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The Scientific Software Initiative at the APS

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ICALEPCS Meeting, Knoxville, TN

Current X-Ray Scientific Software Situation

- 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

Scientific Software Section

- Specific goals:
  - Combine existing analysis and visualization codes with beamline data acquisition software and transform these codes into easy-to-use software
  - Provide a scientific workbench program that is easy to use and learn and from which users can access all the software that is necessary to manage the entire scientific work flow
  - Create new analysis and visualization applications that can be used on all beamlines and that are easily integrated into the standard workbench
  - Develop a software framework, perhaps more than one, that provides tested and debugged scientific routines, such as fitting and visualization, which can be used by developers to create applications
  - Provide high-performance computing
  - Provide documentation, distribution, maintenance, and support

Why Java ?

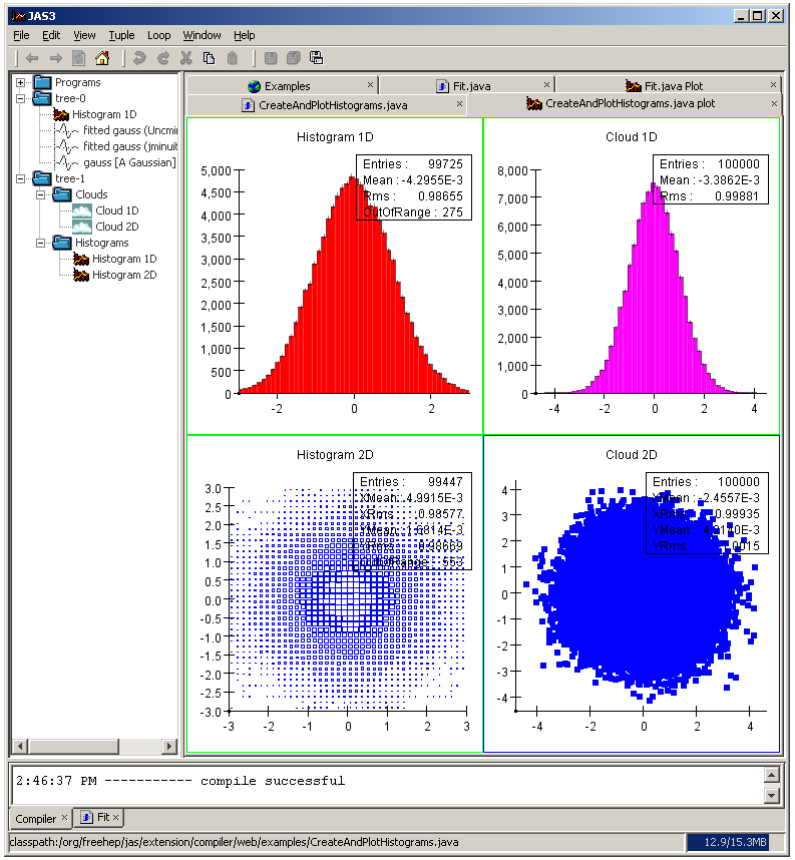
- Java has become a major and important language
- The reason is that most commercial development uses J2EE
  - It is running the financial world
  - There is money to be made improving Java and its tools
- Applications have performance approaching applications written in C
- There is already extensive scientific development in Java
- Advantages
  - 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
  - Eliminates most typos and all syntax errors
- Provides content assist
  - It tells you what to type next and provides documentation, etc.
- Compiles as you write
  - No “write – compile – load – run – figure out what happened” cycle
  - 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
- The above are just a small sample
  - Some of these are available for other languages
  - But generally not at the level they are for Java

Java Analysis Studio (JAS3)

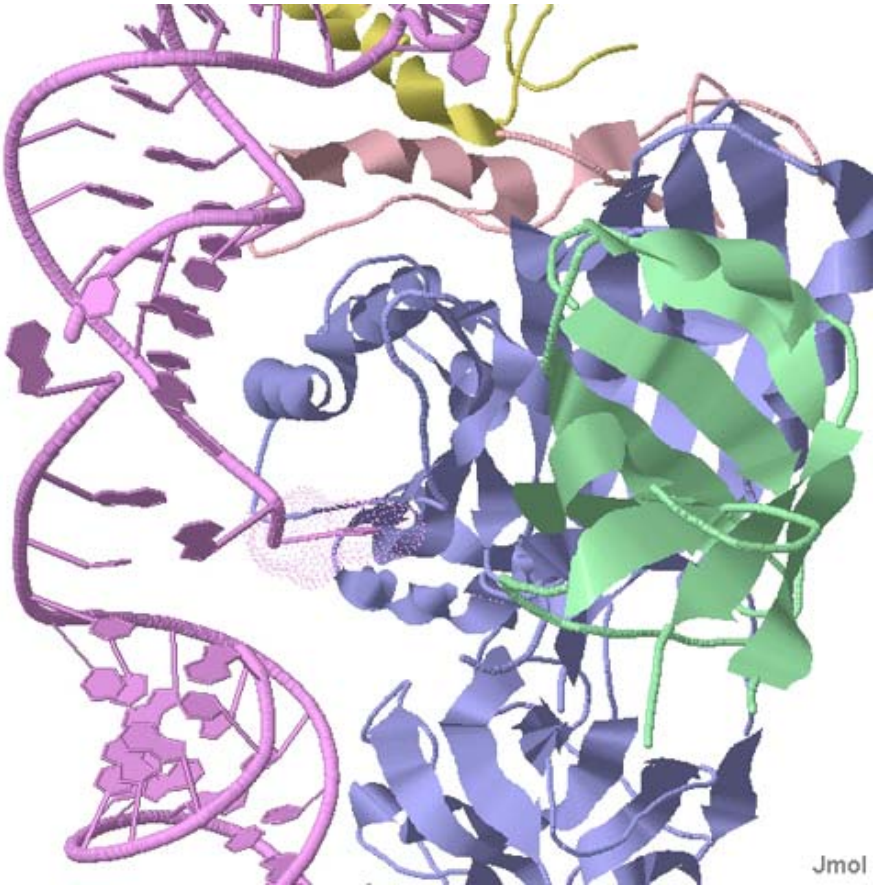
- Developed by and for the High-Energy physics community
- Plotting of 1d, 2d, 3d Histograms, XY plots, Scatter plots, *etc*.
- Open source
- Attractive plotting
- Fitting, other mathematical analysis
  - Primarily from CERN
- Highly modular structure
  - Uses plug-ins



