Transition of GM/CA-CAT data acquisition software from BluIce to JBluIce

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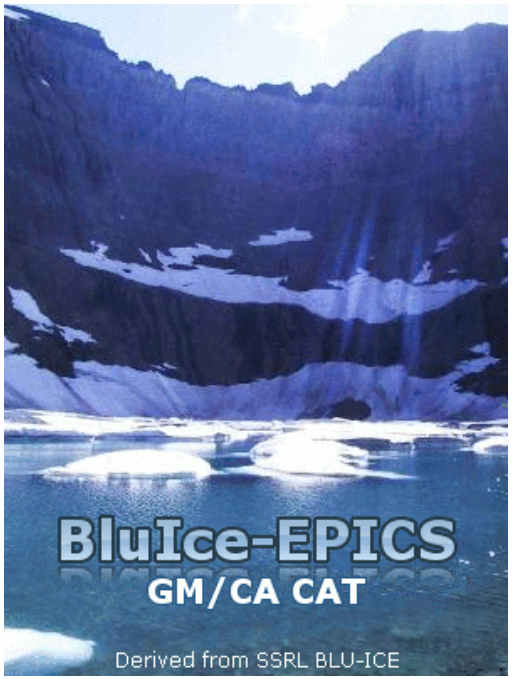
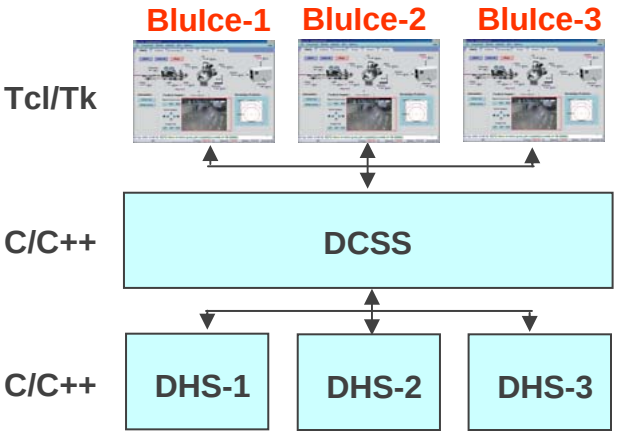


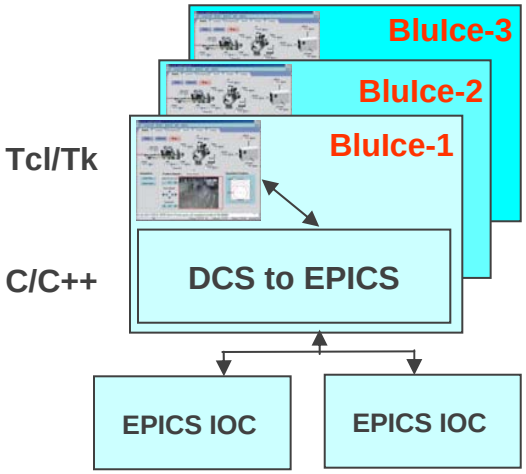
Control Software Requirements

- GM/CA is a macromolecular crystallography beamline
- Our users require:
  - Familiar interface
    - Crystallographers are highly mobile
    - Need to use software at different beamlines with little training
  - Rapid, reliable feature development
    - Crystallographers have many choices of beamlines
    - Advances from other beamlines must be incorporated quickly
    - New features must be released quickly before others do – yet must be high quality

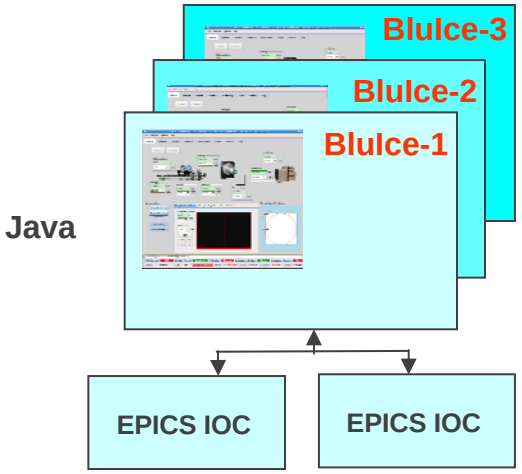
History of JBluIce



BluIce Architecture (SSRL)



