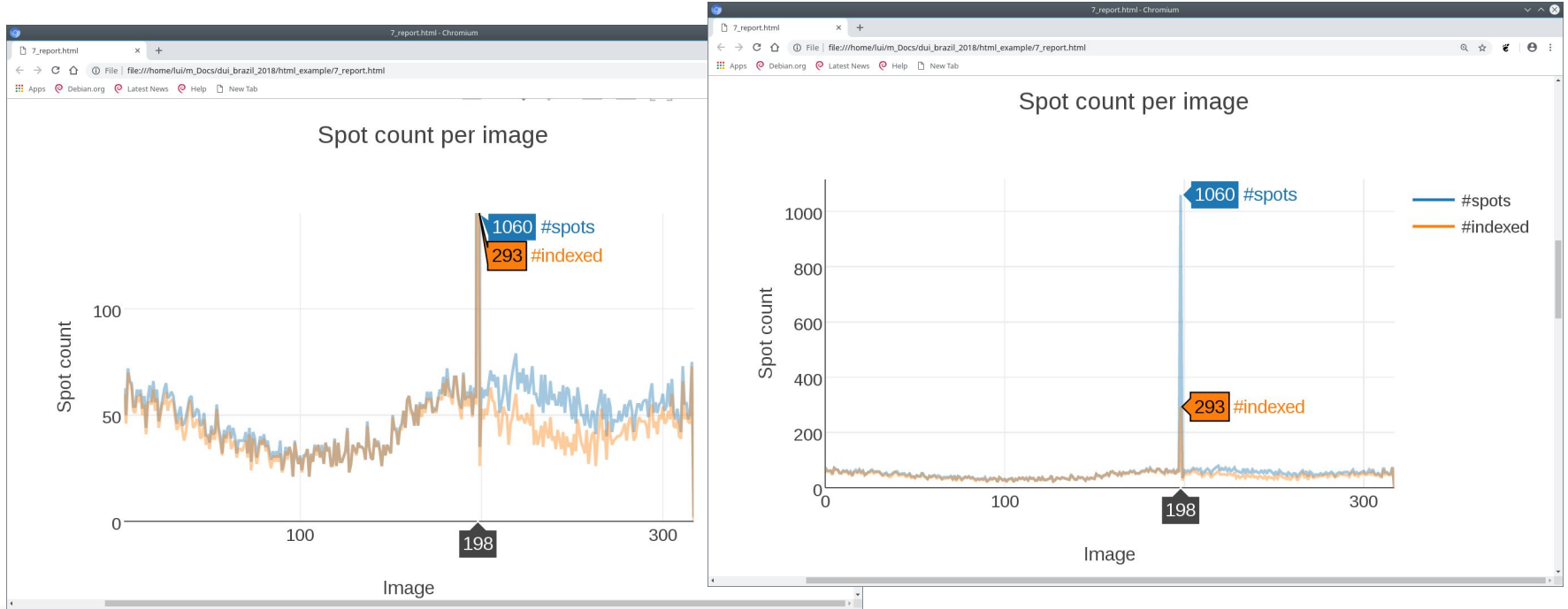
click <<integrate>> to go ahead, or click <<Retry>>

runs:

dials.report

automatically

HTML report view



A case where something went terribly wrong

Navigation Tree



Navigation Tree

The screenshot displays the CCP4 GUI interface. On the left, the History Tree shows a sequence of actions: limport, find_spots, index, refine_bravais_settings, reindex, refine, integrate, export, and another set of reindex, refine, reindex, reindex, and refine. The 'refine' node is currently selected. The main window features a toolbar with icons for find, index, lattice, refine, and integrate, along with buttons for Retry, Run, and Stop. Below the toolbar, the 'refine' section has tabs for Simple and Advanced, with a dropdown menu for 'refinement.parameterisation.scan_varying' set to 'False'. The central area shows a diffraction pattern with several spots labeled with their coordinates, such as (-2, 12, -9), (-2, 10, -9), (-2, 8, -9), (-1, 5, -), (-2, 12, -8), (-2, 10, -8), (-2, 8, -8), (-2, 6, -8), (-2, 10, -7), (-2, 8, -7), (-2, 6, -7), (-2, 12, -6), (-2, 10, -6), (-2, 8, -6), and (-2, 6, -6). The bottom status bar indicates 'X = 1094, Y = 974, I = 16, resolution = 3.4 Å'. At the very bottom, a message reads 'click <<integrate>> to go ahead, or click <<Retry>>'.