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

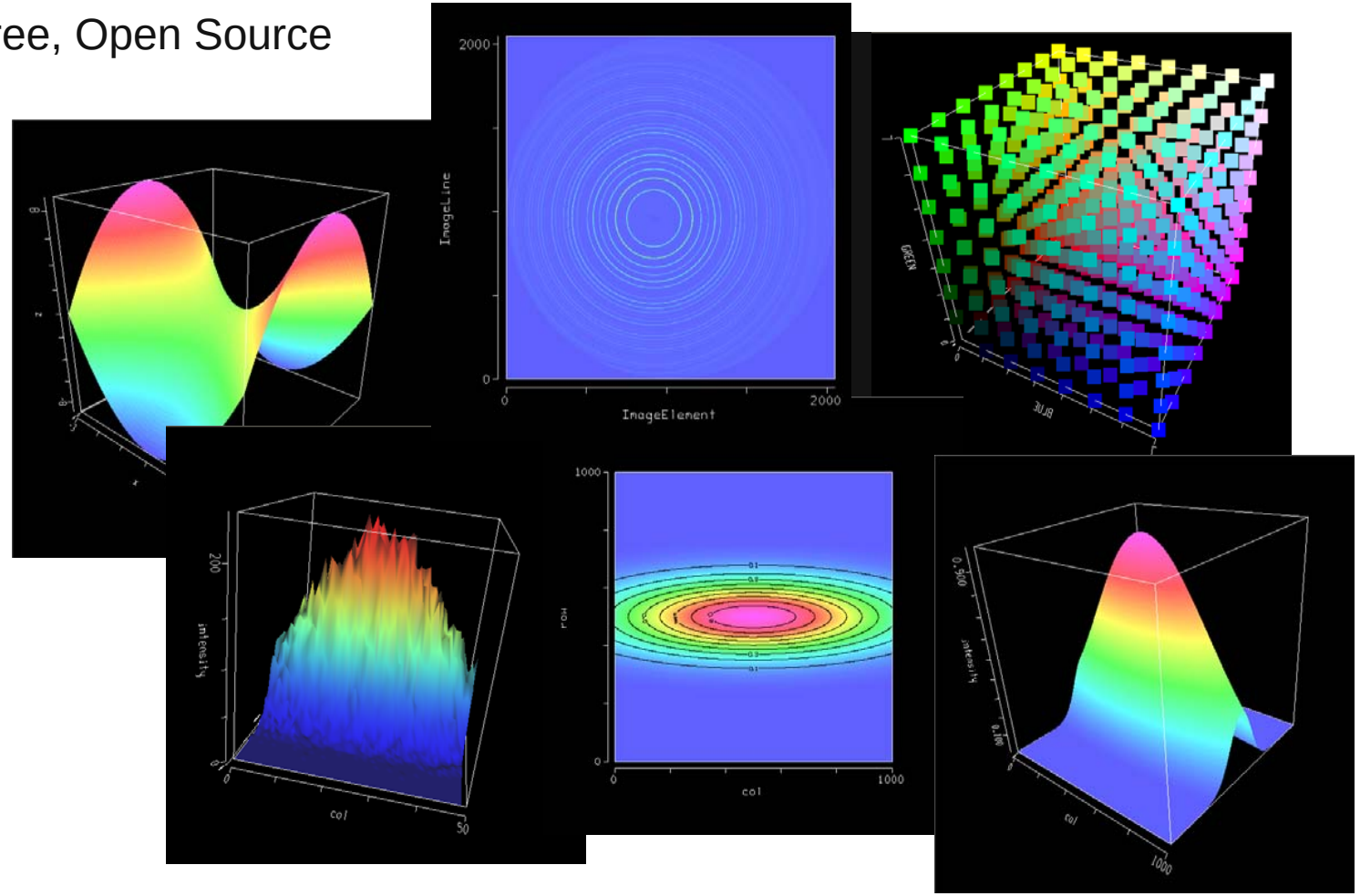
- One of several Java Molecular Graphics packages



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

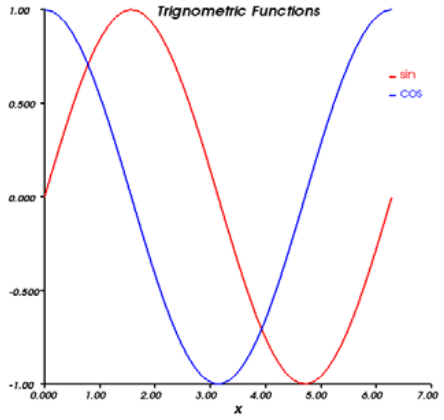
VisAD

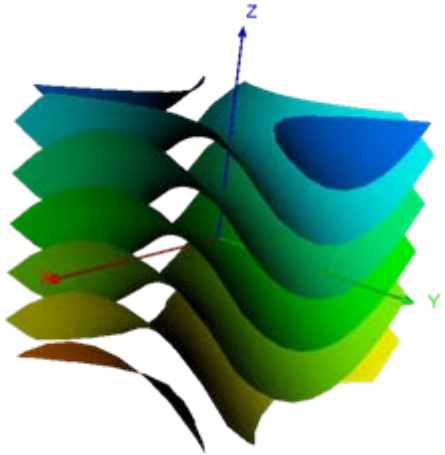
- Space Sciences and Engineering Center (SSEC), and others
- Extensive 2D and 3D visualization package
- Free, Open Source

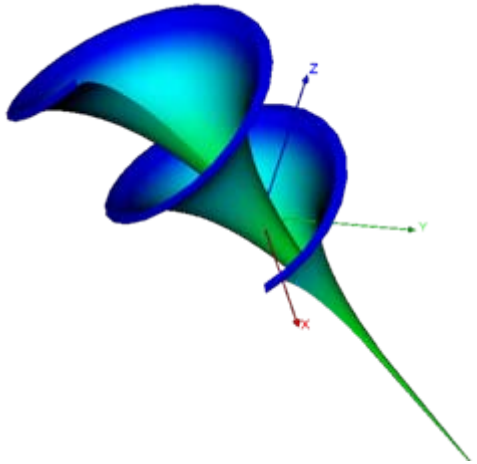


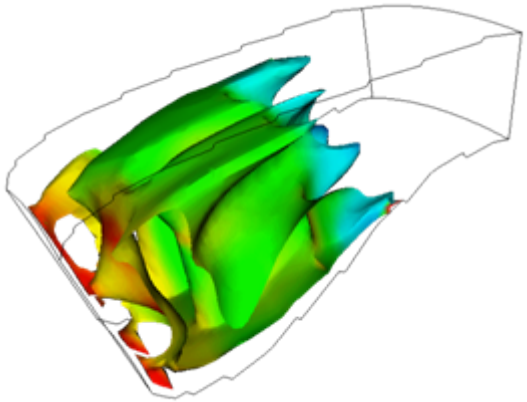
VTK

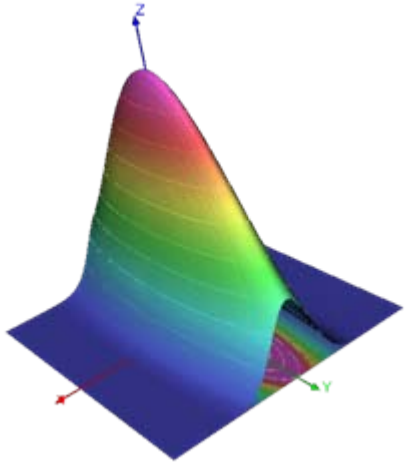
- Software system for 3D computer graphics, image processing, and visualization
- Used by thousands of researchers and developers around the world
- Written in C++
- Has Java wrappers
  - Also, Tcl/Tk, Python
- Free, Open Source