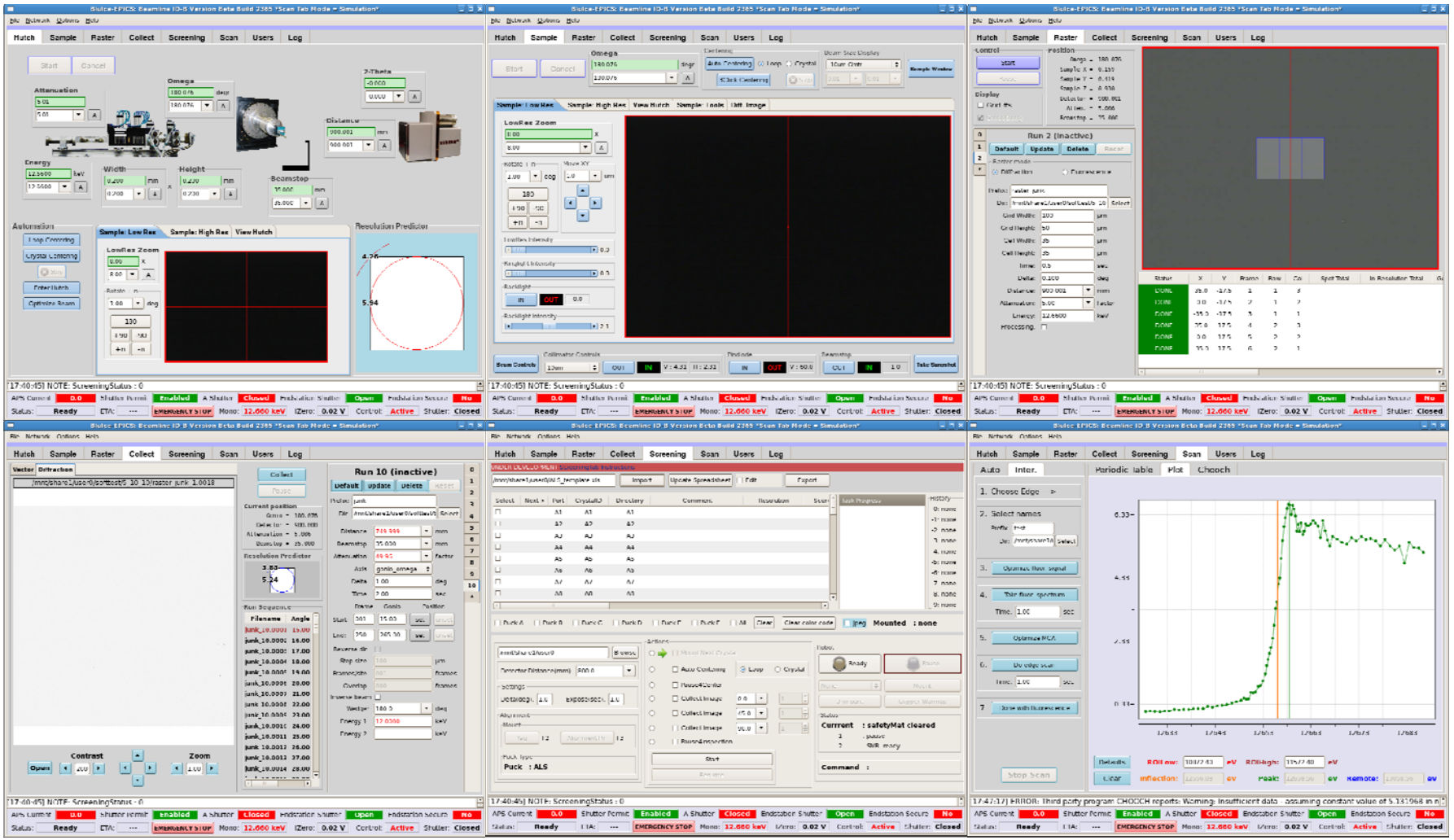
BluIce-EPICS Architecture



JBluIce architecture

- SSRL BluIce: 1997
- GM/CA replaced SSRL BluIce backend: 2003-2005
- GM/CA developed JBluIce: 2008-2010

JBluIce-EPICS: 100% Java in June 2010



What changed from BluIce to JBluIce?

