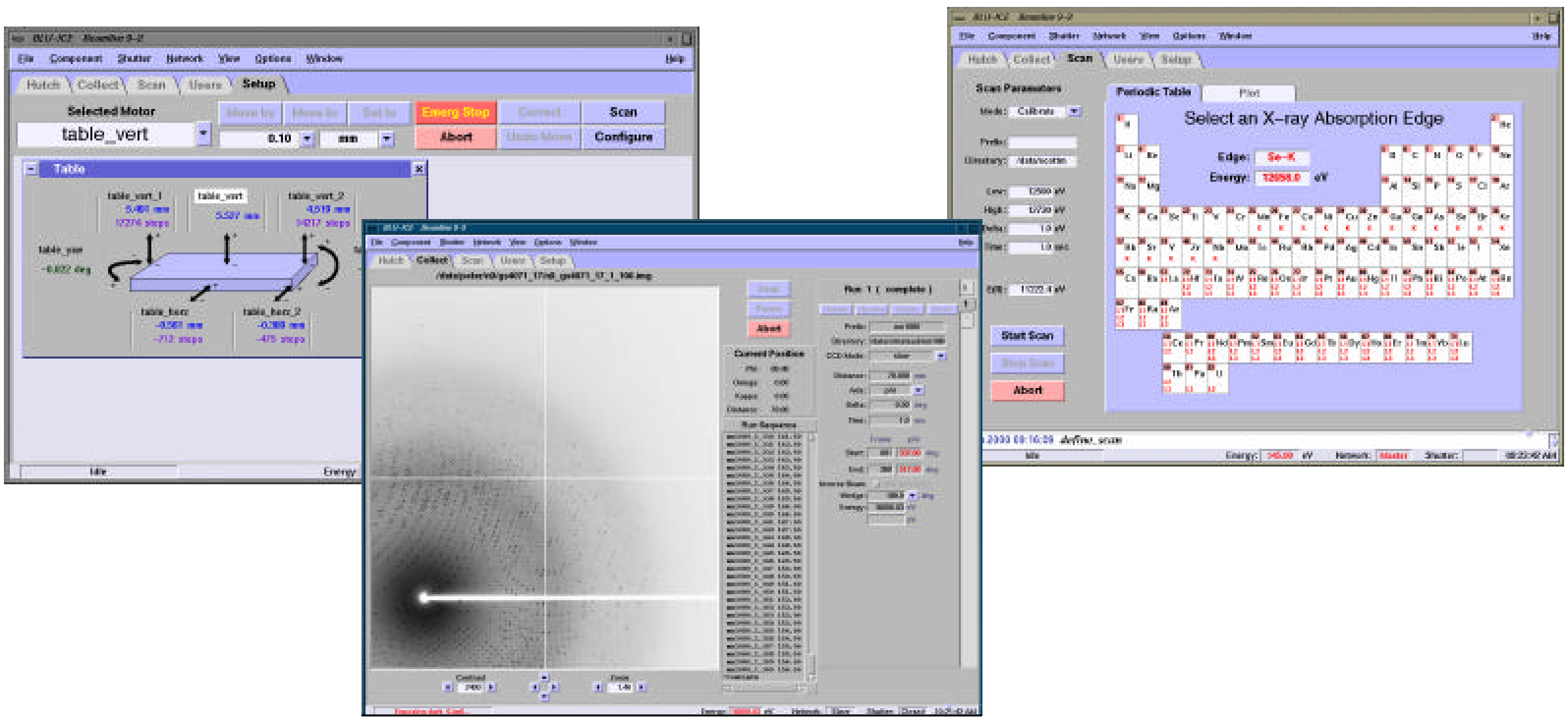
Structural Molecular Biology

Software Development Workshop

September 18th, 2000

Collaborative Data Collection with BLU-ICE



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Overview

Architecture of the Distibuted Control System

- Life cycle of a DCS message.
- Collaboration features.

Hybrid Software Development Strategy

- XOS library for platform-independent C/C++ code.
- Tcl/Tk for platform independent GUI development.

Users’ Favorite Features in BLU-ICE

- GUI focuses on the experiment.
- Simple data collection set up for advanced MAD experiments.

Scripted Devices

- All operations may be scripted in BLU-ICE.
- Same scripts may be run within the DCS server.
- Supports virtual motors with parent-child relationships.