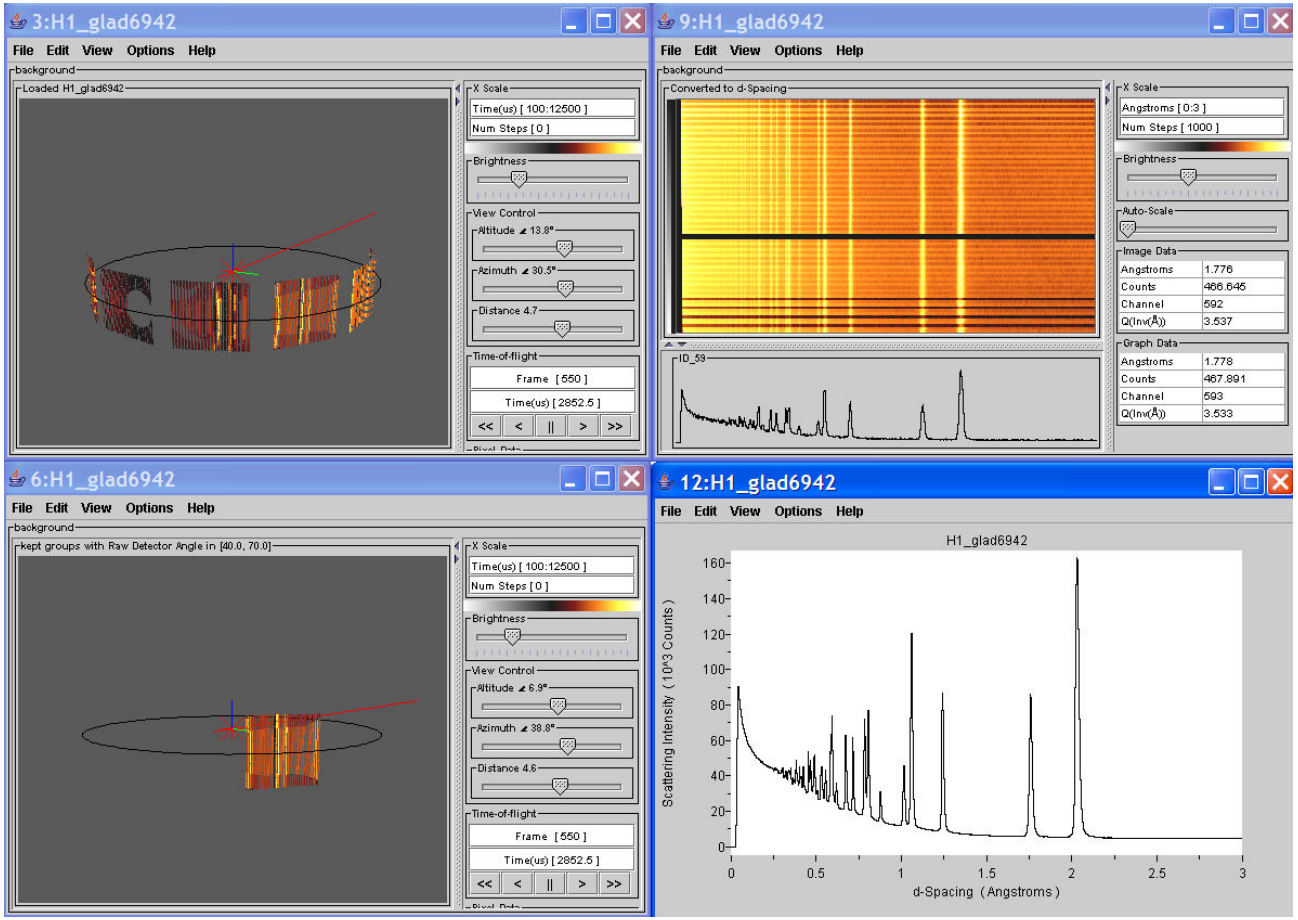






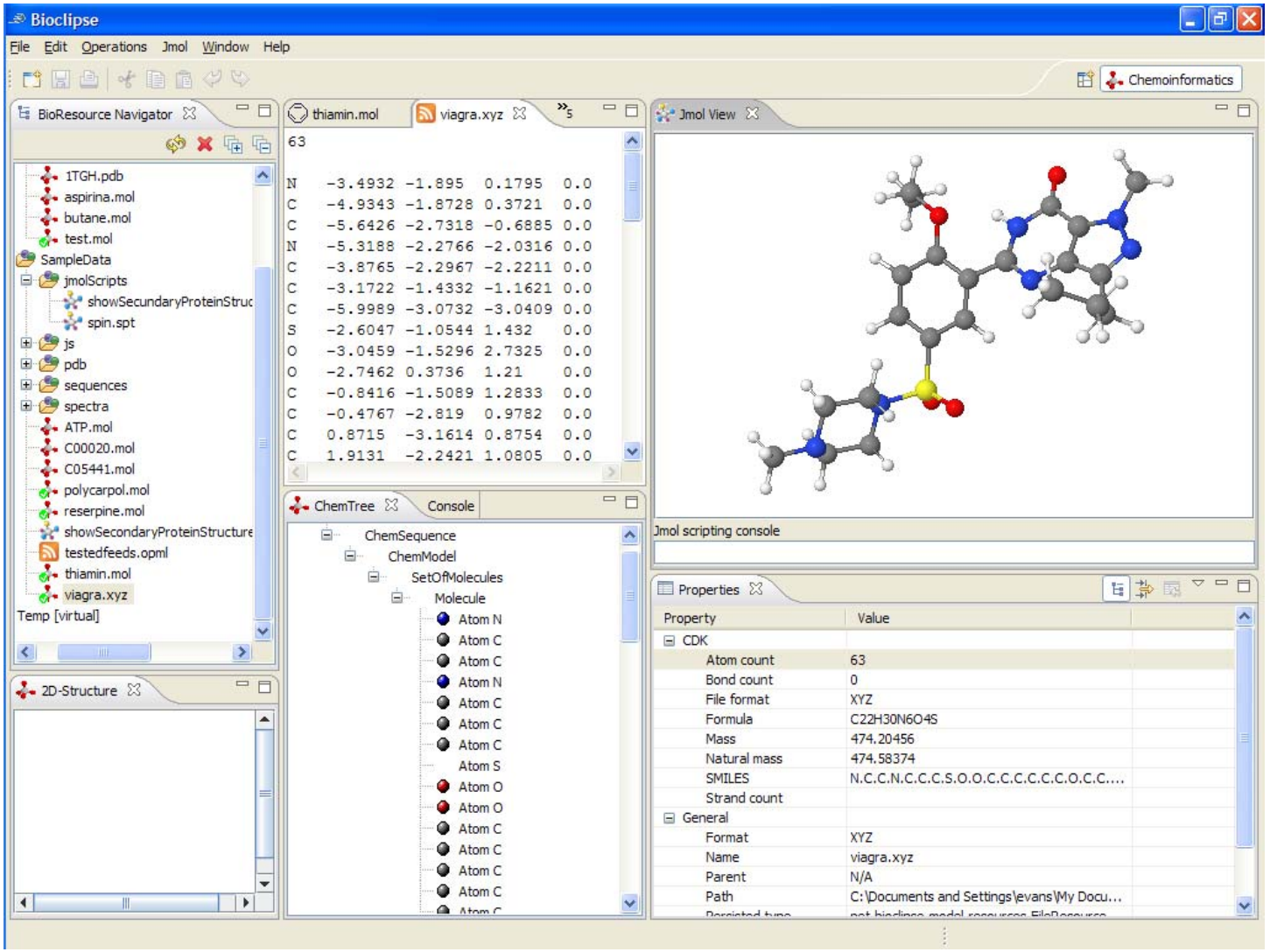
ISAW

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



From: John Hammonds, IPNS

Bioclipse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Jmol View
Jmol scripting console
ChemTree