- **Multiple languages -> single language**
- C++ -> Java
- Architecture changes
- Features

Single language: Advantages

- Easier debugging
  - Full stack trace is always available
  - Step-through debugging always works
- Higher reliability
  - Thanks to easier debugging and JVM protection from memory errors
- Faster development
  - No protocol layer means changes are much easier

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Java: JVM prevents memory errors

- Java removes uncertainty about memory corruption
  - Tools like valgrind and electric fence, and classes like checked pointers, are not required
- Tracking down the sources of crashes was a major issue in 2007-2008

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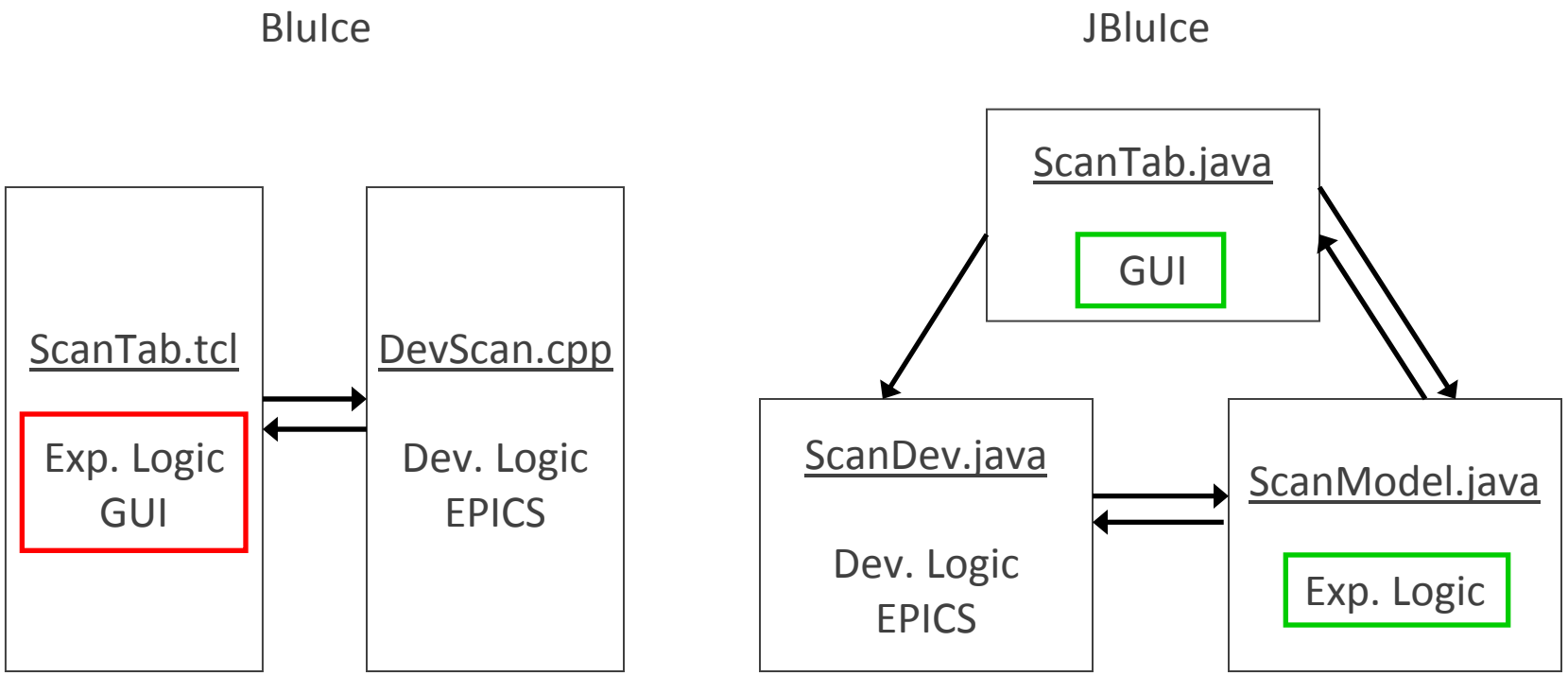
Architecture: Thread-based actions

