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Scientific Software, Java, and Eclipse

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Presented at the EPICS Collaboration Meeting

April 23 - 27, 2007

Deutsches Elektronen Synchrotron DESY, Hamburg, Germany

Outline

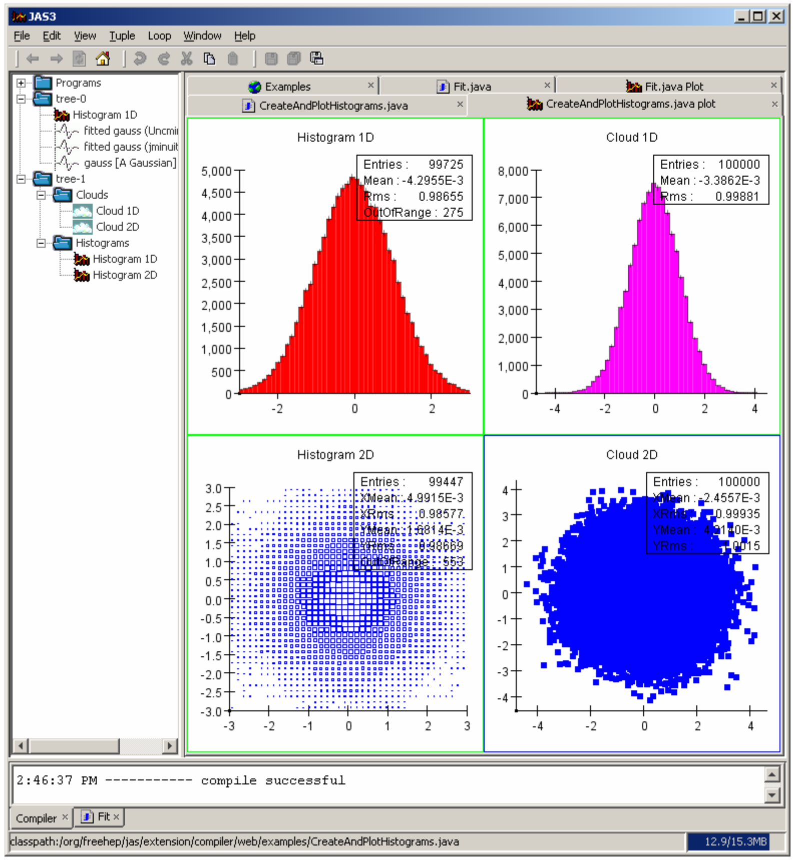
- Scientific Software and Examples
- Java
- X-Ray Software Development at the APS
- Eclipse and Examples

Scientific Software

- The language of choice used to be FORTRAN
  - There are still many legacy FORTRAN codes in use
- C and C++ have become popular
  - Grid computing now tends to be done in C
- Many scientists use Python
  - Reasonably powerful, yet easy to use
  - Allows them to do science rather than software
- There are now a number of significant scientific projects using Java
  - Many started out as C, but have evolved to Java
- Java is now an acceptable, if not the preferred, language for scientific software development

Java Analysis Studio (JAS3)

- Developed by and for the High-Energy physics community
- Plotting of 1d, 2d, 3d Histograms, XY plots, Scatter plots, *etc*.
- Open source
- Attractive plotting
- Fitting, other mathematical analysis
  - Primarily from CERN
- Highly modular structure
  - Uses plug-ins



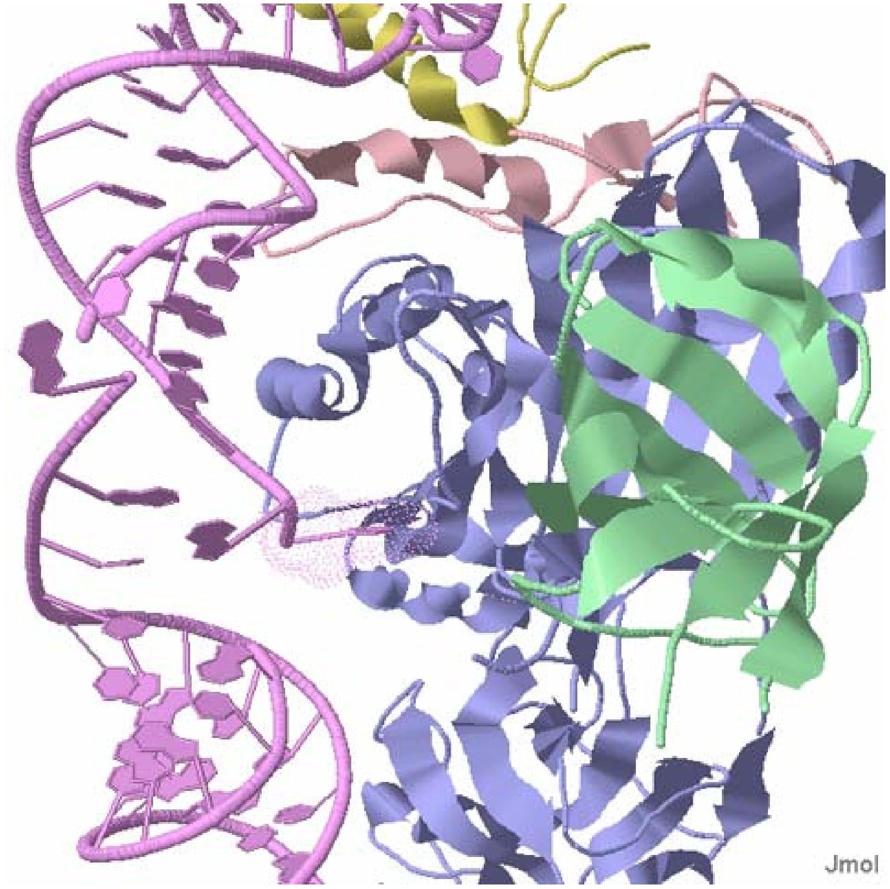
```
2:46:37 PM ----------- compile successful
```

classpath:/org/freehep/jas/extension/compiler/web/examples/CreateAndPlotHistograms.java

JMol – Molecular Viewer

- Commonly used as an applet that can be integrated into web pages to display molecules in a variety of ways
- Also has a standalone application and a development tool kit that can be integrated into other Java applications
- Interactive, 3D
- Free, Open Source