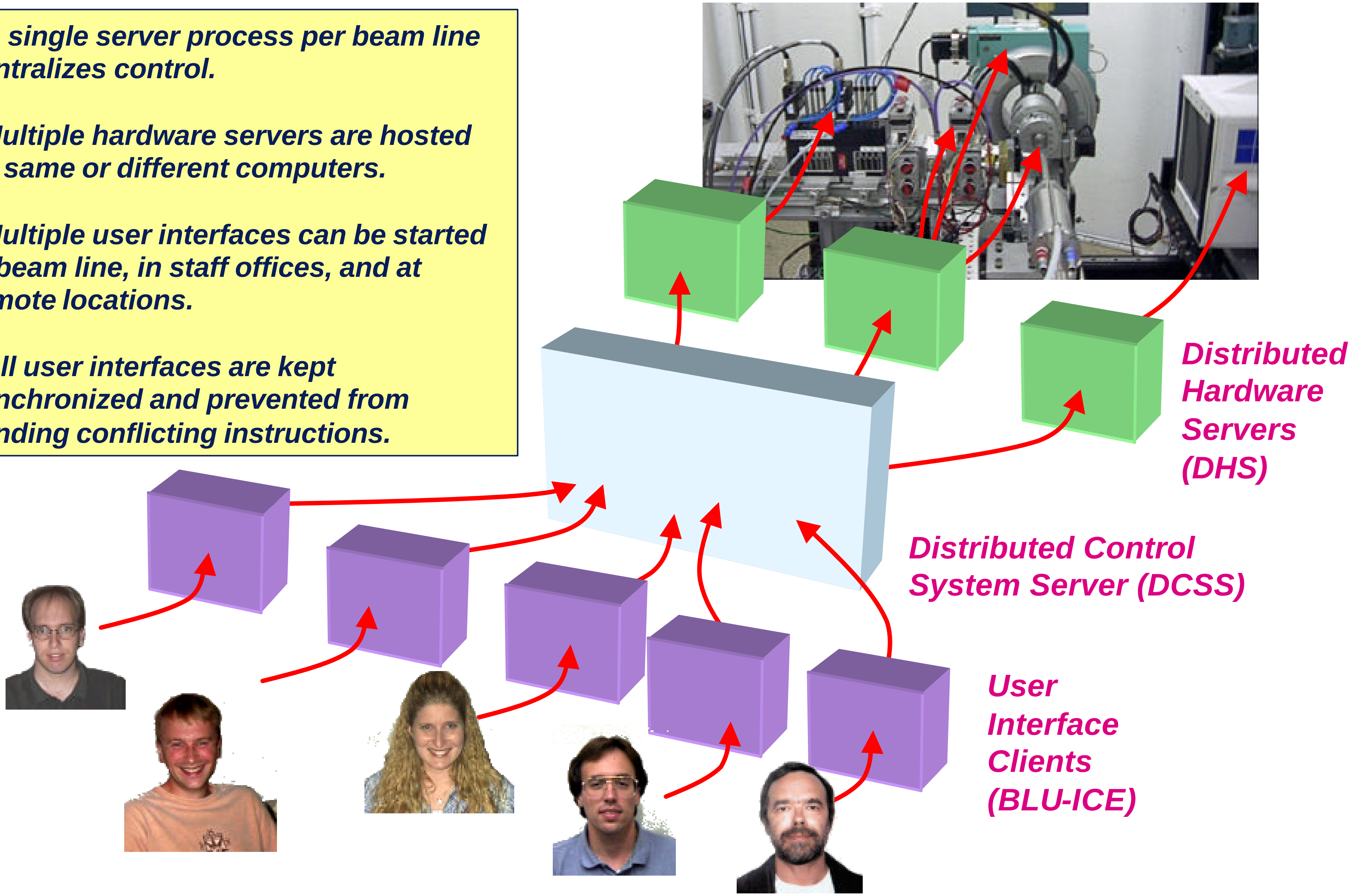
Architecture of the Distributed Control System

- *A single server process per beam line centralizes control.*

- *Multiple hardware servers are hosted on same or different computers.*

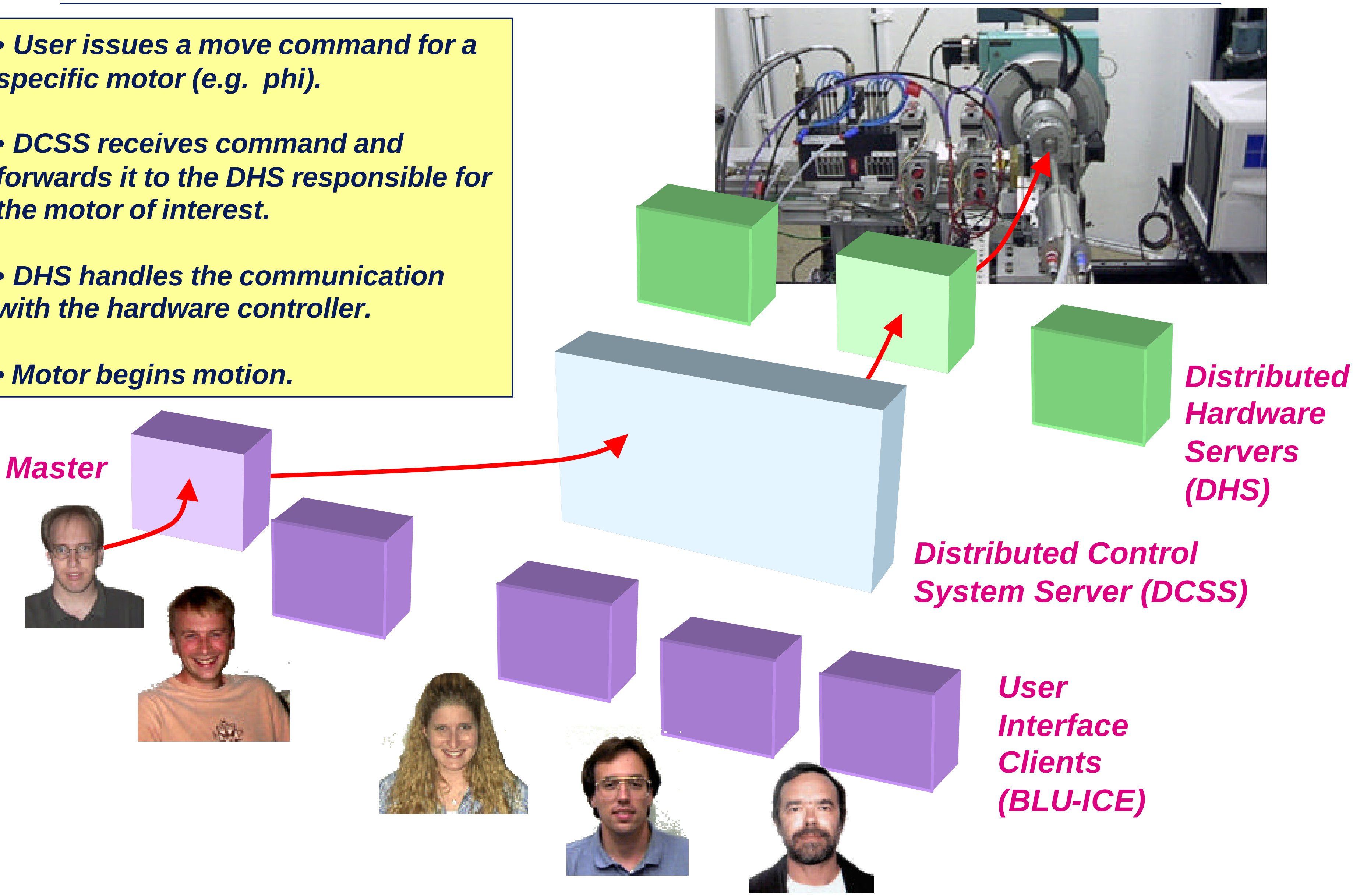
- *Multiple user interfaces can be started at beam line, in staff offices, and at remote locations.*