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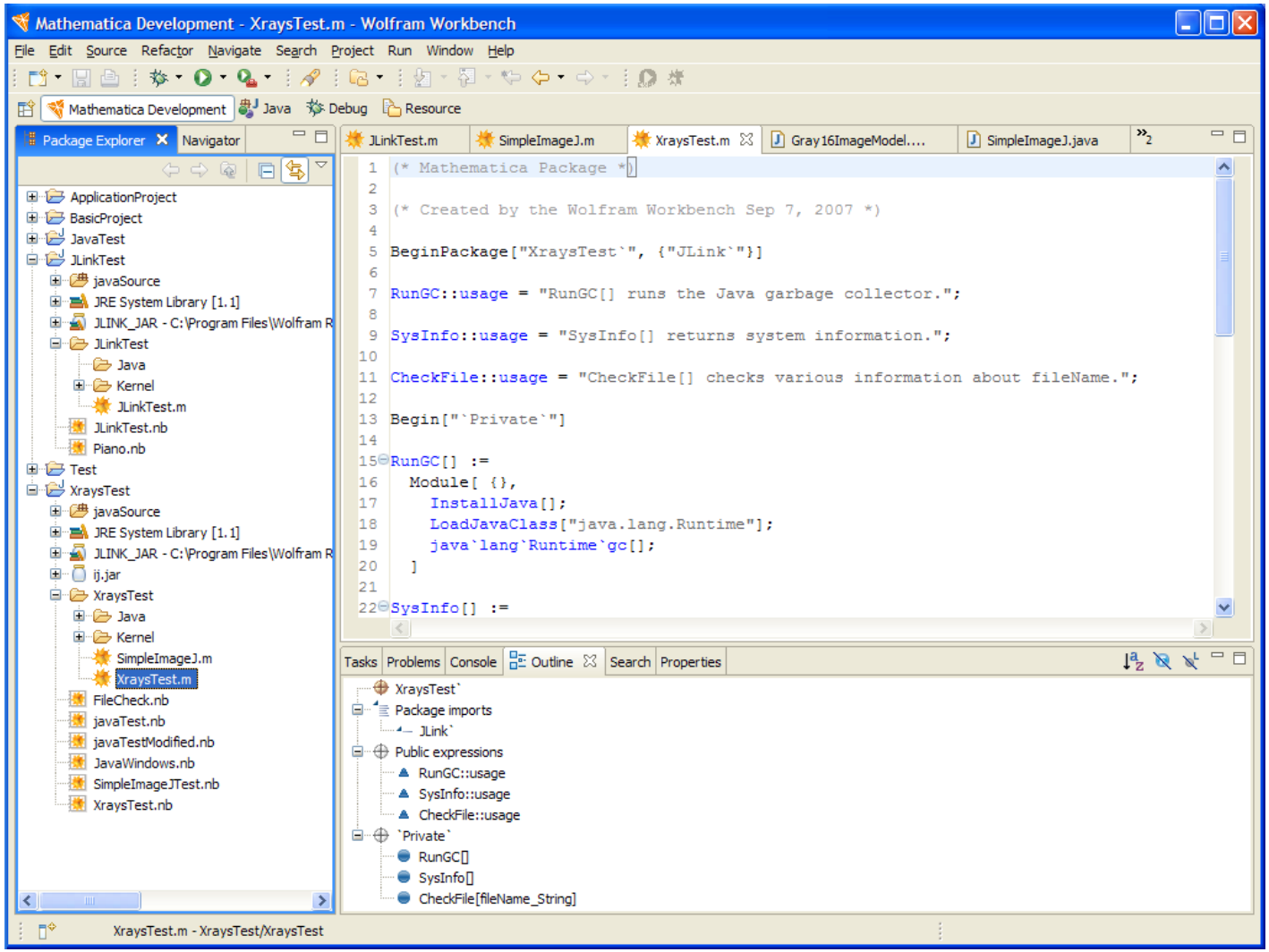
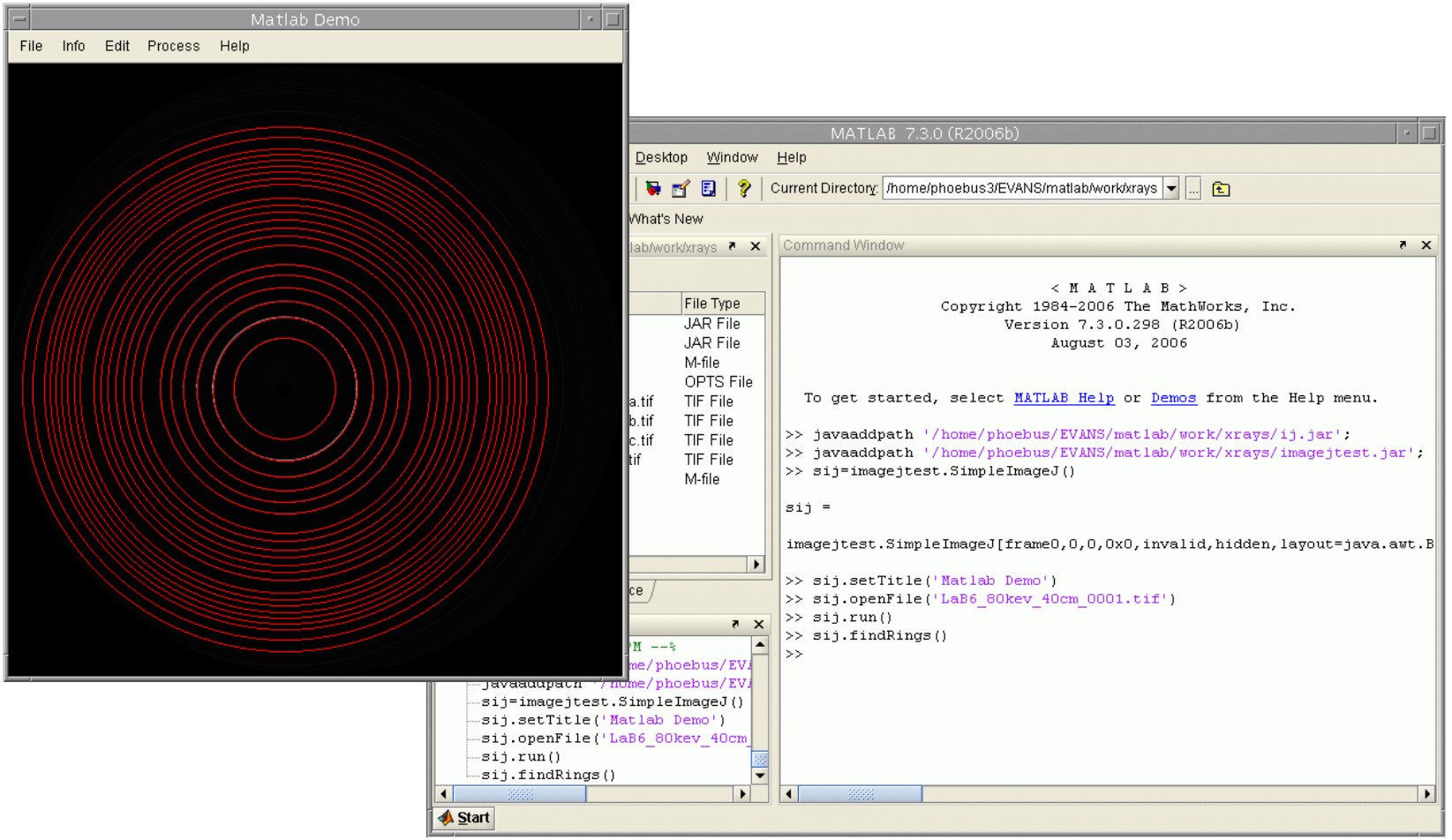
Wolfram Workbench (Mathematica)



Java in Matlab (or IDL or Mathematica or…)

- Matlab has extensive support for Java
  - A scientific software framework can also be used in these apps



Why Eclipse?