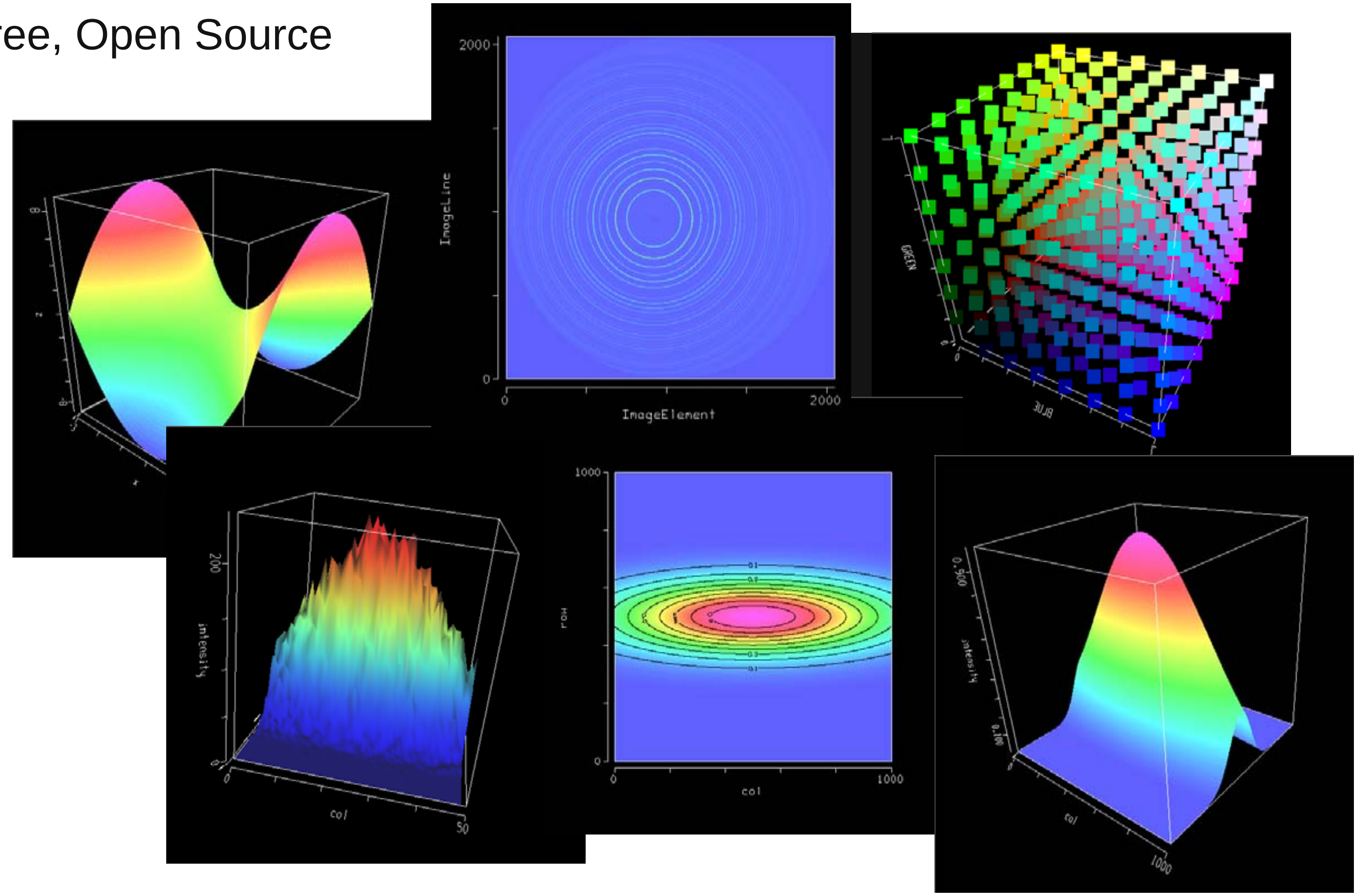
- One of several Java Molecular Graphics packages



Crystal structure of an H/ACA box RNP from Pyrococcus furiosus (PDB CODE: 2HVY)

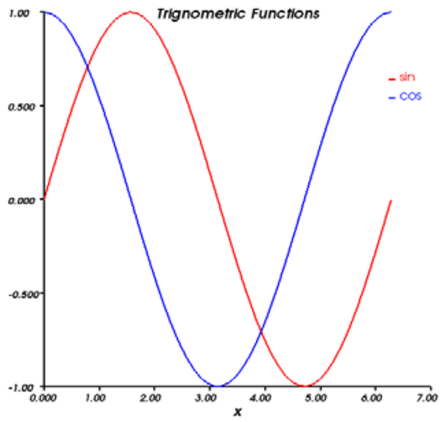
VisAD

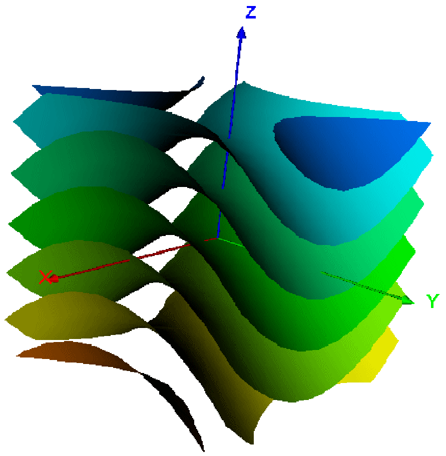
- Space Sciences and Engineering Center (SSEC), and others
- Extensive 2D and 3D visualization package
- Free, Open Source

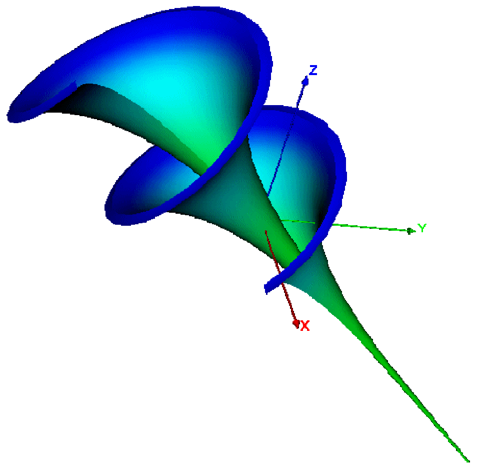


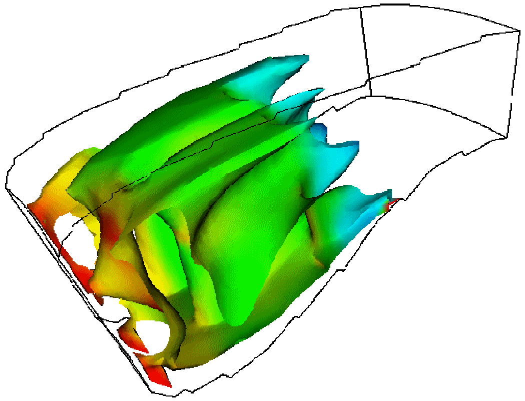
VTK

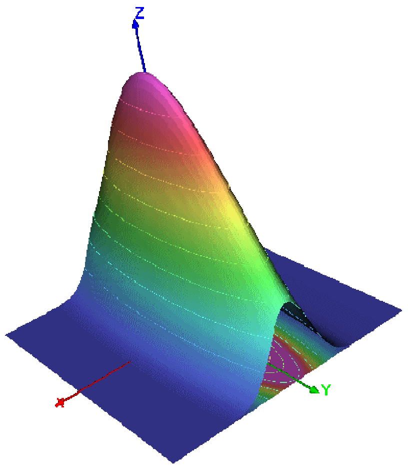
- Software system for 3D computer graphics, image processing, and visualization
- Used by thousands of researchers and developers around the world
- Written in C++
- Has Java wrappers
  - Also, Tcl/Tk, Python
- Free, Open Source











ISAW

- The primary tool for analyzing neutron scattering data at the IPNS
- Has an extensive and sophisticated interface