- *All user interfaces are kept synchronized and prevented from sending conflicting instructions.*



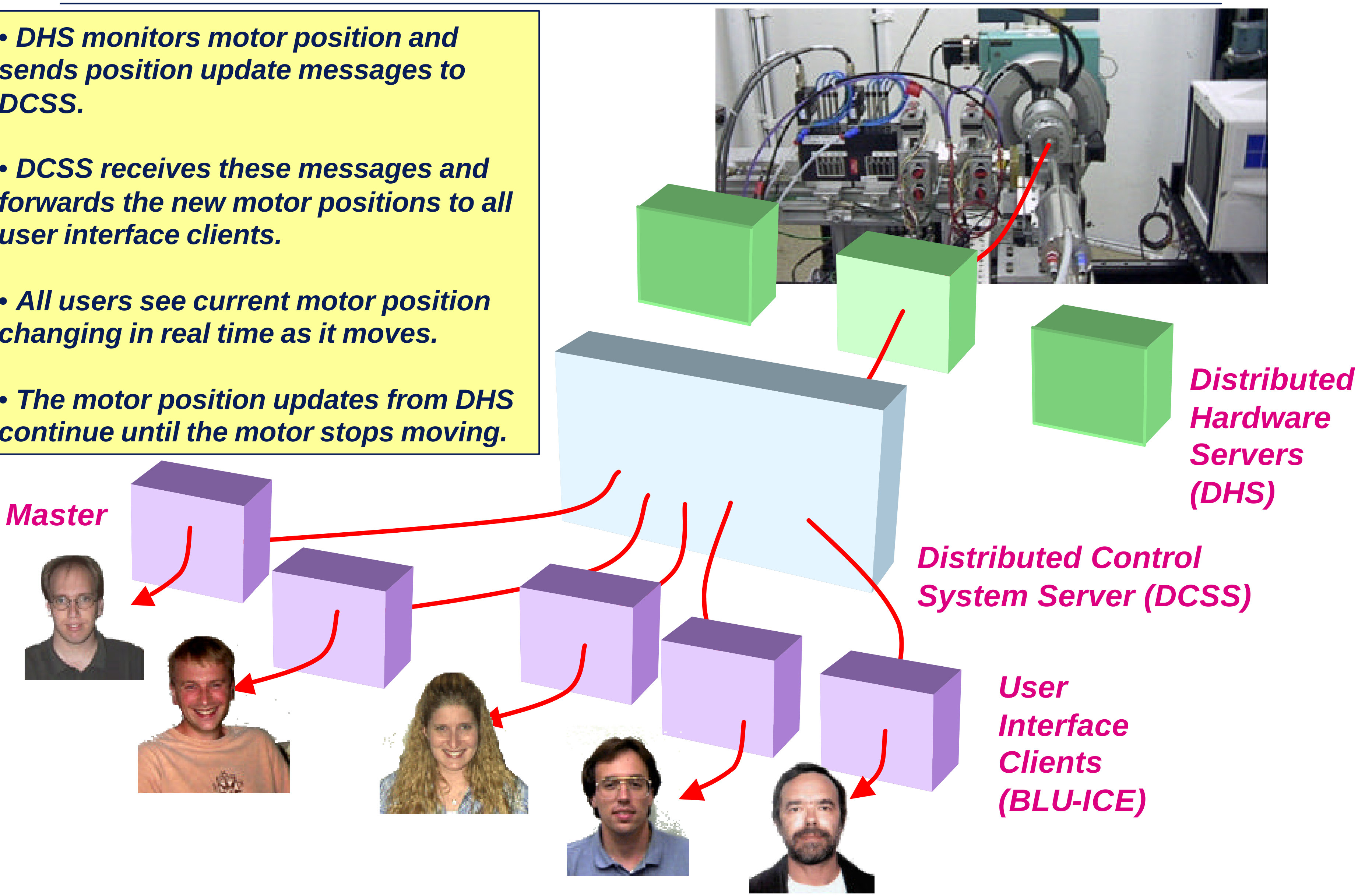
Life Cycle of a Motor Control Command

- *User issues a move command for a specific motor (e.g. phi).*
- *DCSS receives command and forwards it to the DHS responsible for the motor of interest.*
- *DHS handles the communication with the hardware controller.*
- *Motor begins motion.*