- Powerful, flexible, extensible
- Open-source
- Has a huge community with many projects
- Java development environment leads to high productivity
- Deployment via plug-ins appears to solve many problems

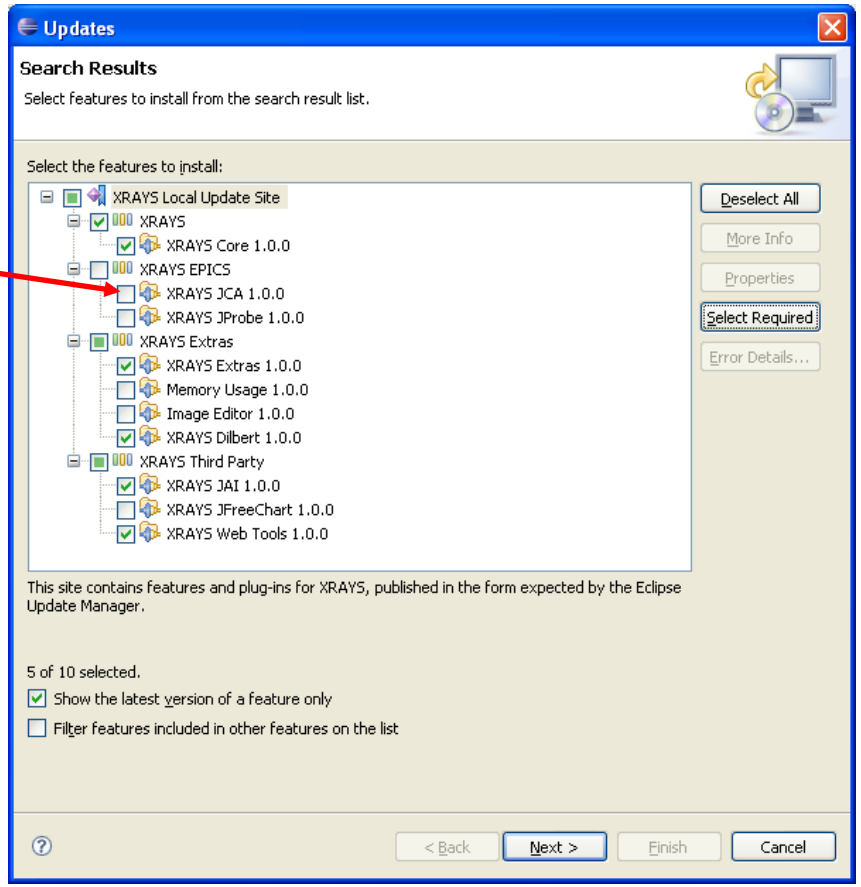
- We intend to use Eclipse, not as an IDE, but as a workbench (IE)
  - Something users will use
  - A way to organize their work

- 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:

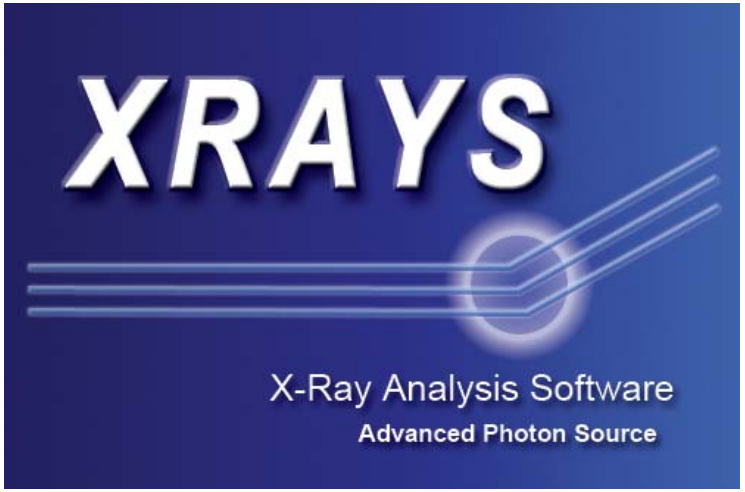
    The Feature “XRAYS JCA” contains org.scatteringsw.xrays.jca which wraps JCA
  - Including DLLs and Shared Objects
- Guarantees they are versions that work with your applications on all platforms you support
- Makes it easy for the user to install and update both your stuff and the 3rd party stuff



Eclipse for Users, not Developers

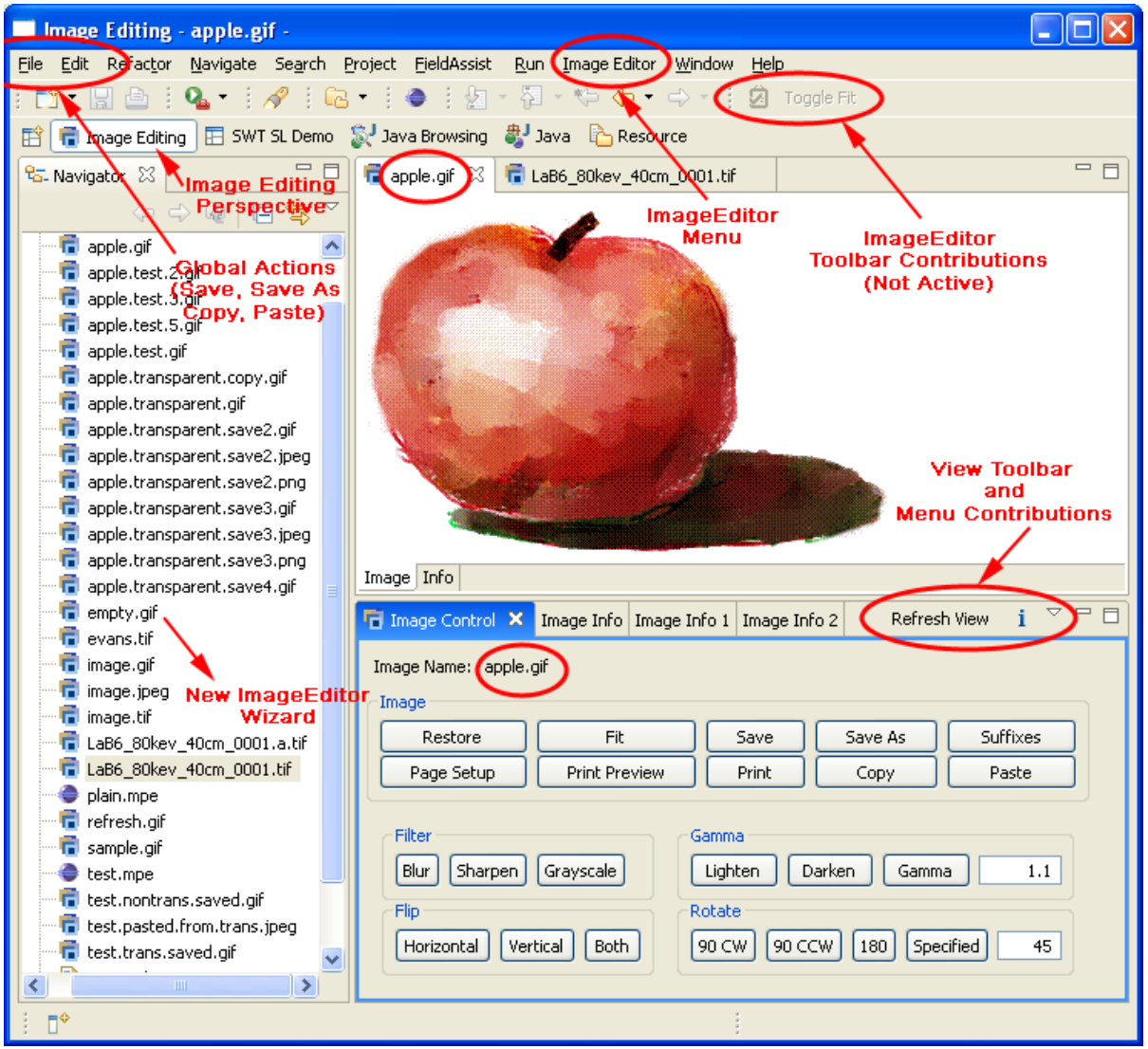
- We intend to use Eclipse as a workbench
- Something a user can come in and be up and running with in a short time
  - Probably with community help
- Each user can use and customize it in his or her own way
- They will probably use it for more than one thing
  - That is why the layout by Perspective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