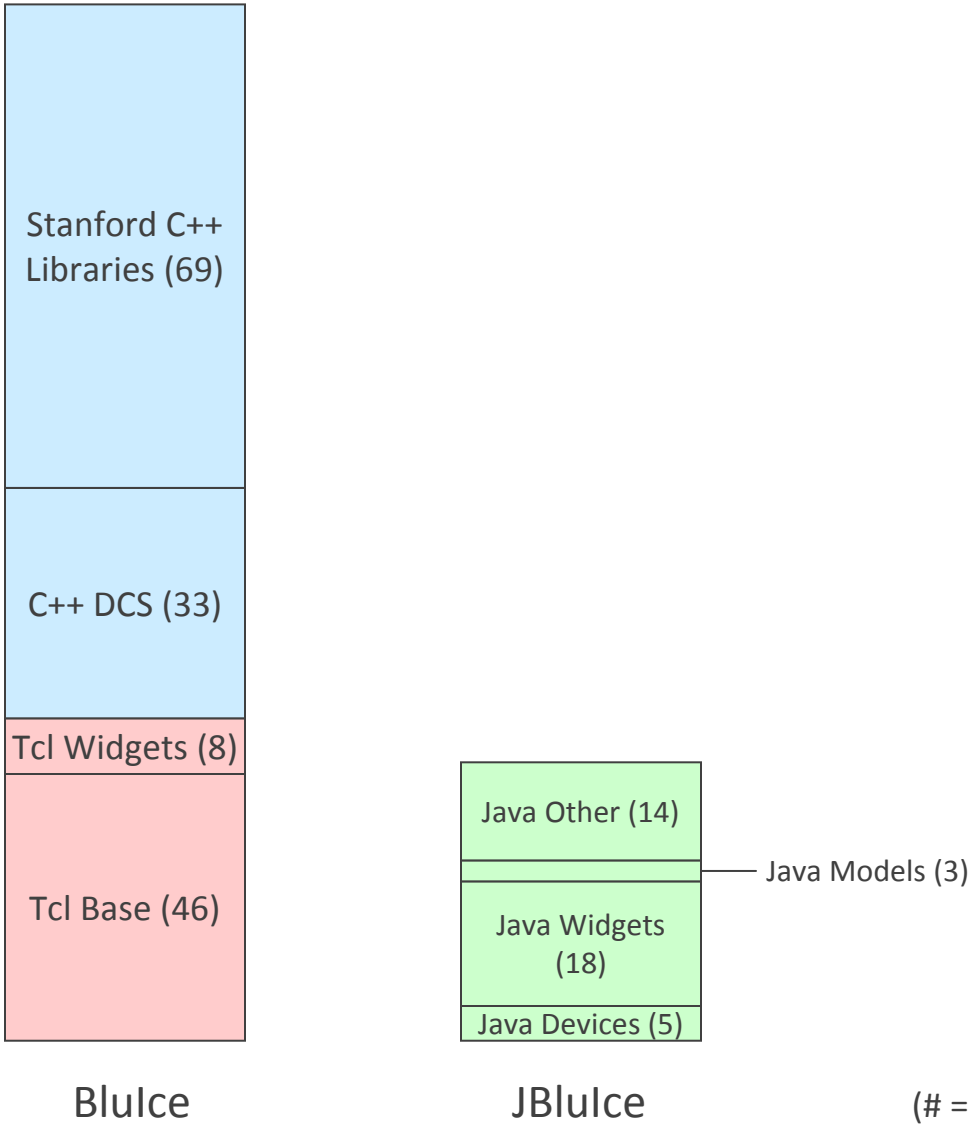
- BluIce-EPICS had some threaded commands, but now all are converted
- Single 1-2 page methods tell the whole story of an action
  - In a thread, the line number tells you a lot about what's happening
  - In a callback-based class, which timers are running, and which callback will be called next?
- Perl scripts are written this way, so porting methods (and keeping in sync) is straightforward

Architecture: Separation of logic, GUI & devices



- SSRL BluIce mixes logic in GUI widgets
- JBluIce usually makes one-line calls to model objects
- Only devices talk to EPICS (except for temporary calls)

Architecture: 3x LOC reduction



- JBluIce has more (relevant) functionality in less LOC than just the BluIce front-end
- Java libraries largely replace Stanford libraries
  - Sockets
  - HTTP
  - Math
- Simplification
  - Replaced sockets with simple HTTP
  - DCS abstraction layer

What changed from BluIce to JBluIce?