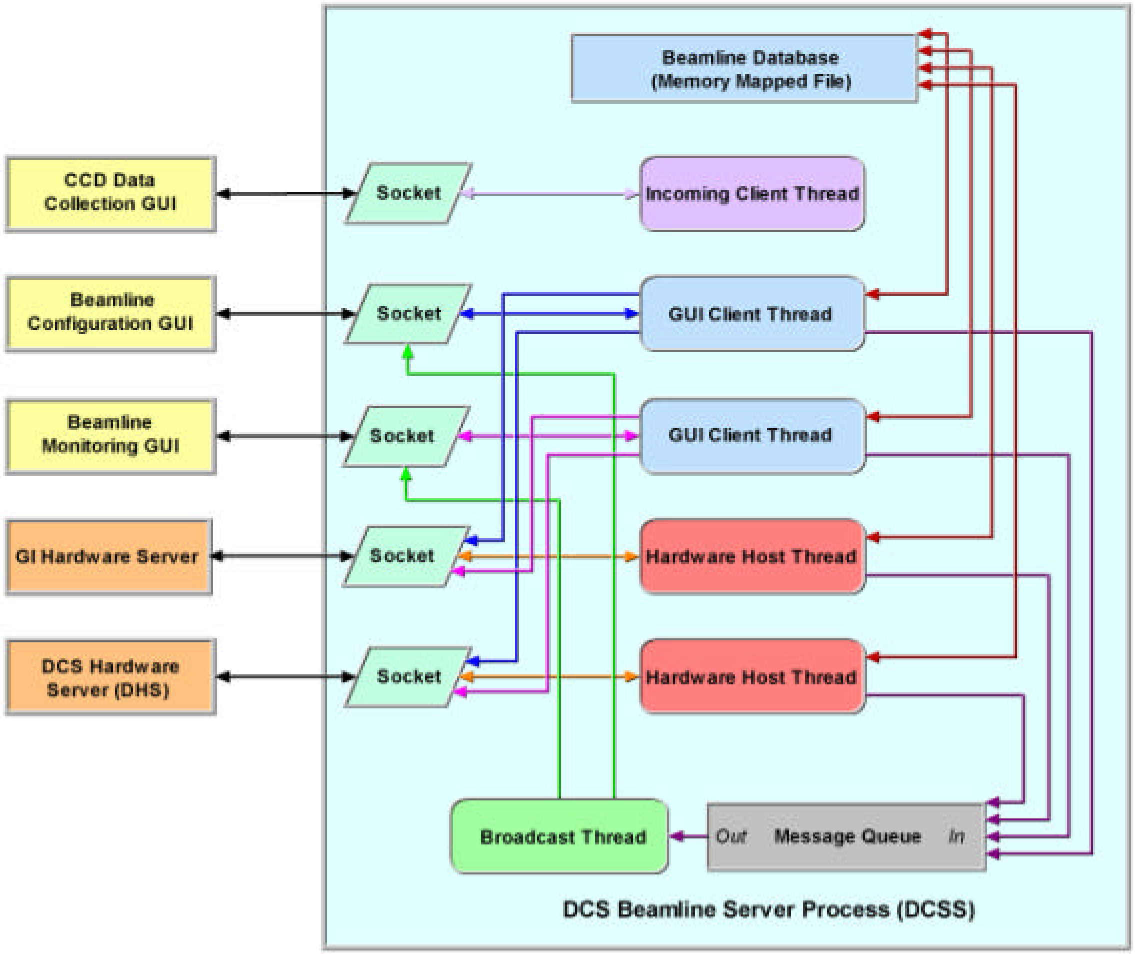


Response to Control Command

- *DHS monitors motor position and sends position update messages to DCSS.*
- *DCSS receives these messages and forwards the new motor positions to all user interface clients.*
- *All users see current motor position changing in real time as it moves.*
- *The motor position updates from DHS continue until the motor stops moving.*



Portability of High Performance C/C++ Server Processes Based on Cross-Operating System (XOS) Library



Supports multithreaded, distributed programs

- Much simplified TCP socket object for rapid network application development.
- Thread creation and synchronization with mutexes and semaphores.
- Memory mapped files.
- Interthread communication.

Portability

- Compile code on Digital Unix, IRIX, OpenVMS, 32-bit Windows.
- Easy to port to new platforms similar to any of the above.

Compile-time approach

- Header file xos.h loads appropriate, system-dependent include files
- Native system calls on each platform for maximum performance
- No runtime overhead for platform independence