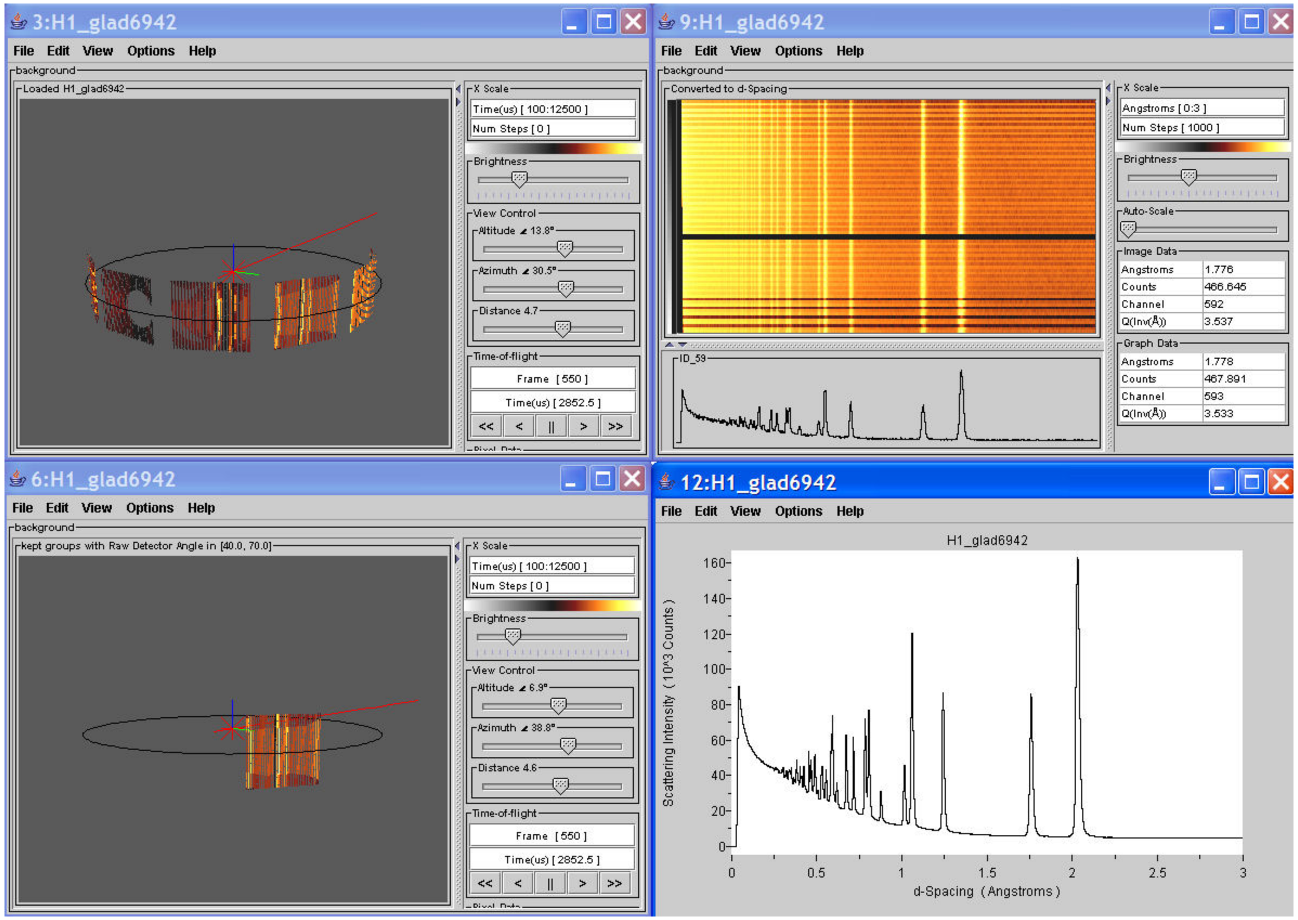


Image Data	
Angstroms	1.776
Counts	466.645
Channel	592
Q(Inv(Å))	3.537

Graph Data	
Angstroms	1.778
Counts	467.891
Channel	593
Q(Inv(Å))	3.533

From: John Hammonds, IPNS

Java ?

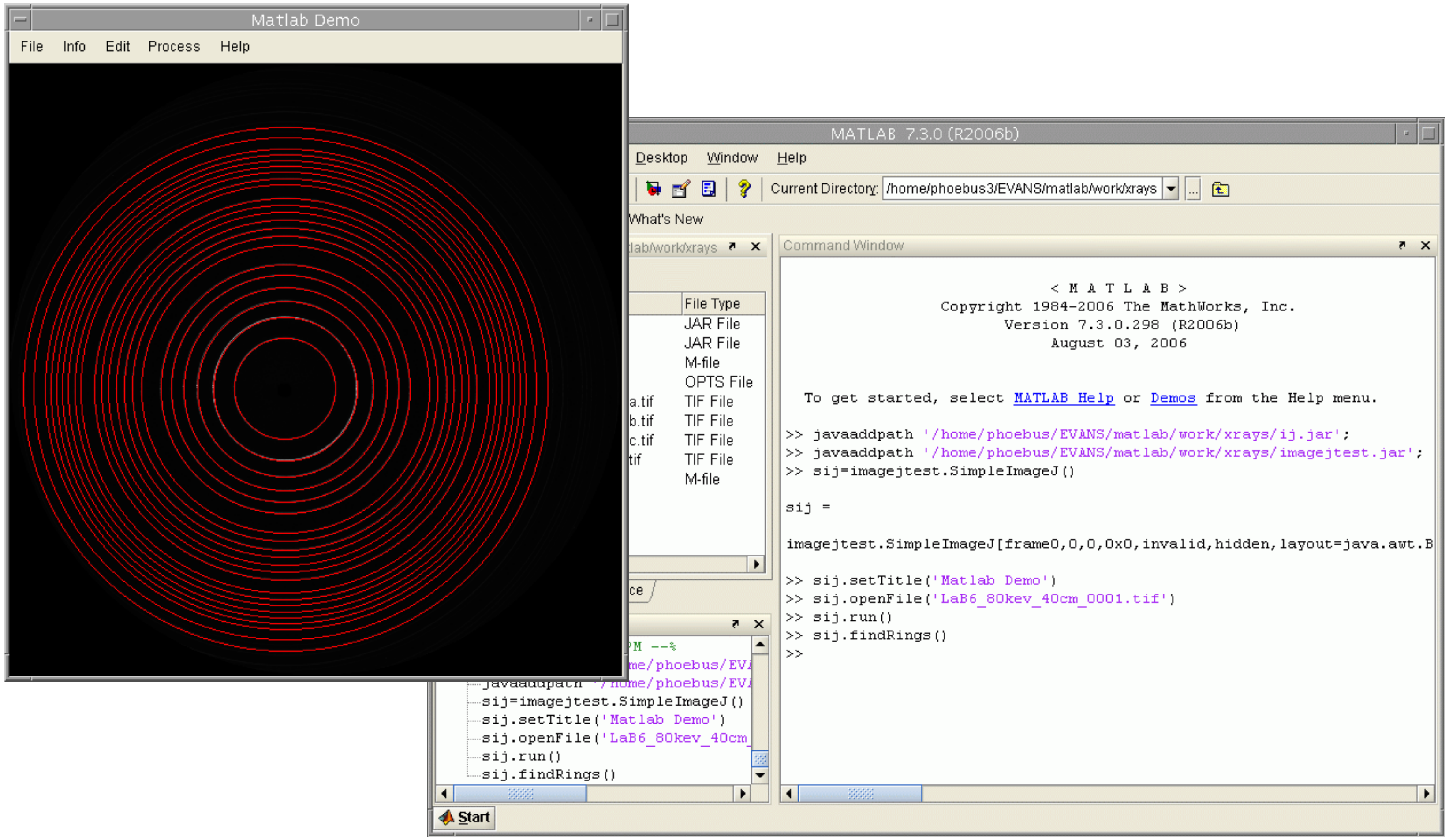
- Java has become a major language
- The reason is that most commercial development uses J2EE
  - There is money to be made improving Java and its tools
- Applications have performance approaching applications written in C
- There is already extensive scientific development in Java
- In my opinion, there is no other viable choice for high-quality, cross-platform, GUI development
  - Huge API
  - Write once, run anywhere
  - Easy to code (compared to C or C++, anyway)
  - Good performance
  - Excellent development tools

Java Development Tools

- Spell checks as you go
  - No “write – compile – load – run – figure out what happened” cycle
  - Probably the one most significant productivity enhancement
- Provides content assist
  - Probably the next most significant productivity enhancement
- Compiles as you write
  - Cycle is now “write – run”
- Massive refactoring
  - E.g. Change a variable name in all your files in all your projects
- Wizards and Tools to help at every stage
  - E.g. Generate getters and setters for all your properties
  - E.g. Add and/or clean up imports
- The above are just a small sample
  - Some of these are available for other languages
  - But usually not at the level they are for Java

Java in Matlab

- Matlab has extensive support for Java
  - Your favorite software framework can also be used in Matlab



```
                    < M A T L A B >
        Copyright 1984-2006 The MathWorks, Inc.
              Version 7.3.0.298 (R2006b)
                    August 03, 2006


  To get started, select MATLAB Help or Demos from the Help menu.

>> javaaddpath '/home/phoebus/EVANS/matlab/work/xrays/ij.jar';
>> javaaddpath '/home/phoebus/EVANS/matlab/work/xrays/imagejtest.jar';
>> sij=imagejtest.SimpleImageJ()

sij =

imagejtest.SimpleImageJ[frame0,0,0,0x0,invalid,hidden,layout=java.awt.B

>> sij.setTitle('Matlab Demo')
>> sij.openFile('LaB6_80kev_40cm_0001.tif')
>> sij.run()
>> sij.findRings()
>>
```

```
sij=imagejtest.SimpleImageJ()
sij.setTitle('Matlab Demo')
sij.openFile('LaB6_80kev_40cm
sij.run()
sij.findRings()
```