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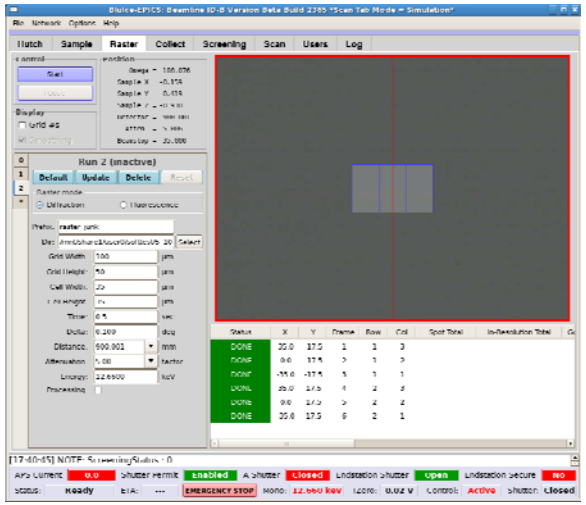
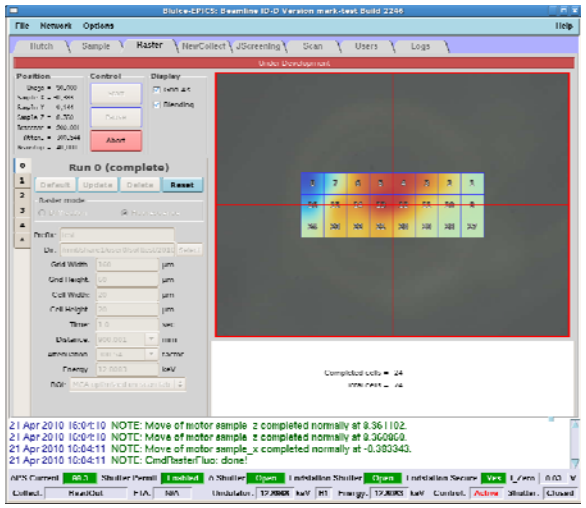
- **Features**