XRAYS



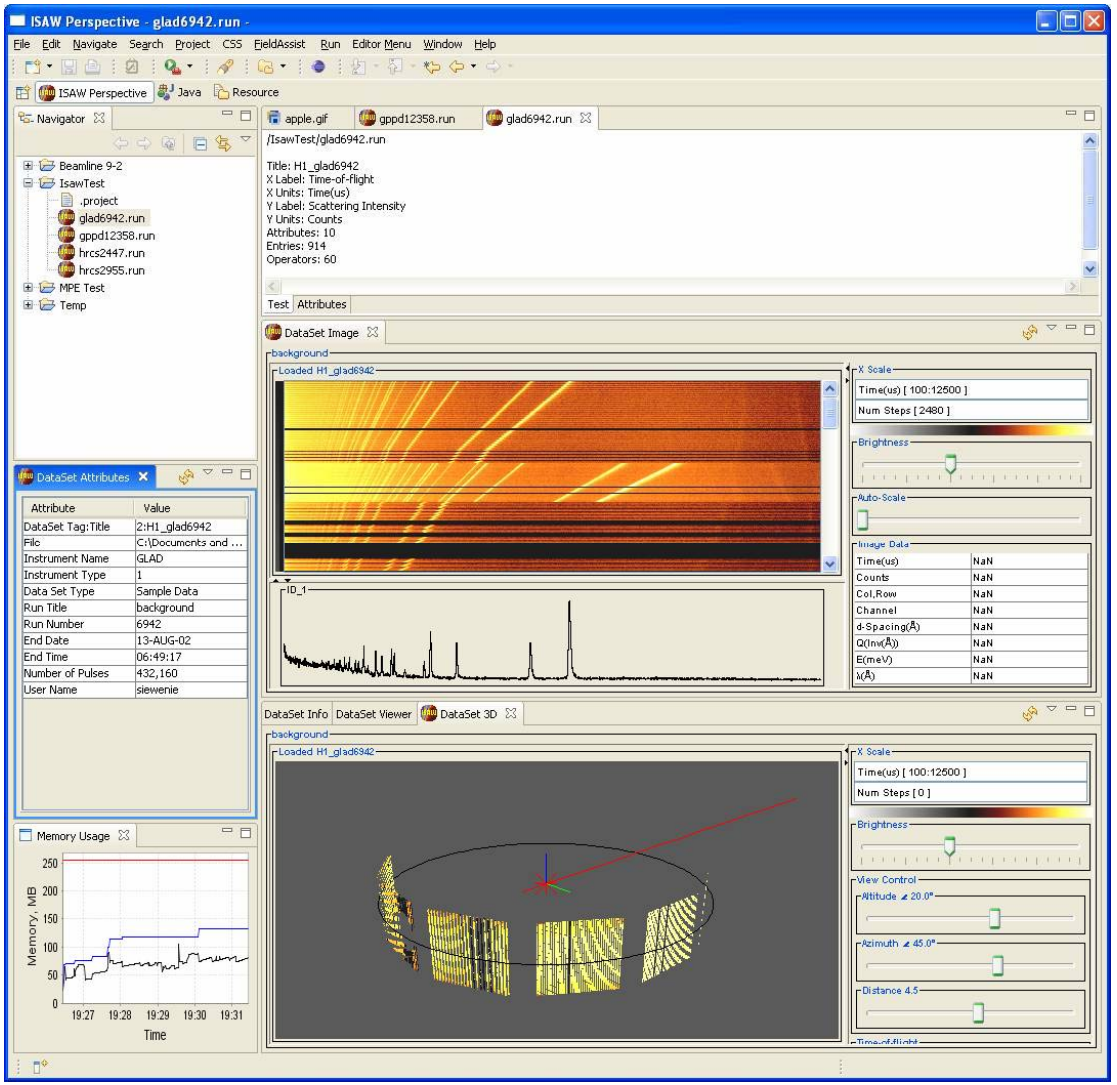
- Stands for X-Ray Analysis Software
  - (or X-Ray Software)
- It is expected to grow into a large suite of analysis and visualization applications
- These will include:
  - Scientific workbench program
  - New analysis and visualization applications
  - Updating and coordination of existing analysis 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
  - Currently more than 3000 Java source files in 120 projects
  - 38 Java projects intended for distribution (org.scatteringsw.xrays.xxx)
  - 10 ready-to-deploy features (collections of plug-ins) in 4 categories

