Data Integration with DUI:

Dr. Luis Fuentes-Montero (Luiso)
Levels of interaction with Dials

Ease of use

xia2

DUI

Command line tools

Programmer's API

Degree of control
Levels of interaction with Dials

Ease of use

xia2

DUI

Command line tools

Programmer's API

Degree of control
What is DUI?
What is DUI?

Drive Under Influence
What is DUI?

Drive Under Influence

X
What is DUI?

Dials User Interface
What is DUI?

**Dials User Interface**
What is DUI?

Dials User Interface
DUI Running DIALS
DUI Running DIALS
DUI Running DIALS
DUI Running DIALS
DUI Running DIALS

failed to << check_gray_outs() >>
update_pbar_msg = click dials icon to run refine
found val, = True
run_clicked
.CurrentWidget(ref) = 'mini_dials_w_GUI.custom_widgets.ParamWidget object at 0x7f7f23d6b98'
cmd_tmp = ["refine", \'.refinement.parameterisation.scan_varying=True']
starting motion

[[ 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.debug_logs=/memdisk/dui_files/11_refine.debug.log
output.log=/memdisk/dui_files/11_refine.log']

<< here

path_to_log = /memdisk/dui_files/11_refine.log
DUI Running DIALS

failed to << check_gray_out() >>
update_pbar_msg = click dials icon to run refine
found val, v = True
run_clicked
...CurrentWidget(ren) = <mini_dials_w_GUI.custom_widgets.ParamWidget object at 0x7fef23d6b9b8>

cmd_tmp = ['refine', 'refinement.parameterisation.scan_varying=True']
starting motion

'cmd_lat_to_run = ['dials.refine', 'refinement.parameterisation.scan_varying=True', 'input.experiments

[[ 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_logs=memdisk/dui_files/11_refine.debug.log

bash memdisk:python2.7
DUI Running DIALS
```python
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
```
Embedded image viewer
Embedded image viewer
Embedded image viewer

Adjustable Image Palette
Embedded image viewer

Updates With Processing Steps
Embedded image viewer

Updates With Processing Steps
Embedded image viewer

Updates With Processing Steps
Embedded image viewer

Updates
With
Processing
Steps
Embedded image viewer

Updates With Processing Steps
Running Dials visualisation “commands”
Running Dials visualisation “commands”
Running Dials visualisation “commands”

Click Here
Running Dials visualisation “commands”
Running Dials visualisation “commands”

Or Click Here
Log Text
Log Text

Processing Commands

Shows output of processing commands.

CCP4
diamond
DIALS
HTML report view
HTML report view runs: dials.report automatically
HTML report view

runs:

dials.report

automatically
HTML report view

runs:
dials.report
automatically
HTML report view

runs:
dials.report
automatically
HTML report view

A case where something went terribly wrong
Navigation Tree

Never be afraid to:

navigate
Never be afraid to: navigate
Navigation Tree

Never be afraid to:
navigate
Navigation Tree

Never be afraid to:

navigate
https://github.com/ccp4/DUI/issues
Links:
- http://dials.diamond.ac.uk/
- https://github.com/ccp4/DUI/issues

Giving feedback

Github account: ccp4brazil
Password: brazilccp4