Features: Raster

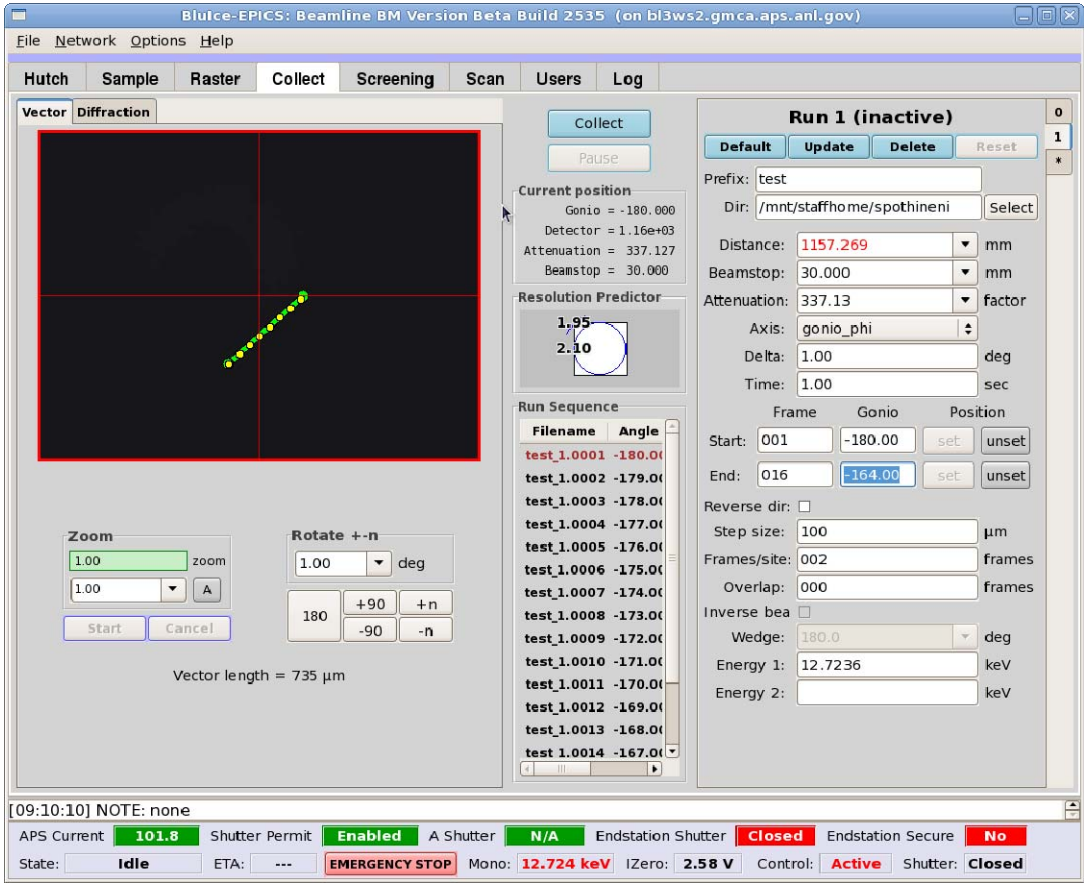




- 2008-2: Initial release
- 2009-2: Fl. raster
- 2010-1: Multiple run tabs
- Two uses
  - Find invisible crystals
  - Find the best diffracting areas of large crystals
- Diffraction vs. fluorescence
  - Diffraction is always relevant
  - Fluorescence is 4x faster and causes less radiation damage

Features: Vector collect

- Data collection along an arbitrary 3D vector
  - To define, center endpoints and click “set”
- Uses
  - Collect along rod-shaped crystals
  - Raster crystals that don’t fit the rigid raster tab grid
- Visualization over live video
- Parameters for:
  - Frames per site
  - Site spacing
  - Overlap



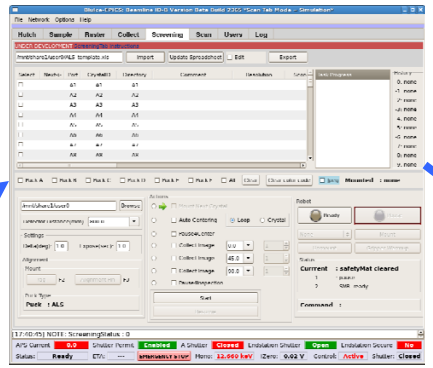
Features: Integrated motion tracking

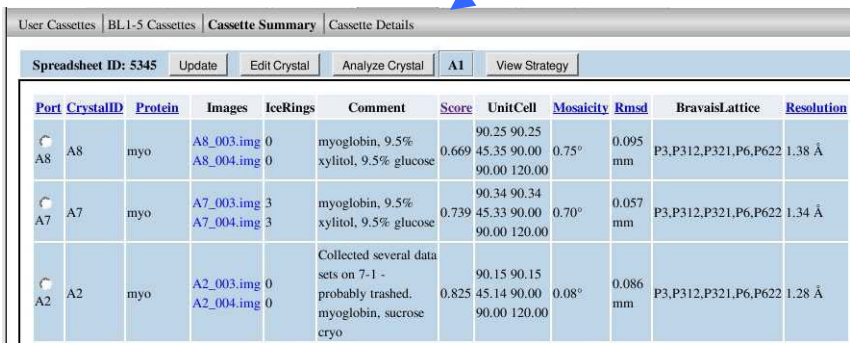
Tracking output

```
[14.530] estimateMoveTime(): motionTime=2.1s accelTime=200.00s accelCurve=100.00s ...
[14.531] elap.=  0.0s  inPos=1 runPrg=0 actPos=-0.0000 ...
[14.633] elap.=  0.1s  inPos=1 runPrg=0 actPos=0.0281  ...
...
[15.959] elap.=  1.4s  inPos=0 runPrg=1 actPos=87.2386 ...
[16.061] elap.=  1.5s  inPos=0 runPrg=1 actPos=89.9528 ...
[16.163] elap.=  1.6s  inPos=0 runPrg=0 actPos=89.9997 ...
[16.265] elap.=  1.7s  inPos=1 runPrg=0 actPos=89.9998 ...
[16.367] elap.=  1.8s  inPos=1 runPrg=0 actPos=89.9998 ...
[16.469] elap.=  1.9s  inPos=1 runPrg=0 actPos=89.9998 ...
[16.478] Tracking ended. Real in-motion time for motor gonio_omega was 1.9s (92.3% of est.)
[16.478] Motor gonio_omega, no errors detected.
```