X-Ray Software Development at the APS

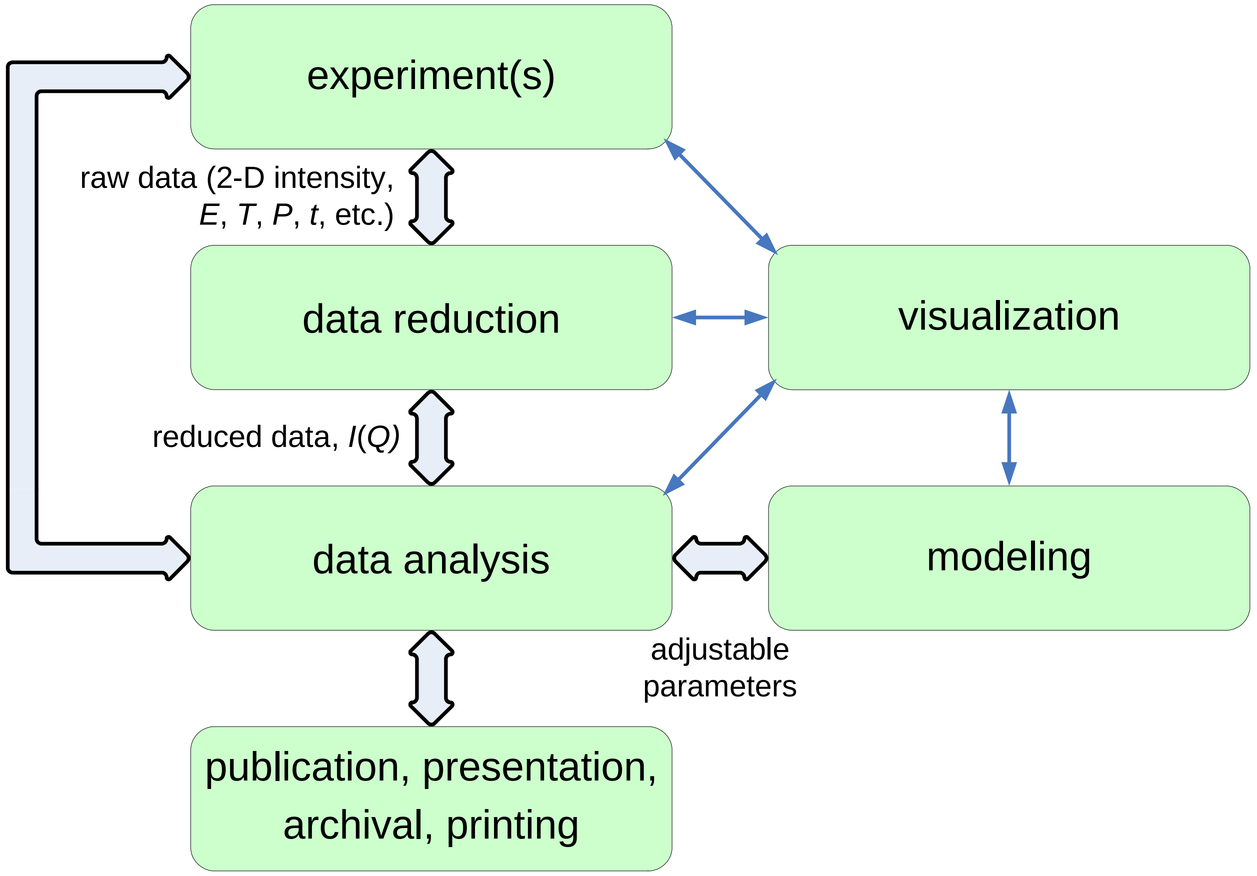
- Best described as "Uncoordinated"
- Wide variety of languages
  - FORTRAN, C, C++, Perl, Tcl/Tk, Python, Java, …
- Visualization relies on (different) commercial products
  - IDL, IGOR, Matlab, …
- Each beamline tends to do its own thing
- Modeling and Analysis is not well integrated with Data Acquisition
- Lack of real-time data reduction
- Little high-performance computing
- Little remote access
- No common data format

- A Scientific Software Section was formed to help remedy this situation

XRAYS

- Stands for X-Ray Analysis Software
  - (or X-Ray Software)
- It is expected to grow into a large suite of analysis and visualization applications
- These will include:
  - Scientific workbench program
  - New analysis and visualization applications
  - Updating and coordination of existing analysis and visualization applications
  - A framework of software routines that developers can use to write applications
- It currently consists mostly of exploration and prototype applications
  - This is the groundwork for what we really want to do
  - More than 1200 Java source files in 60 projects
  - 38 Java projects intended for distribution (gov.anl.xrays.xxx)
  - 10 ready-to-deploy features (collections of projects) in 4 categories

We Want to Manage the Entire Experimental Data Flow



Eclipse

- Eclipse is an Open Source community
- It was started in 2001 by IBM
  - IBM donated a lot of research
  - Controlled the early development, but later relinquished control
- It is now controlled by the Eclipse Foundation
  - Strategic members contribute up to $500K and 8 developers
  - Currently 17 strategic members
  - Currently more than 150 developers

- Out of the box it looks like a Java IDE (Integrated Development Environment)
- It is really a Plug-in manager
  - That happens to come with Java Development plug-ins.
  - You can make it be most anything you want

XRAYS Rationalization for Eclipse

- Providing coordination is a primary goal
- Resources are limited
- Have to choose something
  - Eclipse seems like the best choice
  - Powerful, flexible, extensible
  - Open-source
  - Huge community with many projects
- Java development environment leads to high productivity
- Deployment via plug-ins appears to solve many problems

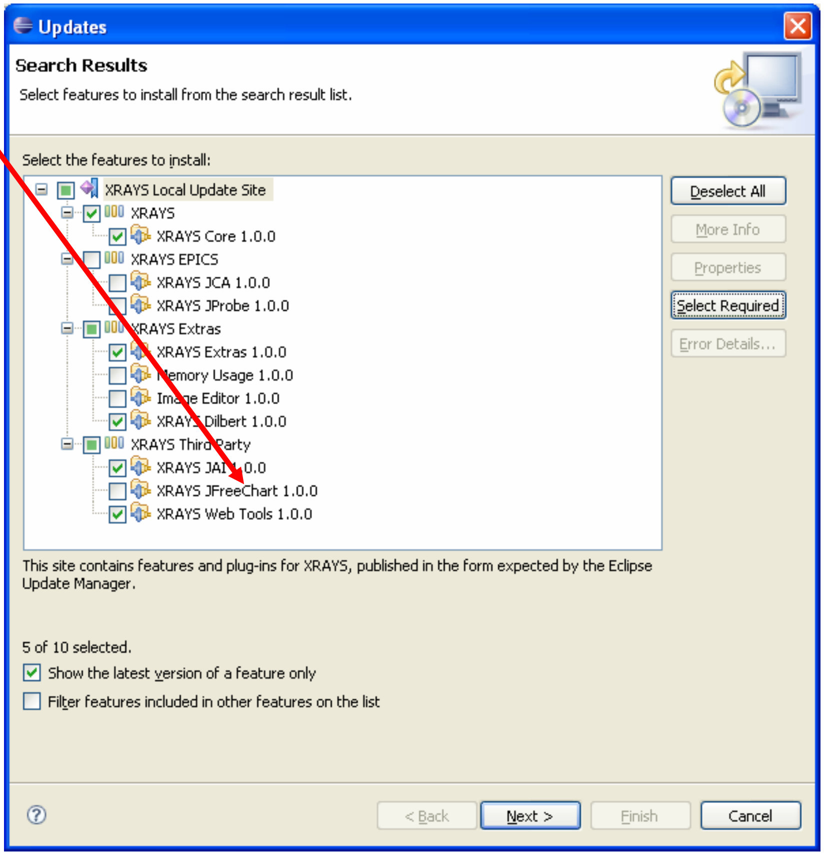
- We intend to use Eclipse, not as an IDE, but as a workbench
  - Something users will use

- Downsides
  - Most x-ray beamline staff and users are not using Eclipse now
  - 95% will be unhappy [with anything we do]

Deployment is a Major Reason for Using Eclipse

- Both Java and Eclipse are multi-platform
- Updates are easily made through the Eclipse update mechanism
- You can wrap 3rd party applications in your own plug-ins
  - For example:

    The Feature "XRAYS JFreeChart" contains gov.anl.xrays.jfreechart which wraps JFreeChart
  - Including DLLs and Shared Objects
- Guarantees they are versions that work with your applications on all supported platforms
- Makes it easy for the user to install and update both your stuff and the 3rd party stuff


Updates

Search Results

Select features to install from the search result list.