Never
be afraid to:
navigate

Navigation Tree

The screenshot shows the CCP4 GUI interface. On the left is a History Tree with a blue box around the 'refine' node under 'find_spots'. The central panel contains buttons for 'find', 'index', 'lattice', 'refine', and 'integrate', along with 'Retry', 'Run', and 'Stop' buttons. Below these are 'Simple' and 'Advanced' tabs for the 'refine' section, with a dropdown menu for 'refinement.parameterisation.scan_varying' set to 'False'. The bottom section contains four tables for experimental parameters:

Beam		Crystal			Scan		Detector	
X (mm)	Y (mm)	a	b	c	Image Range	Distance (mm)	Number of Panels	
212.64	219.87	39.76	42.45	42.34	1 90	192.16	Gain	
Wavelength (Å)		α	β	γ	Oscillation	Max res (Å)	1.0	
0.9795		90.04	90.0	89.96	Exposure Time	1.0		

The right panel shows an 'Image View' of a diffraction pattern with spots labeled with coordinates like (9, 7, 5), (9, 6, 4), (9, 5, 3), (8, 7, 5), (8, 6, 4), (8, 5, 3), (8, 4, 2), (7, 6, 4), (7, 5, 3), (7, 4, 2), (6, 7, 5), (6, 6, 4), (6, 5, 3), and (6, 4, 2). A status bar at the bottom indicates 'X = 1038, Y = 1036, I = 7, resolution = 3.6 Å'. A footer note says 'click <<integrate>> to go ahead, or click <<Retry>>'.

Never
be afraid to:
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Navigation Tree

The screenshot displays the CCP4 GUI interface. On the left, the History Tree shows a sequence of actions: limport, find_spots, index, refine_bravais_settings, reindex, refine, integrate, export, and another set of refine, reindex, and index actions. The main panel features a toolbar with icons for find, index, lattice, refine, and integrate, along with buttons for Retry, Run (DIALS), and Stop. Below the toolbar, the find_spots parameters are shown in a Simple/Advanced view, including spotfinder thresholds for dispersion gain, sigma_background, sigma_strong, and global_threshold, as well as the number of processors (mp.nproc) set to 12. A 'Reset to Default' button is also present. At the bottom left, a summary panel provides details for the Beam (X: 212.48 mm, Y: 220.0 mm, Wavelength: 0.9795 Å), Crystal (a, b, c axes), Scan (Image Range: 1-90, Oscillation: 1.0, Exposure Time: 1.0), and Detector (Distance: 190.18 mm, Gain: 1.0, Max res: 1.01 Å). The Image View window on the right shows a diffraction pattern with several spots highlighted by green boxes. The status bar at the bottom indicates the current spot coordinates: X = 1117, Y = 1042, I = 11, resolution = 4.2 Å. A footer note reads: 'click <<index>> to go ahead, or click <<Retry>>'.

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be afraid to:
navigate

Navigation Tree

The screenshot displays the CCP4 GUI interface. On the left, the History Tree shows a sequence of actions: limport, find_spots, index, refine_bravais_settings, reindex, refine, integrate, and a sub-tree for integration.mp.nproc=6. The main window features a toolbar with icons for find, index, lattice, refine, and integrate, along with buttons for Retry, Run, and Stop. Below the toolbar are configuration panels for Simple and Advanced settings, including integration.profile.fitting (True), integration.background.algorithm (glm), integration.mp.nproc (6), and mtz output name (hkl_out.mtz). The bottom left contains a summary table for Beam, Crystal, Scan, and Detector parameters. The right side shows the Image View with a grid of diffraction patterns, each labeled with Miller indices (h, k, l).

Beam		Crystal			Scan		Detector		
X (mm)	Y (mm)	a	b	c	Image Range	Distance (mm)	Number of Panels	Gain	Max res (Å)
212.62	219.89	42.36	42.36	39.71	1 90	191.77		1.0	1.01
Wavelength (Å)		α	β	γ	Oscillation				
0.9795		90.0	90.0	90.0	1.0				
		Exposure Time							
		1.0							

click << Retry >> or navigate elsewhere in the tree

Never
be afraid to:
navigate

<https://github.com/ccp4/DUI/issues>

The screenshot shows the GitHub interface for the repository `ccp4/DUI`. The browser address bar displays `https://github.com/ccp4/DUI/issues`. The repository name `ccp4 / DUI` is shown at the top, along with statistics: 14 Watchers, 2 Stars, and 3 Forks. Below the repository name, there are tabs for `Code`, `Issues 57`, `Pull requests 0`, `Wiki`, and `Insights`. A search bar contains the filter `is:issue is:open`. A `New issue` button is visible on the right. The main content area shows a list of issues with the following details:

- 57 Open** (28 Closed)
- Author, Labels, Projects, Milestones, Assignee, Sort
- #85 some data-sets are not well handled by embedded image viewer in DUI**
#85 opened 22 days ago by luisodls
- #84 handle spaces in dir names when importing**
#84 opened 22 days ago by luisodls
- #83 grey out "Open Reciprocal Lattice Viewer" prior to spot finding**
#83 opened on 11 Oct by dagewa High priority
- #82 Inconsistent naming**
#82 opened on 11 Oct by dagewa
- #81 Please add resolution limit to integrate simple tab**



Links:

- <http://dials.diamond.ac.uk/>
- <https://github.com/ccp4/DUI/issues>

Giving feedback

Github account: **ccp4brazil**

Pasword: **brazilccp4**