- Tracking guarantees motors are in position, and handles errors and timeouts
- In Tcl/C++, tracking was added in the background
  - DCS protocol didn't support tracking
  - Tracking was done in the background but could be ignored
- In Java, tracking determines when a move finishes
  - Moves always complete, by timeout if necessary
  - Move results are more informative because they incorporate tracking

Features: Editable spreadsheet and WebIce integration

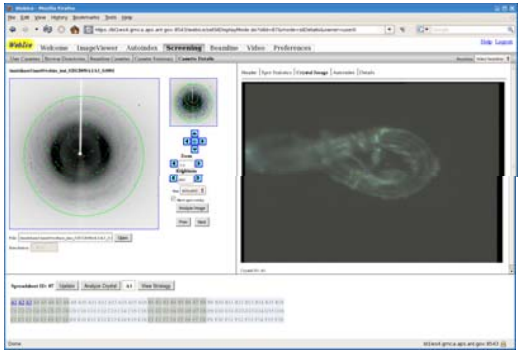




User Cassettes | BL1-5 Cassettes | **Cassette Summary** | Cassette Details

Spreadsheet ID: 5345 Update | Edit Crystal | Analyze Crystal | A1 | View Strategy

Port	CrystalID	Protein	Images	IceRings	Comment	Score	UnitCell	Mosaicity	Rmsd	BravaisLattice	Resolution
A8	A8	myo	A8_003.img A8_004.img	0 0	myoglobin, 9.5% xylitol, 9.5% glucose	0.669	90.25 90.25 45.35 90.00 90.00 120.00	0.75°	0.095 mm	P3,P312,P321,P6,P622	1.38 Å
A7	A7	myo	A7_003.img A7_004.img	3 3	myoglobin, 9.5% xylitol, 9.5% glucose	0.739	90.34 90.34 45.33 90.00 90.00 120.00	0.70°	0.057 mm	P3,P312,P321,P6,P622	1.34 Å
A2	A2	myo	A2_003.img A2_004.img	0 0	Collected several data sets on 7-1 - probably trashed. myoglobin, sucrose cryo	0.825	90.15 90.15 45.14 90.00 90.00 120.00	0.08°	0.086 mm	P3,P312,P321,P6,P622	1.28 Å



- New features built in to the initial converted screening tab:
  - Spreadsheet can be edited and saved without using OpenOffice or Excel
  - Screening results are sent automatically to WebIce
- 2010-1: WebIce scores can be loaded back in to BluIce

Features: 5x startup time reduction

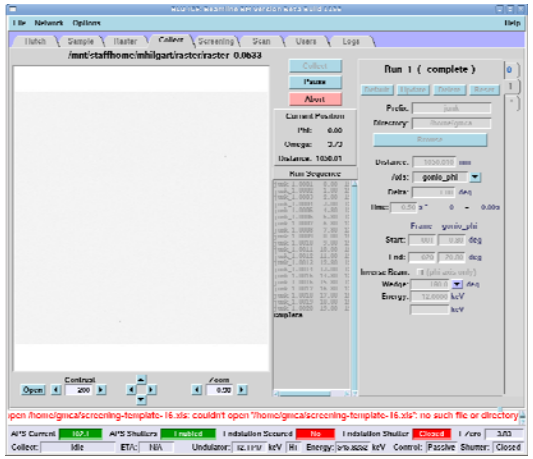
BluIce: 16 seconds

JBluIce: 2.8 seconds

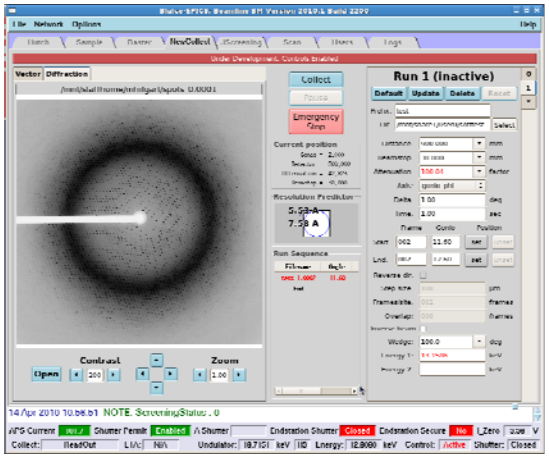
- Tests were performed on the same computer
- Improvement due mostly to connecting PVs in parallel at startup
  - PV requests are sent at once
  - Callbacks are sent as PVs connect