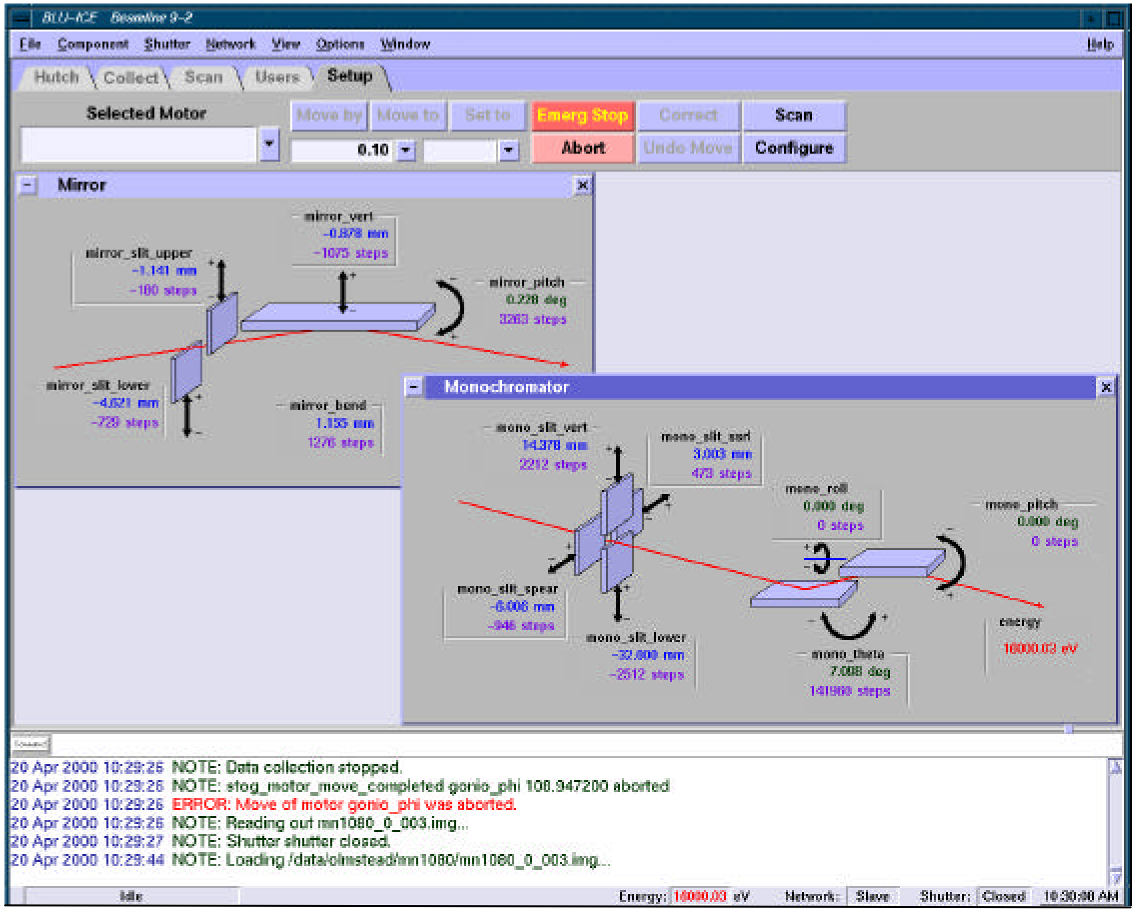
Reliability

- Simpler APIs for more reliable code.
- Less need to study different platforms.

New C++ version under development

- Object oriented, STL based, with error handling via C++ exceptions.
- Cross-platform user authentication and permissions-based file I/O.
- Generalized communication streams for uniform network communication, interthread messaging and file I/O with transparent encryption, compression, etc.
- Cross-platform, cross-vendor, database interface.

Tcl/Tk Features Are Key to the Development of BLU-ICE



Platform Independent

- Tcl/Tk runs on any Unix, VMS, Mac, and 32-bit Windows computer.
- Scripts can also be bundled with Tcl/Tk binaries.

Rapid Development

- Required only a fraction of the code necessary if written in C, C++, or Java.
- Easy maintenance critical at the beam lines.

Object Orientation

- The [Incr Tcl] extension to Tcl provides object-oriention.
- Migration to [Incr Tcl] is simplifying the BLU-ICE code.

Active Canvas

- Binding of events to canvas objects facilitates highly graphical, very interactive user interfaces.

Event based concurrency

- Much simpler than multithreading models for GUI development.

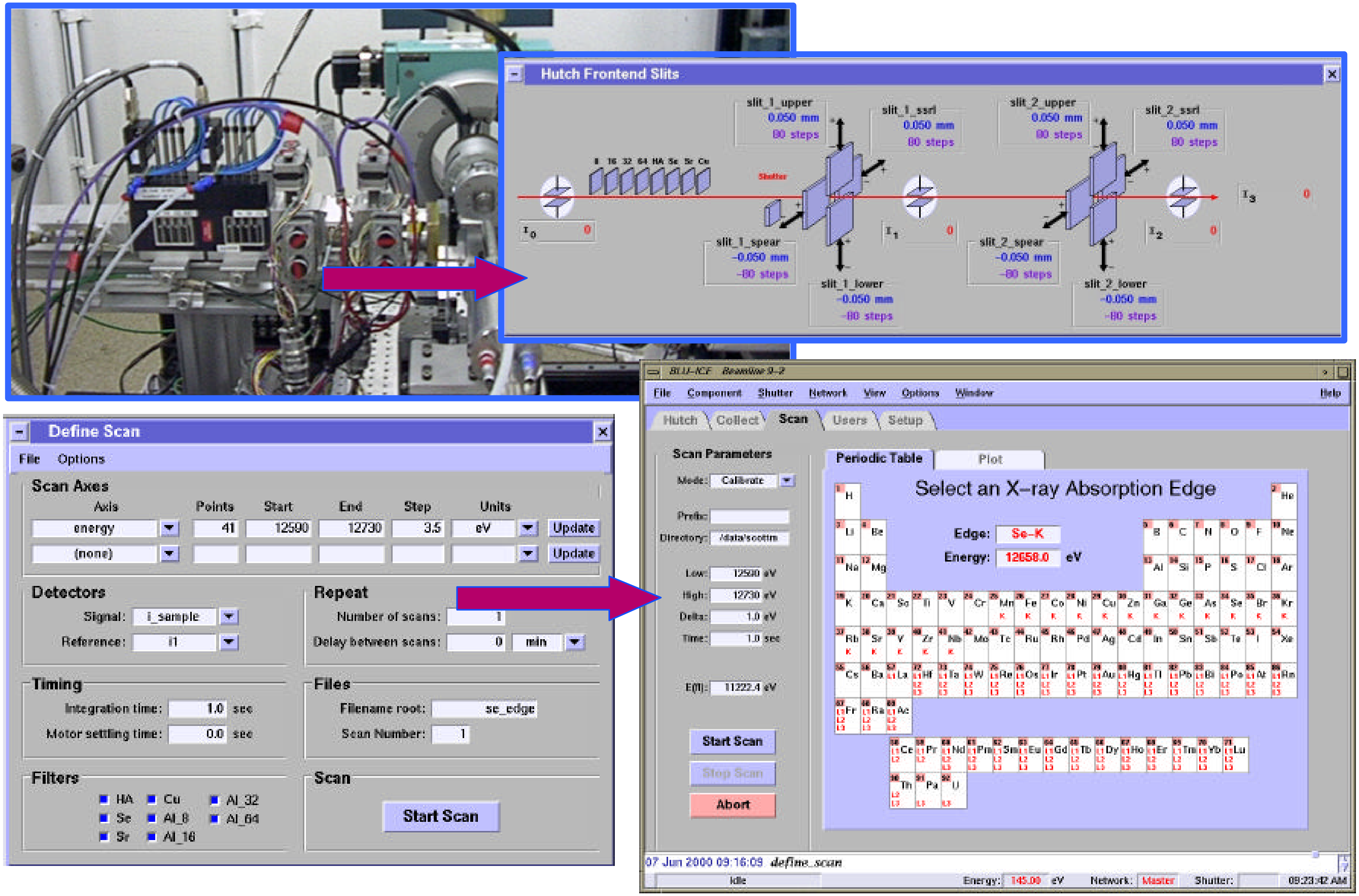
Command Prompt with Scripting

- Command prompt and a full featured programming language for scripting.
- User can script any operation in BLU-ICE using control structures, variables, procedures, file I/O, even classes.