Select the features to install:

- [■] XRAYS Local Update Site
  - [✓] XRAYS
    - [✓] XRAYS Core 1.0.0
  - [ ] XRAYS EPICS
    - [ ] XRAYS JCA 1.0.0
    - [ ] XRAYS JProbe 1.0.0
  - [■] XRAYS Extras
    - [✓] XRAYS Extras 1.0.0
    - [ ] Memory Usage 1.0.0
    - [ ] Image Editor 1.0.0
    - [✓] XRAYS Dilbert 1.0.0
  - [■] XRAYS Third Party
    - [✓] XRAYS JAI 1.0.0
    - [ ] XRAYS JFreeChart 1.0.0
    - [✓] XRAYS Web Tools 1.0.0

This site contains features and plug-ins for XRAYS, published in the form expected by the Eclipse Update Manager.

5 of 10 selected.

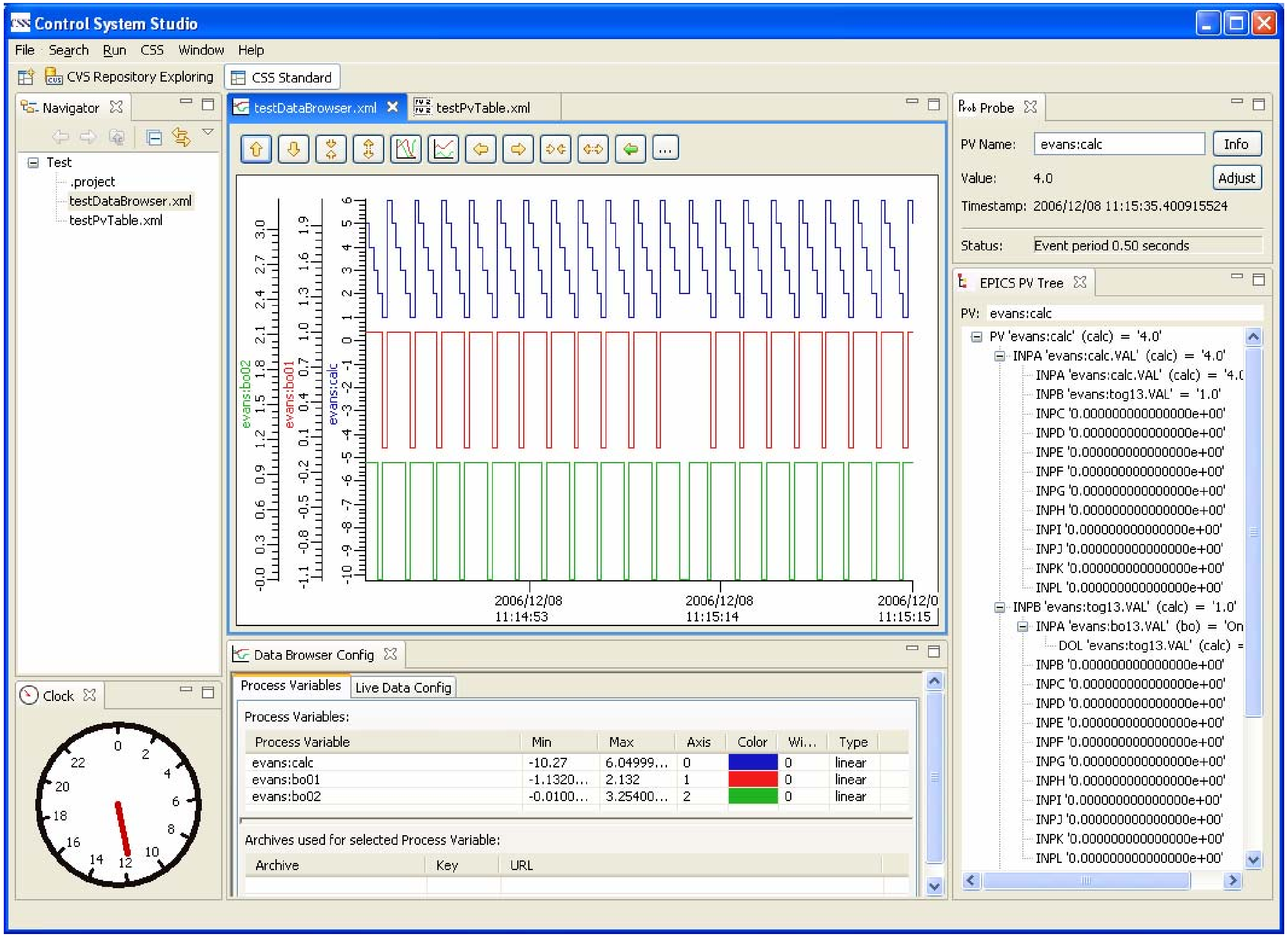
[✓] Show the latest version of a feature only

[ ] Filter features included in other features on the list

Eclipse for Users, not Developers

- We intend to use Eclipse as a workbench
- Something a user can come in and be up and running with in a short time
  - Probably with community help
- Each user can use and customize it in his or her own way
  - (That is what Eclipse provides)
- They will probably use it for more than one thing
  - That is why the layout by Perspective is important
  - You just switch perspectives to change tasks
- I think this paradigm is better than using RCP applications
  - You provide the plug-ins
  - The user manages his Workbench as he or she pleases

EPICS Control System Studio



PV Name: evans:calc

Value: 4.0

Timestamp: 2006/12/08 11:15:35.400915524

Status: Event period 0.50 seconds

PV: evans:calc

```
PV 'evans:calc' (calc) = '4.0'
  INPA 'evans:calc.VAL' (calc) = '4.0'
    INPA 'evans:calc.VAL' (calc) = '4.0
    INPB 'evans:tog13.VAL' = '1.0'
    INPC '0.000000000000000e+00'
    INPD '0.000000000000000e+00'
    INPE '0.000000000000000e+00'
    INPF '0.000000000000000e+00'
    INPG '0.000000000000000e+00'
    INPH '0.000000000000000e+00'
    INPI '0.000000000000000e+00'
    INPJ '0.000000000000000e+00'
    INPK '0.000000000000000e+00'
    INPL '0.000000000000000e+00'
  INPB 'evans:tog13.VAL' (calc) = '1.0'
    INPA 'evans:bo13.VAL' (bo) = 'On
      DOL 'evans:tog13.VAL' (calc) =
    INPB '0.000000000000000e+00'
    INPC '0.000000000000000e+00'
    INPD '0.000000000000000e+00'
    INPE '0.000000000000000e+00'
    INPF '0.000000000000000e+00'
    INPG '0.000000000000000e+00'
    INPH '0.000000000000000e+00'
    INPI '0.000000000000000e+00'
    INPJ '0.000000000000000e+00'
    INPK '0.000000000000000e+00'
    INPL '0.000000000000000e+00'
```