Image Editor as an Experiment Prototype

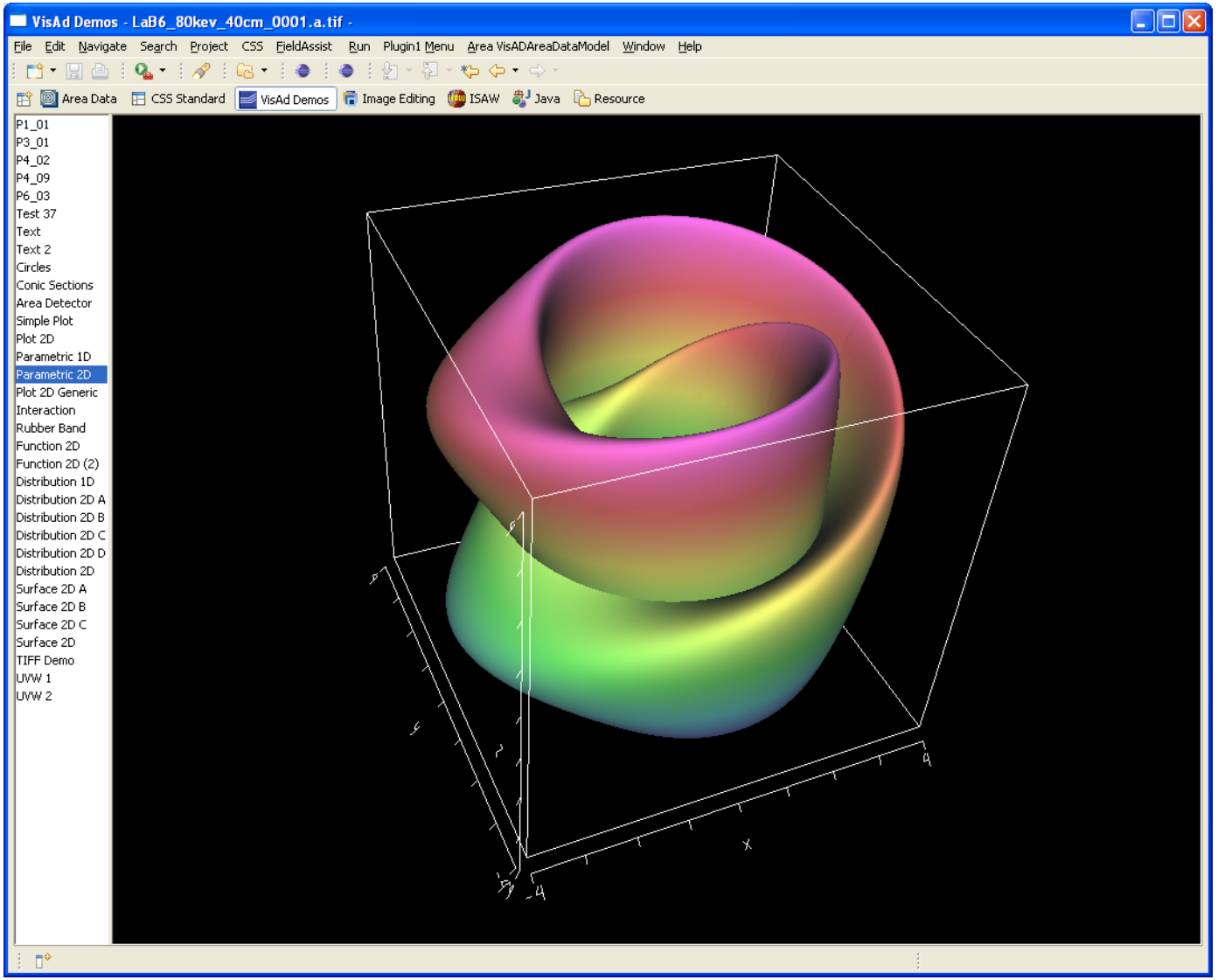


Prototype Implementation of ISAW

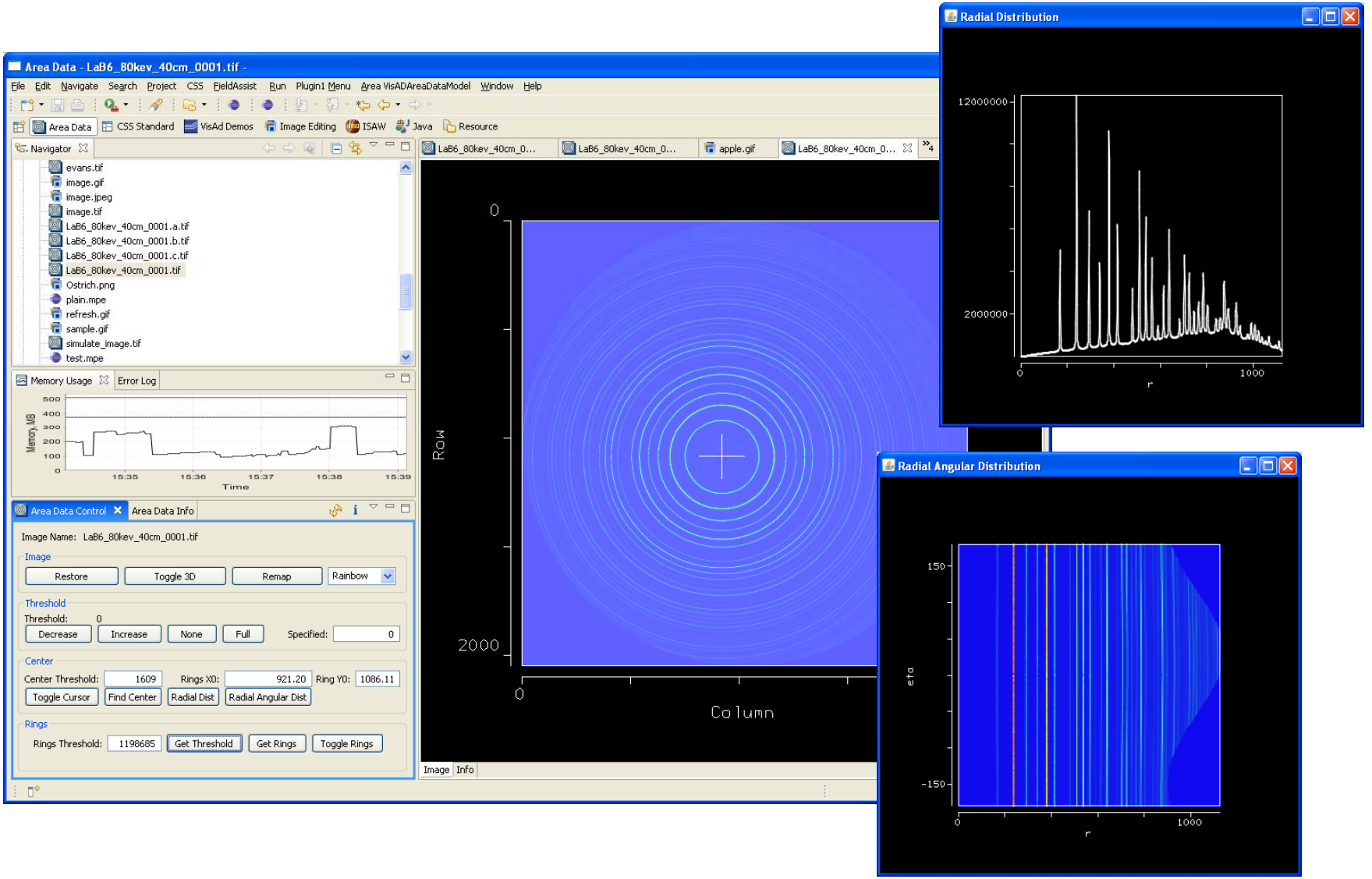
- Includes:
  - A Perspective
  - An Editor for ISAW DataSets
    - *.run, .isd*
  - Some Views
- All work together
  - Views change when the edited file changes



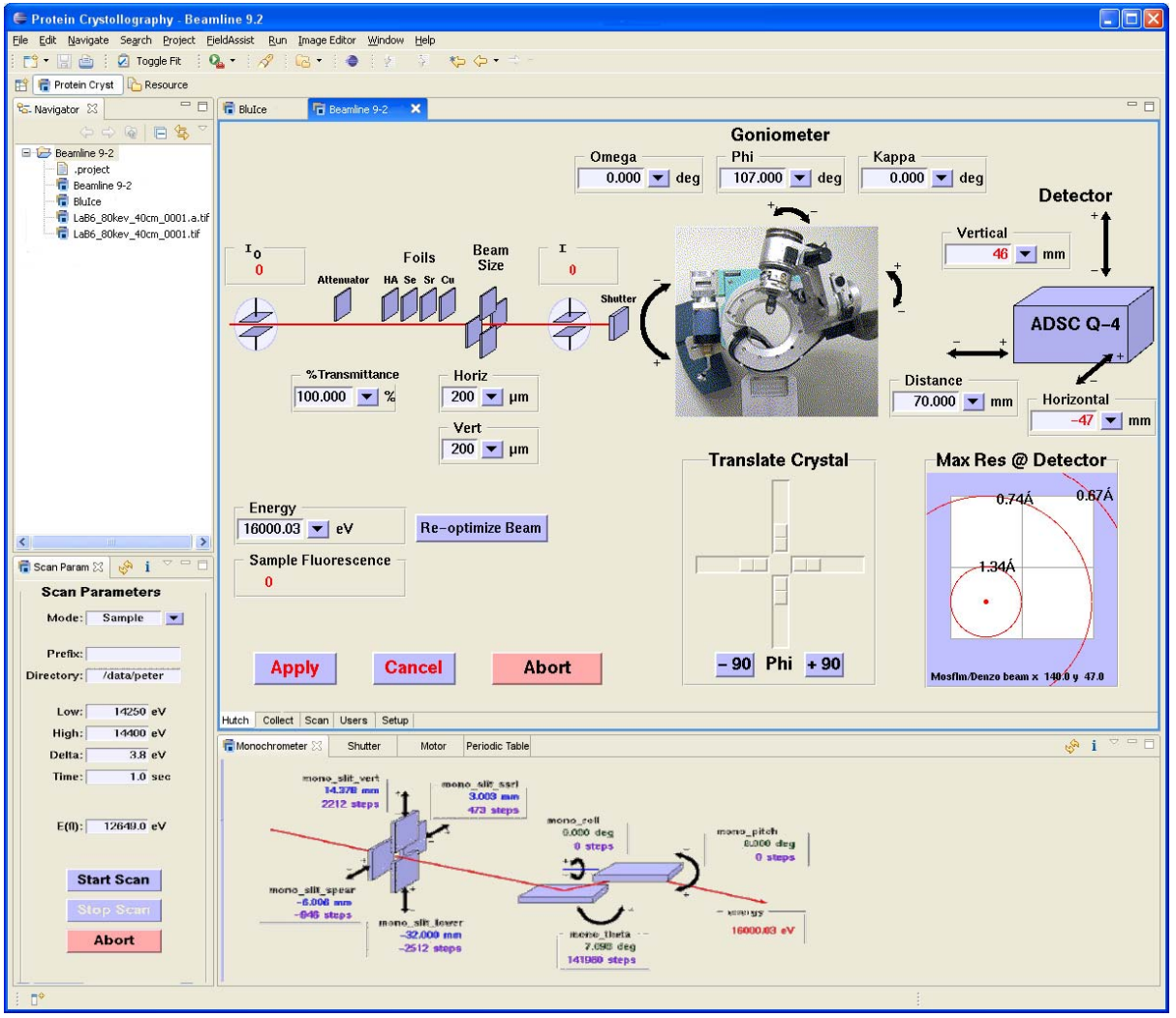
A Perspective Can be a Single Application