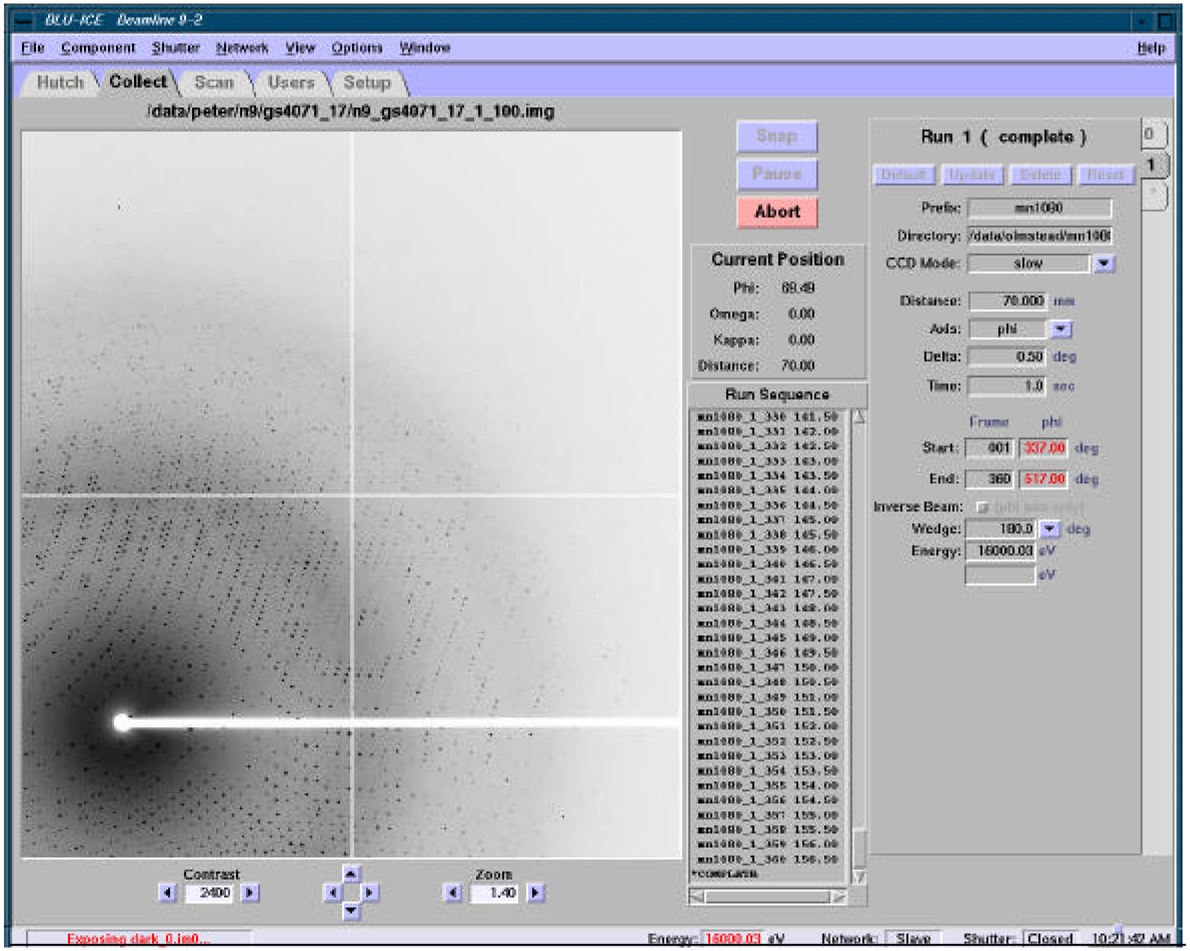
Extensible in C/C++

- Tcl was designed to be extended readily in C. Extensions can be loaded dynamically.
- High performance code, multiple threads and so on are best implemented in extensions.

Extending the GUI Building Philosophy to Support Users



Collaborative Data Collection Control with BLU-ICE



Intuitive MAD Data Collection

- Multiple runs can be defined and started together.
- Supports multiple energies, inverse beam, and wedges.

Run Sequence Preview

- Lists details of data frames to be collected for each run.
- Changes as data collection parameters are edited.

