# DUI2 and the Evolution Toward XUI: Enhancing Crystallographic Data Processing

DUI2 has long served as a valuable interface for users across the experience spectrum—from introducing young crystallographers to the basics of data processing, to offering advanced control for expert users. However, recent advancements in experimental techniques and the evolution of the DIALS suite and its pipelines have significantly changed how users interact with these tools, prompting a need for a new generation of graphical interfaces.

## Current Strengths of DUI2

DUI2’s two primary strengths are:  
- Image Viewer: This overlays the results of spot finding, indexing, and integration directly onto the experimental images. It provides essential visual feedback for decision-making up to the integration stage.  
- Control Tree/Graph: This allows users to explore and compare different processing paths. When multiple experiments are conducted on the same crystal, it enables merging these paths into a unified workflow.

However, after the integration step, the image viewer becomes less relevant, as subsequent steps rely solely on integrated intensities. At this point, analyzing reports generated by DIALS commands becomes more informative than visual inspection.

## Limitations and the Need for a New Interface

While DUI2 has been adapted to run some of the programs invoked by pipelines like xia2.multiplex, its legacy design limits further development. The increasing reliance on automated pipelines has also reduced DUI2’s usage.

To address these limitations, a new GUI—tentatively referred to as XUI—is being developed. This interface is designed to support modern workflows and provide more intuitive control over complex pipelines.

## User Interaction Flow in XUI

Here is a typical user interaction with the new software, in chronological order:

1. Directory Selection: The user selects the directory containing the diffraction images.

2. Integration Launch: The user initiates xia2.integrate, and XUI creates a corresponding node in the processing tree.

3. Result Inspection: After integration, XUI presents two inspection modes:

- Tab 1: A text-based table showing numerical results and icons for each sweep (one row per sweep).

- Tab 2: Graphical plots showing spots per image (one graph per sweep), arranged in a grid layout.

4. Decision Point: The user decides whether to:

- Edit and re-run integration:

- Modify parameters and re-launch xia2.integrate, or

- Open the legacy DUI2 interface, preloaded with a tree that replicates the xia2.integrate execution.

- Proceed to Multiplexing: If satisfied, the user continues to the next step.

5. Node Structure: Based on the user’s choice, the next node in the tree becomes either a sibling or a child of the previous node.

6. Multiplexing: XUI runs xia2.multiplex and displays a dendrogram representing the relationships between datasets.

7. Interactive Refinement: The user can peek into branches of the dendrogram and selectively re-run xia2.multiplex to refine the results.

## Design Philosophy of the New GUI

Unlike DUI2, which emphasizes image visualization, XUI focuses on processing statistics, completeness, and data quality across all crystals. Users will be able to:  
- Eliminate entire experiments or specific sweeps from further processing.  
- Control execution by selecting or excluding datasets based on metrics such as completeness, missing wedges, or incorrect space groups.

This approach retains the tree-based control philosophy of DUI2 but introduces modern tools for dataset management and decision-making.

## Legacy Support and Modular Tools

- DUI2 will remain available for users who prefer its interface or require its image viewer.  
- The image viewer will be modularized into a standalone tool, capable of opening diffraction images independently of any DIALS processing.  
- The new GUI will be compatible with steps previously executed by xia2.integrate, xia2.ssx, or xia2.multiplex, ensuring seamless integration between legacy and modern workflows.