Tcl/Java integration

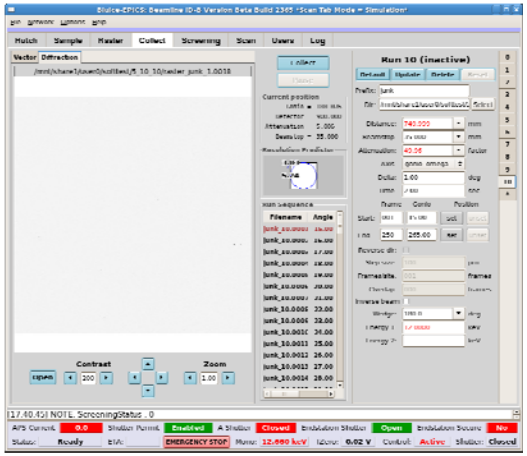
100% Tcl: 2008-1



During conversion



100% Java: 2010-2



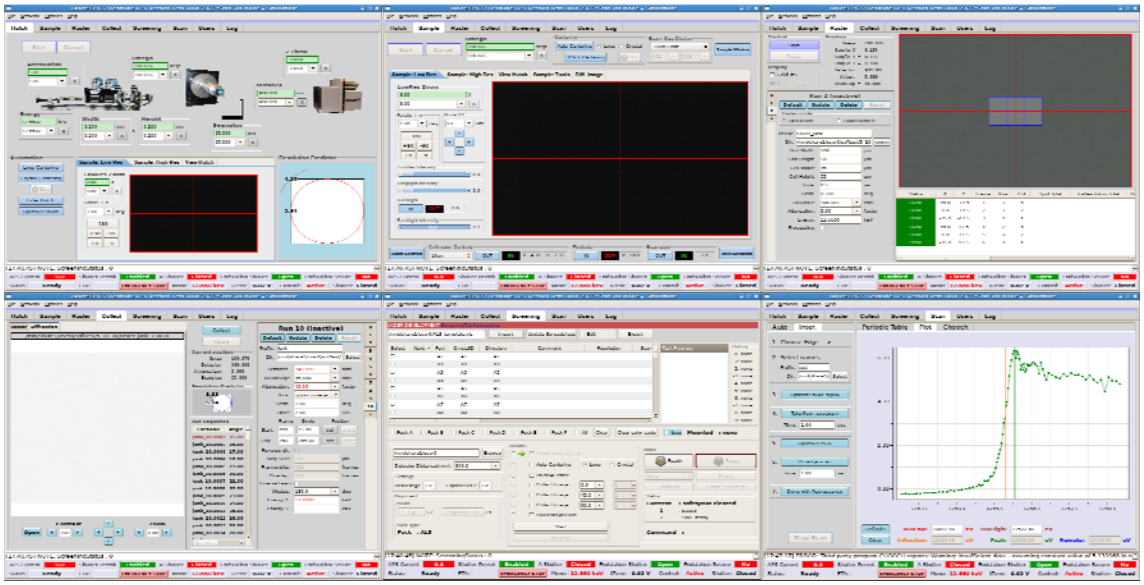
- Raster was an initial test
- 1-3 tabs were converted per run
- TkXext embedded Java windows in Tcl
- Named pipes were used for sending commands between processes

Release

- 2.5 years of development
  - Raster: 2008-2
  - Fl. raster: 2009-2
  - Screening: 2009-3
  - Collect: 2010-1
  - Hutch, Sample, Scan: 2010-2
- Testing
  - Fully functional 4 weeks before users
  - Change cutoff 2 weeks before users
  - Crystallographers tested daily for the last 4 weeks
- Smooth release so far
  - No serious bugs found in 1.5 weeks of users

Conclusion

- Users' demands guide development
  - Familiar interface
    - Throughout development, interface is kept the same
  - Rapid, reliable feature development
    - Architecture has been streamlined to enable fast development and high reliability
- Future plans: concentrate on features



JBluIce-EPICS

JBluIce Developers	EPICS Developers	Design Suggestions and Testing	Management
Mark Hilgart	Sergey Stepanov	Craig Ogata	Janet Smith
Sudhir Pothineni	Oleg Makarov	Ruslan Sanishvili	Robert Fischetti
		Michael Becker	
		Nagarajan Venugopalan	
		Derek Yoder	