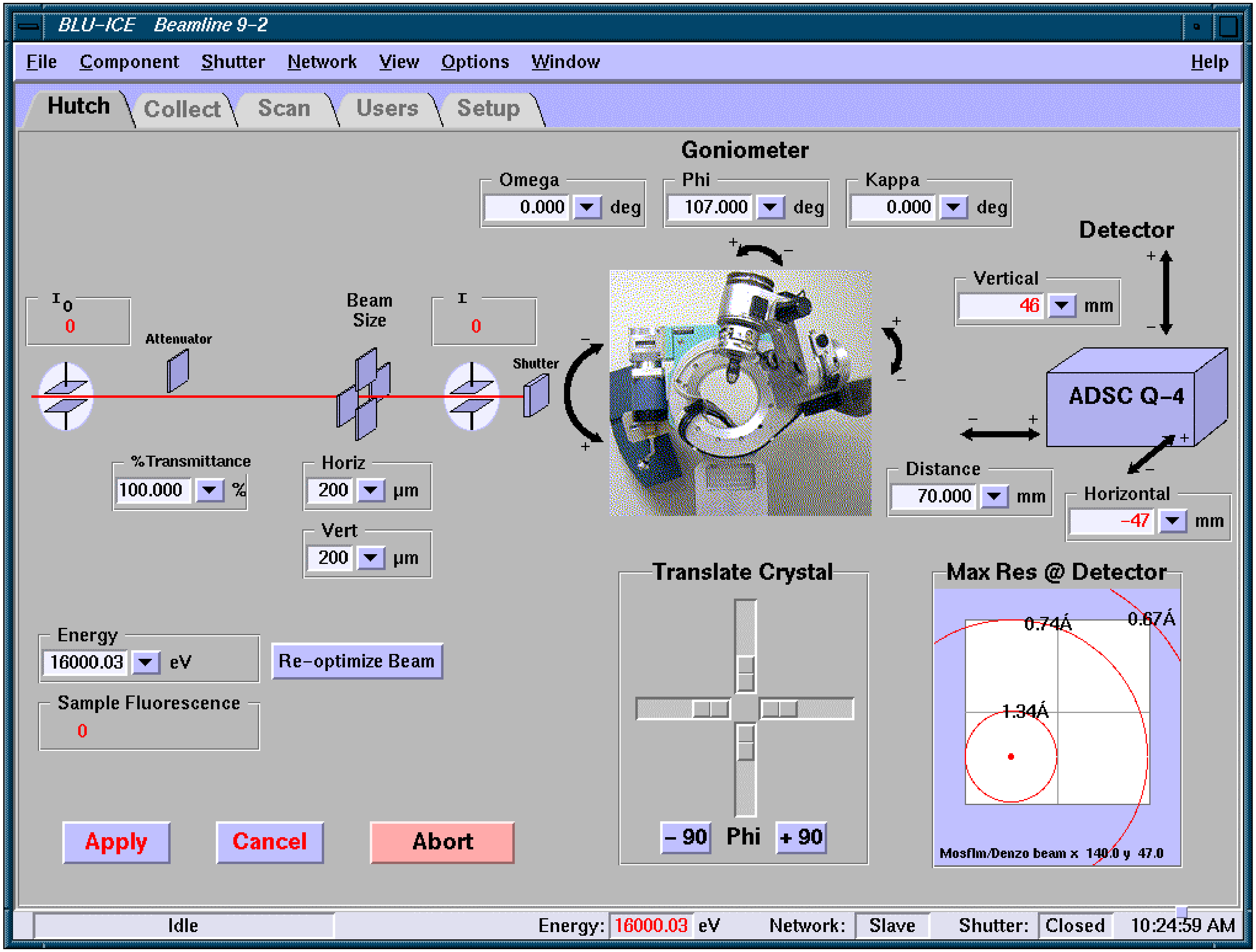
Robust Pause/Restart Capability

- Data collection may be paused at any time.
- Next frame to collect may be selected in sequence window.

Supports Multiple Instances

- Multiple instances of BLU-ICE may monitor data collection.
- All instances show run definitions being edited.
- New diffraction images are displayed on all instances.
- Data collection continues even if all BLU-ICE instances exit.

BLU-ICE Experimental Setup Window



Example Scripted Device: TABLE_VERT

```
proc table_vert_move { new_table_vert } {

   # import device variables
   variable table_pitch

   # move the two motors
   move  table_vert_1  to  [ table_vert_1_calculate $new_table_vert $table_pitch ]
   move  table_vert_2  to  [ table_vert_2_calculate $new_table_vert $table_pitch ]

   # wait for the moves to complete
   wait_for_devices  table_vert_1  table_vert_2
}


proc table_vert_1_calculate { tv tp } {

   # import device variables
   variable table_pivot
   variable table_v1_z
   variable table_pivot_z

   # calculate position of table_vert_1 given vertical height and pitch
   return [ expr  $tv + ( $table_v1_z - $table_pivot_z ) * tan ( [ rad $tp ] )  ]
}
```

DCSS Scripting Engine: Server-side Motion Control Scripting

Scripting capability of BLU-ICE embedded in DCSS

- [Incr Tcl] interpreter executes as one thread within DCSS.
- Interpreter runs the non-GUI portions of BLU-ICE.
- Scripting Engine can run any scripts developed within BLU-ICE.

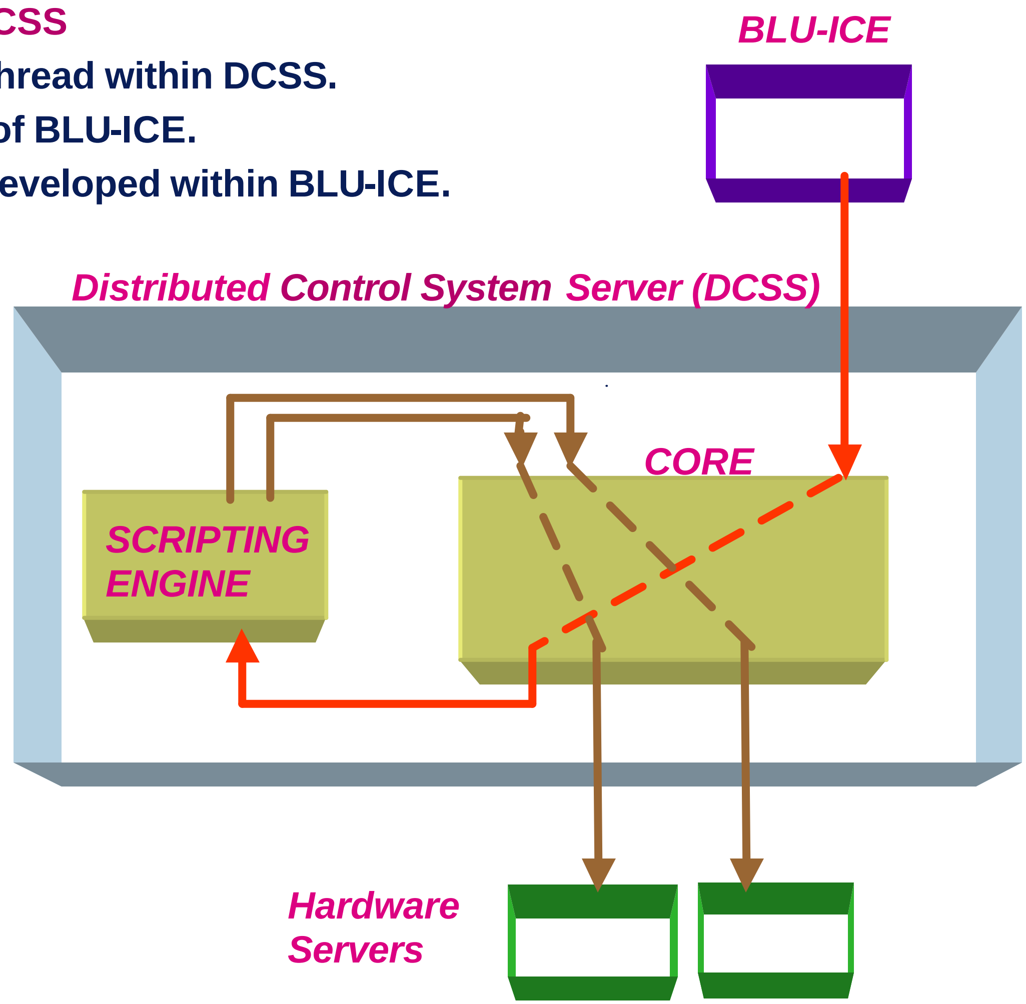
Scripting Engine connects to DCSS core twice