Area Data Editor



X-Ray Experiment

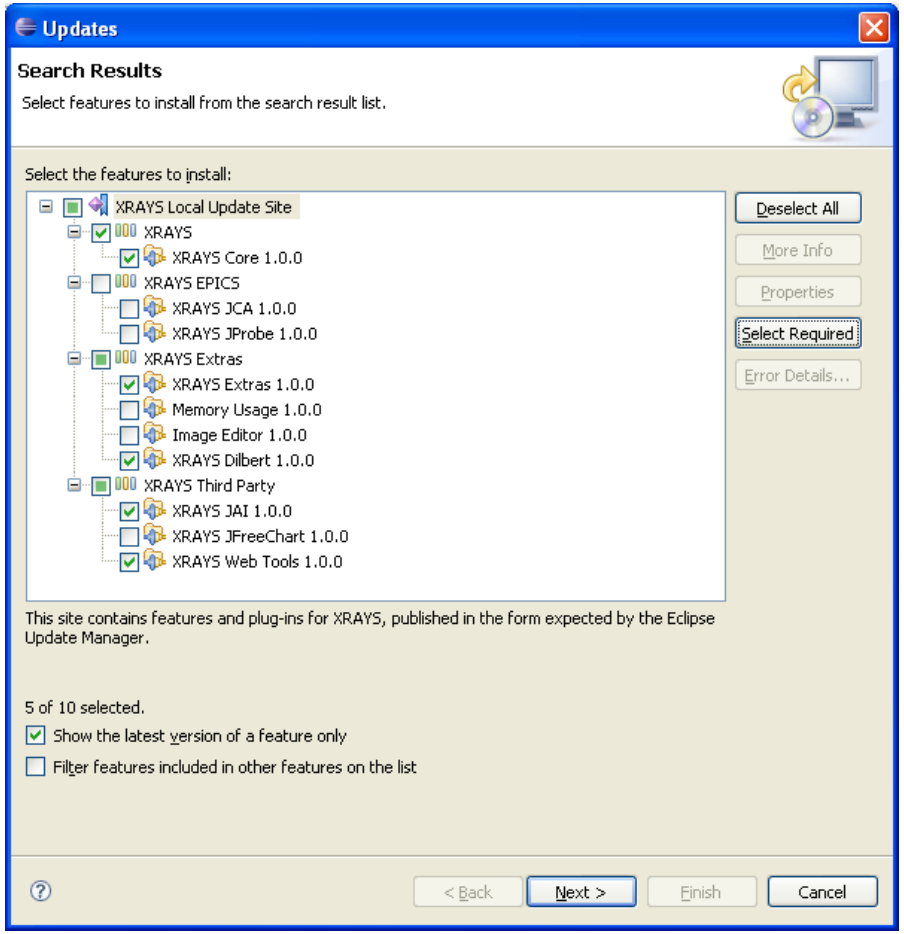


Images from: BLU-ICE and the Distributed Control System, NOBUGS III, January 2000

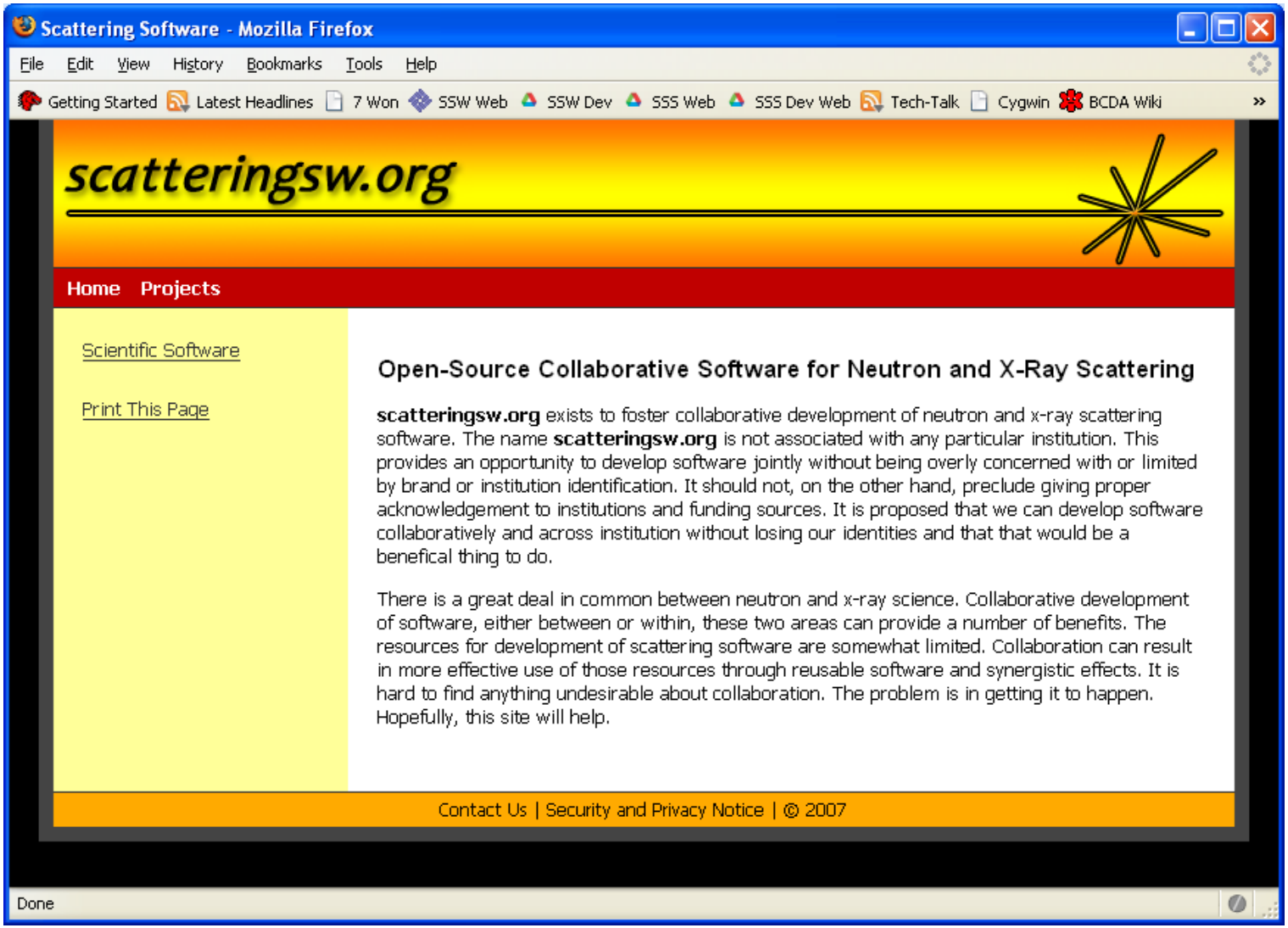
Deployable Plug-ins

- These Eclipse projects are available through the Eclipse update mechanism at http://www.scatteringsw.org/XRAYS/updates

- 10 features in 4 categories consisting of ~25 plug-ins
- Work in Progress
  - Not thoroughly tested
  - Not fully documented
- Not really scientific software
  - But potentially useful



scatteringsw.org



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- Pete Jemian – Group Leader of the APS BCDA group
  - Is invaluable in helping provide the direction for this effort.

Thank You

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