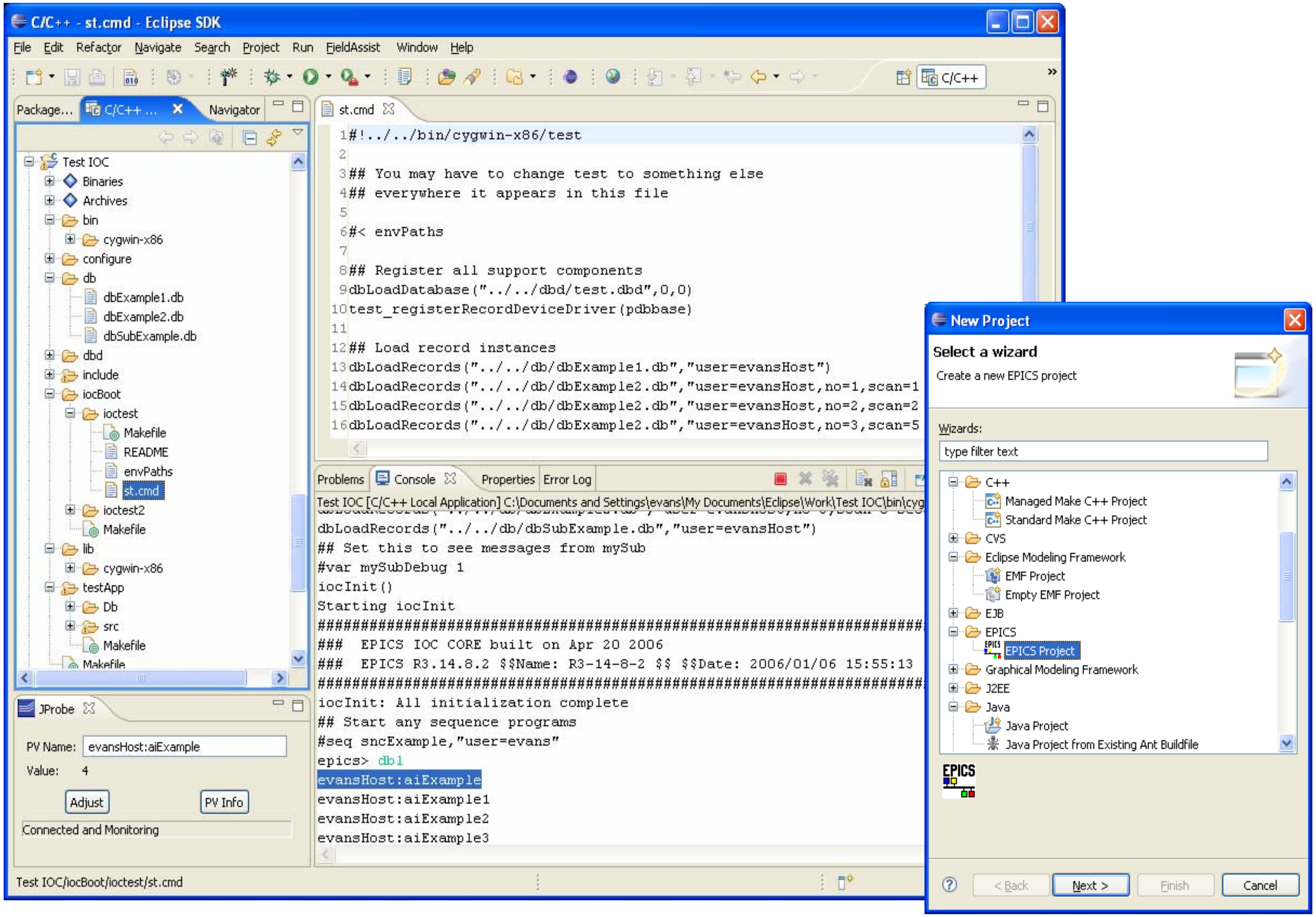
Process Variables:

Process Variable	Min	Max	Axis	Color	Wi...	Type
evans:calc	-10.27	6.04999...	0	🟦	0	linear
evans:bo01	-1.1320...	2.132	1	🟥	0	linear
evans:bo02	-0.0100...	3.25400...	2	🟩	0	linear

Archives used for selected Process Variable:

Archive	Key	URL

EPICS IDE : IOC Development



```
#!../../bin/cygwin-x86/test

## You may have to change test to something else
## everywhere it appears in this file

#< envPaths

## Register all support components
dbLoadDatabase("../../dbd/test.dbd",0,0)
test_registerRecordDeviceDriver(pdbbase)

## Load record instances
dbLoadRecords("../../db/dbExample1.db","user=evansHost")
dbLoadRecords("../../db/dbExample2.db","user=evansHost,no=1,scan=1
dbLoadRecords("../../db/dbExample2.db","user=evansHost,no=2,scan=2
dbLoadRecords("../../db/dbExample2.db","user=evansHost,no=3,scan=5
```

Test IOC [C/C++ Local Application] C:\Documents and Settings\evans\My Documents\Eclipse\Work\Test IOC\bin\cyg

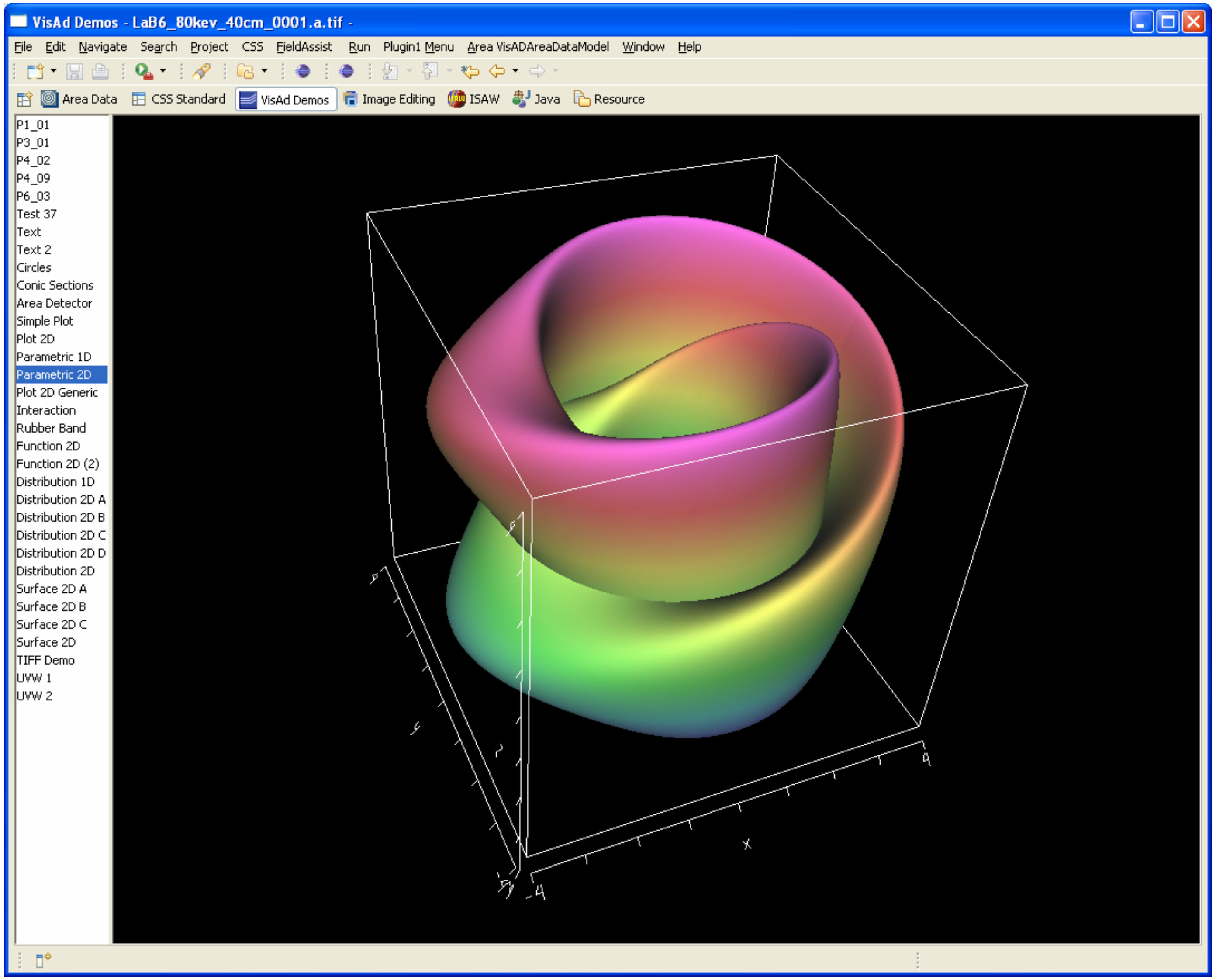
```
dbLoadRecords("../../db/dbSubExample.db","user=evansHost")
## Set this to see messages from mySub
#var mySubDebug 1
iocInit()
Starting iocInit
############################################################################
###  EPICS IOC CORE built on Apr 20 2006
###  EPICS R3.14.8.2 $$Name: R3-14-8-2 $$ $$Date: 2006/01/06 15:55:13
############################################################################
iocInit: All initialization complete
## Start any sequence programs
#seq sncExample,"user=evans"
epics> dbl
evansHost:aiExample
evansHost:aiExample1
evansHost:aiExample2
evansHost:aiExample3
```