- Once as a Hardware Server serving "Scripted Devices."
- Once as a "User Interface Client."

Scripted device command routing

- Request for a move of a scripted device is routed to the Scripting Engine hardware server interface.
- Scripting Engine runs a script that issues move requests for the child motors.

Children motors may also be scripted devices with their own children!



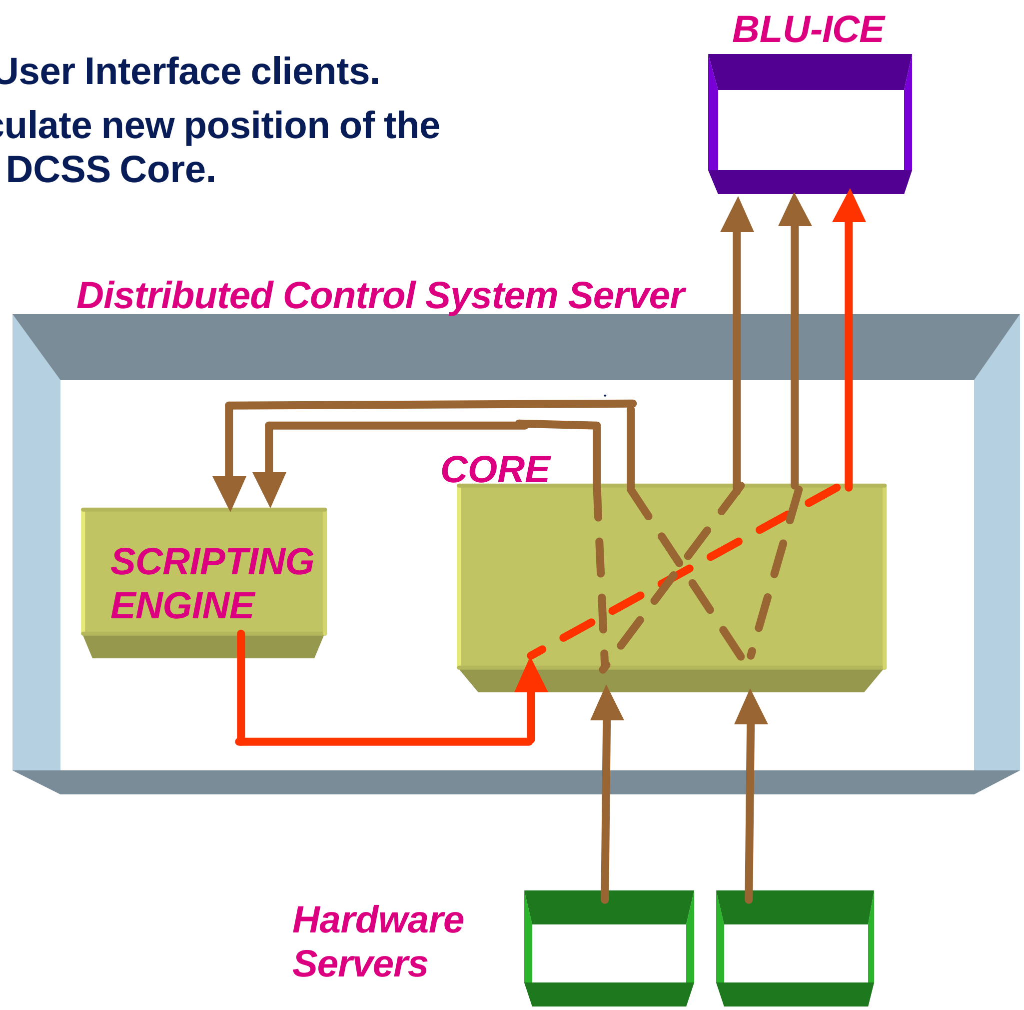
Scripted Devices: Path of a Response Message

Response messages flow backwards.

- Real-motor position updates go to all User Interface clients.
- Scripting Engine runs scripts that calculate new position of the Scripted Device and sends updates to DCSS Core.
- DCSS Core forwards the updated Scripted Device positions to all User Interface client.
- BLU-ICE gets a continuous stream of updated positions for both real motors and scripted devices.
- System works recursively, handling nested Scripted Devices.

Possible Uses for Scripted Devices Unlimited

- Sophisticated device control with many intermediate states.
- Complex limit checking for collision avoidance.
- New data collection schemes.



Acknowledgements

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