PV Name: evansHost:aiExample
Value: 4
Connected and Monitoring

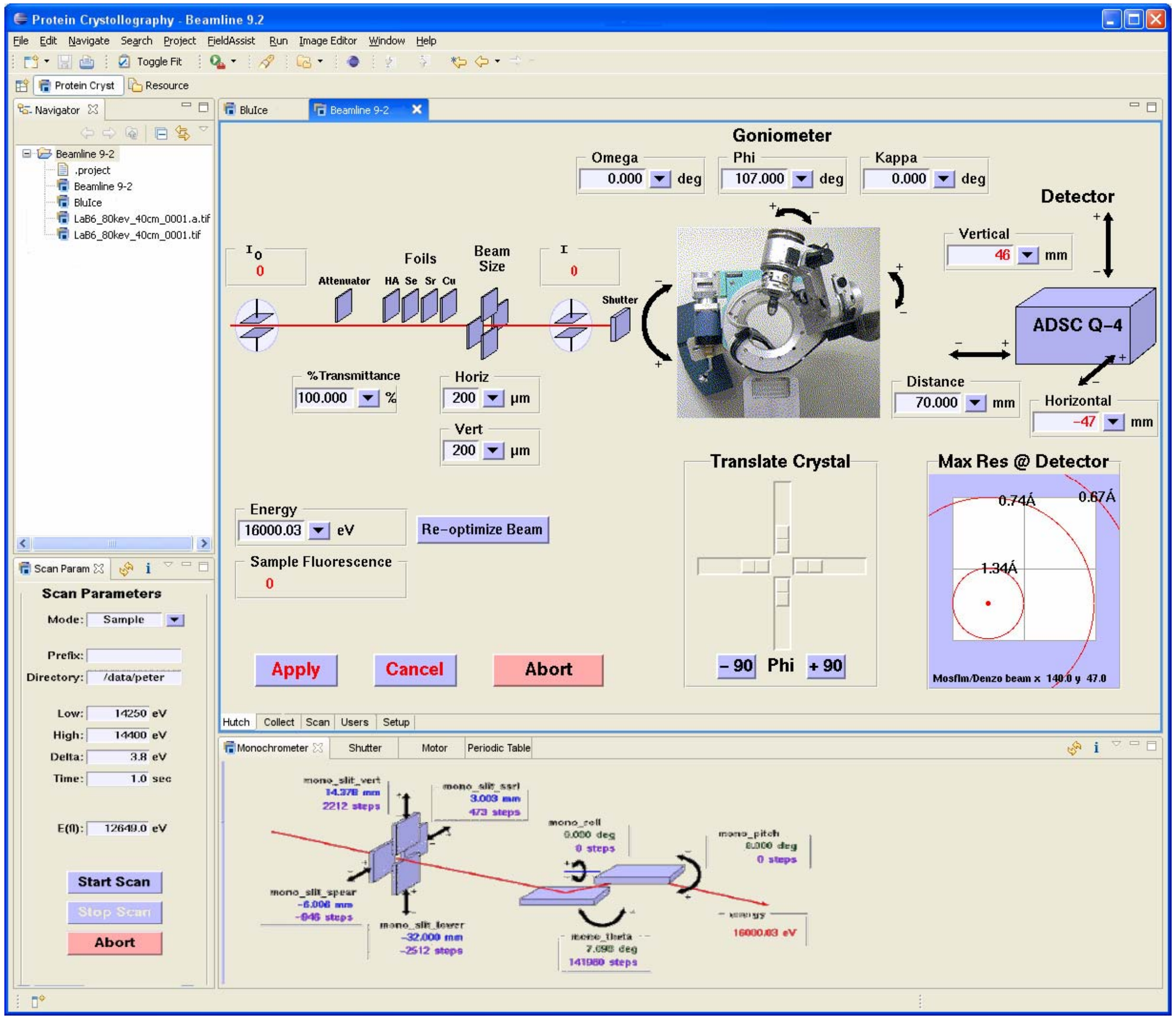
Test IOC/iocBoot/ioctest/st.cmd

Select a wizard
Create a new EPICS project

A Perspective Can be a Single Application



X-Ray Experiment



Beamline 9-2
.project
Beamline 9-2
BluIce
LaB6_80kev_40cm_0001.a.tif
LaB6_80kev_40cm_0001.tif

Omega 0.000 deg
Phi 107.000 deg
Kappa 0.000 deg
Vertical 46 mm
Distance 70.000 mm
Horizontal -47 mm
I₀ 0
I 0
%Transmittance 100.000 %
Horiz 200 µm
Vert 200 µm
Energy 16000.03 eV
Sample Fluorescence 0
-90 Phi +90
0.74Å 0.67Å 1.34Å
Mosflm/Denzo beam x 140.0 y 47.0

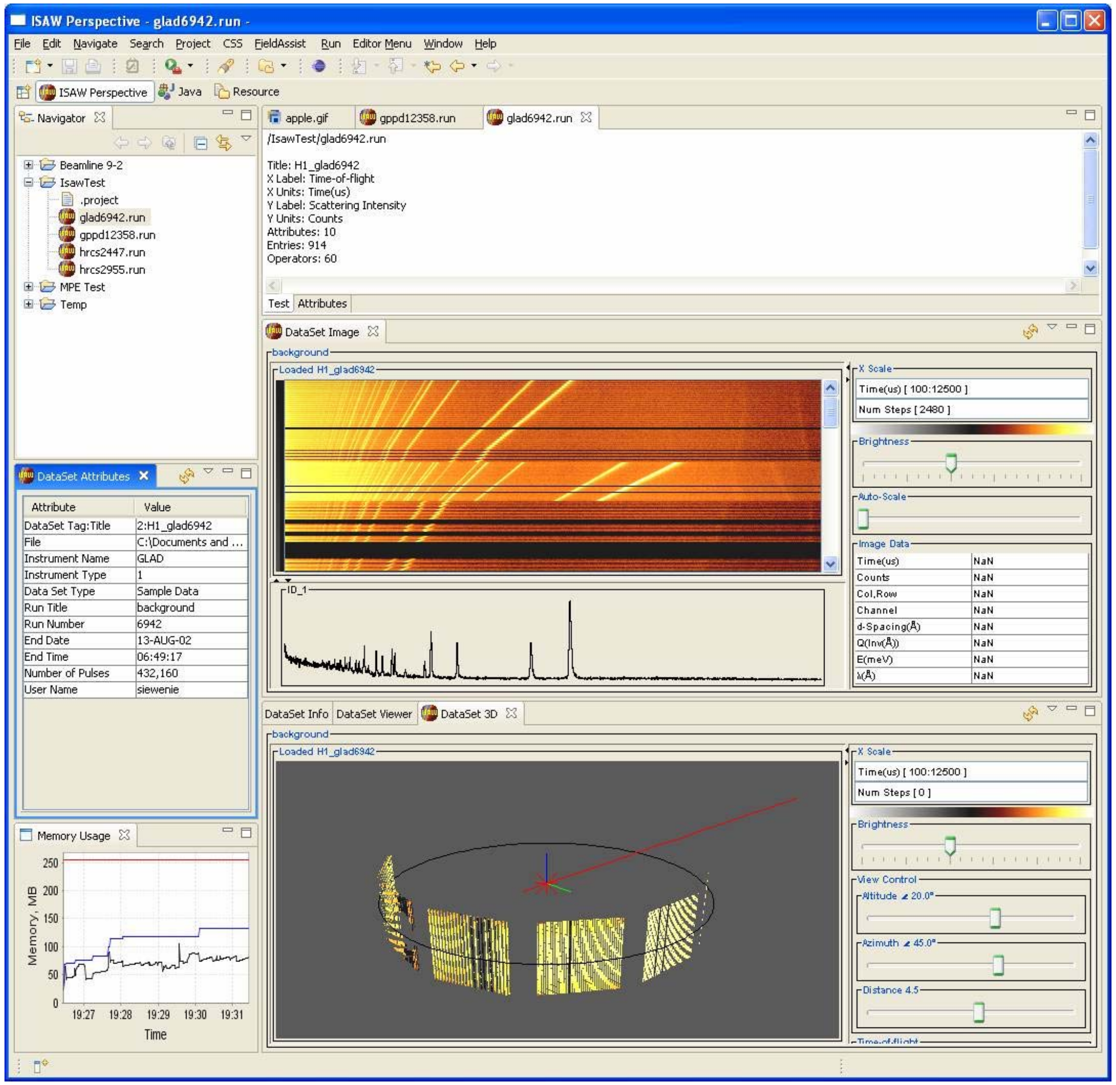
Scan Parameters
Mode: Sample
Prefix:
Directory: /data/peter
Low: 14250 eV
High: 14400 eV
Delta: 3.8 eV
Time: 1.0 sec
E(f1): 12649.0 eV

mono_slit_vert 14.378 mm 2212 steps
mono_slit_ssrl 3.003 mm 473 steps
mono_roll 0.000 deg 0 steps
mono_pitch 0.000 deg 0 steps
mono_slit_spear -6.008 mm -946 steps
mono_slit_lower -32.000 mm -2512 steps
mono_theta 7.098 deg 141960 steps
energy 16000.03 eV

Images from: BLU-ICE and the Distributed Control System, NOBUGS III, January 2000

Prototype Implementation of ISAW

- Includes:
  - A Perspective
  - An Editor for ISAW DataSets
    - *.run, .isd*
  - Some Views
- All work together
  - Views change when the edited file changes



/IsawTest/glad6942.run

Title: H1_glad6942
X Label: Time-of-flight
X Units: Time(us)
Y Label: Scattering Intensity
Y Units: Counts
Attributes: 10
Entries: 914
Operators: 60

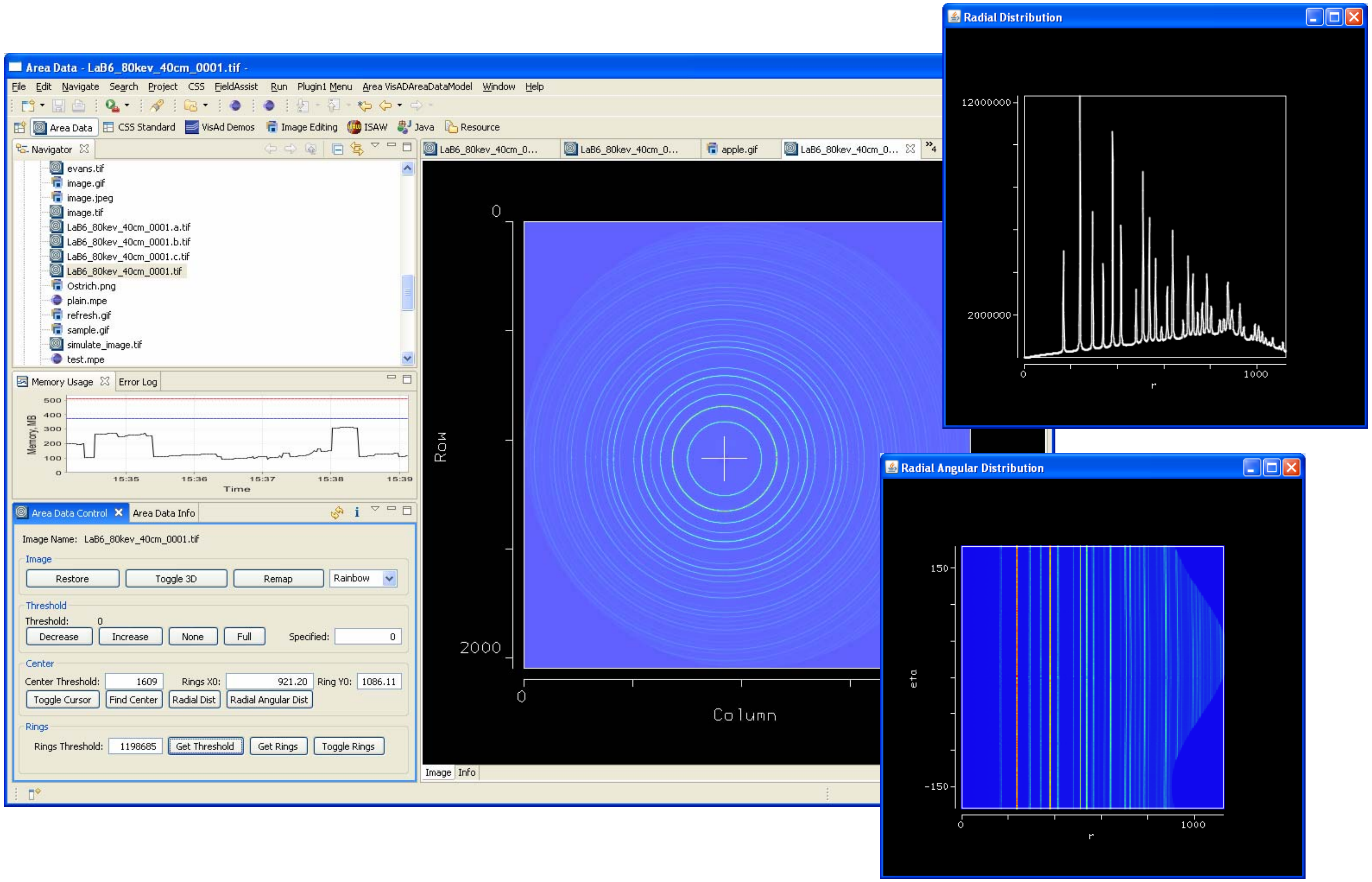
Attribute	Value
DataSet Tag:Title	2:H1_glad6942
File	C:\Documents and ...
Instrument Name	GLAD
Instrument Type	1
Data Set Type	Sample Data
Run Title	background
Run Number	6942
End Date	13-AUG-02
End Time	06:49:17
Number of Pulses	432,160
User Name	siewenie

Time(us) [100:12500]
Num Steps [2480]

Time(us)	NaN
Counts	NaN
Col,Row	NaN
Channel	NaN
d-Spacing(Å)	NaN
Q(Inv(Å))	NaN
E(meV)	NaN
λ(Å)	NaN

Time(us) [100:12500]
Num Steps [0]

Area Data Editor - First Scientific Application



Area Data - LaB6_80kev_40cm_0001.tif -
File Edit Navigate Search Project CSS FieldAssist Run Plugin1 Menu Area VisADAreaDataModel Window Help
Area Data | CSS Standard | VisAd Demos | Image Editing | ISAW | Java | Resource
Navigator
evans.tif
image.gif
image.jpeg
image.tif
LaB6_80kev_40cm_0001.a.tif
LaB6_80kev_40cm_0001.b.tif
LaB6_80kev_40cm_0001.c.tif
LaB6_80kev_40cm_0001.tif
Ostrich.png
plain.mpe
refresh.gif
sample.gif
simulate_image.tif
test.mpe
Memory Usage | Error Log
Memory, MB
Time
Area Data Control | Area Data Info
Restore | Toggle 3D | Remap | Rainbow
Decrease | Increase | None | Full
Toggle Cursor | Find Center | Radial Dist | Radial Angular Dist
Get Threshold | Get Rings | Toggle Rings
LaB6_80kev_40cm_0... | LaB6_80kev_40cm_0... | apple.gif | LaB6_80kev_40cm_0...
Row
Column
Image | Info
Radial Distribution
12000000
2000000
r
Radial Angular Distribution
eta
150
-150
r
1000

Image Name: LaB6_80kev_40cm_0001.tif

Image

Threshold

Threshold: 0

Specified: 0

Center

Center Threshold: 1609 Rings X0: 921.20 Ring Y0: 1086.11

Rings

Rings Threshold: 1198685

Thank You

This has been a

Scientific Software Presentation

Thank You

This has been a

Scientific Software Presentation