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Report on the 2006 XSD Scientific Software Workshop

Kenneth Evans, Jr.

Presented at the APS/Users Monthly Operations Meeting

September 27, 2006

Argonne National Laboratory, Argonne, IL

The Workshop is Part of a Larger Initiative

- The purpose is to establish a coordinated software development program at the APS

- Step 1: A study group was formed last fall
  - To see what others are doing, in particular DANSE
- Step 2: A workshop committee was formed
  - As part of the APS upgrade process
  - The committee sent out requests for input to over 100 members of the community and has compiled the responses
  - The members have provided their own expertise
  - The workshop was held on August 29
  - There will be a report with findings and recommendations
- Step 3: A Scientific Software Section has been formed in BCDA
  - Hiring 2 software developers has been requested

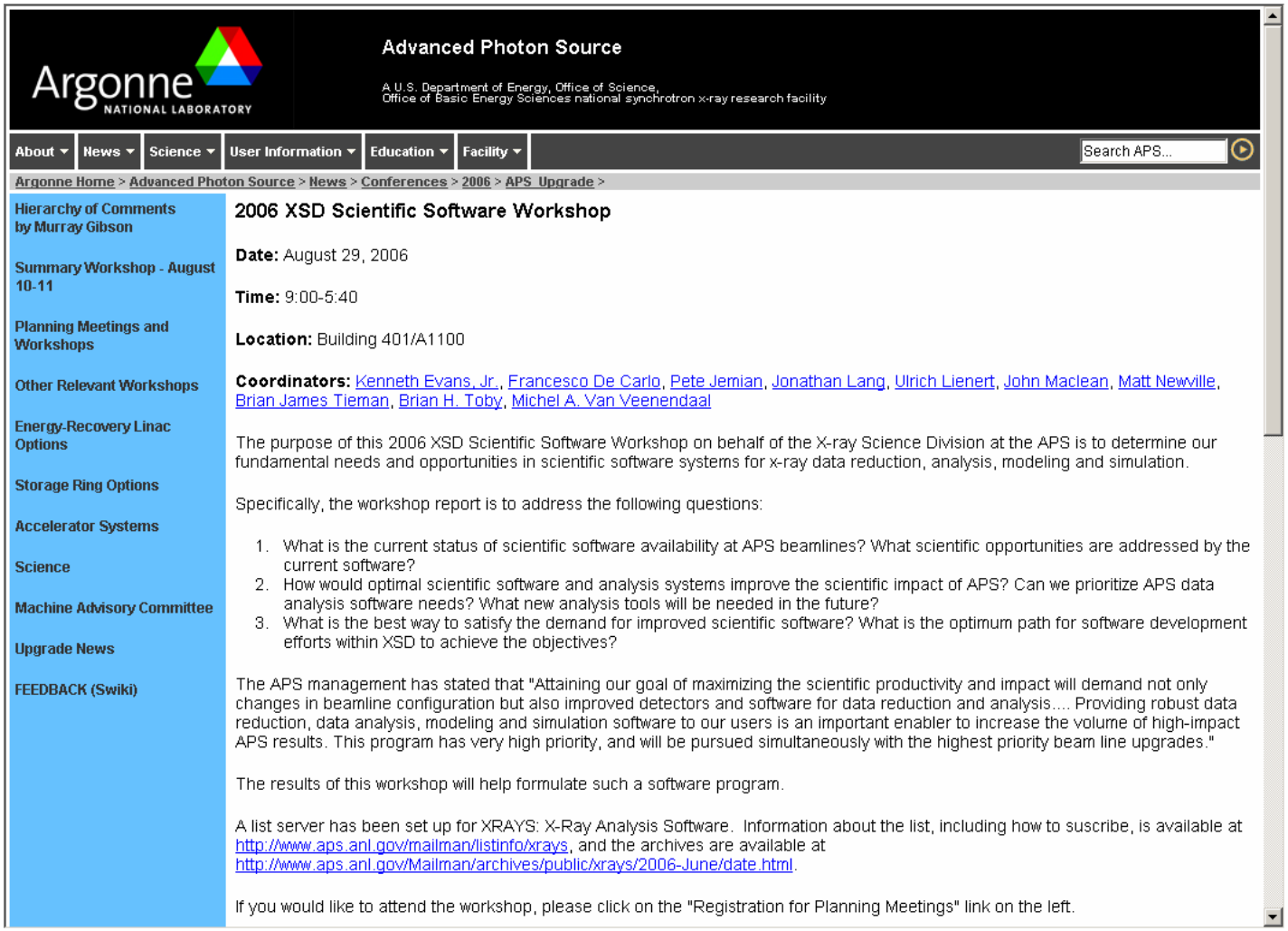
The Committee

- Kenneth Evans, Jr.
- Francesco De Carlo
- Pete Jemian
- Jonathan Lang
- Ulrich Lienert
- John Maclean
- Matt Newville
- Brian James Tieman
- Brian H. Toby
- Michel A. Van Veenendaal

- If you want input into the process, please contact a member of the committee
  - They will be glad to help
  - Your input is important

The Best Source of Information is the Workshop Web Page

- Look under Conferences & Workshops



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Advanced Photon Source

A U.S. Department of Energy, Office of Science,
Office of Basic Energy Sciences national synchrotron x-ray research facility

About | News | Science | User Information | Education | Facility | Search APS...

Argonne Home > Advanced Photon Source > News > Conferences > 2006 > APS_Upgrade >

Hierarchy of Comments by Murray Gibson

Summary Workshop - August 10-11

Planning Meetings and Workshops

Other Relevant Workshops

Energy-Recovery Linac Options

Storage Ring Options

Accelerator Systems

Science

Machine Advisory Committee

Upgrade News

FEEDBACK (Swiki)

2006 XSD Scientific Software Workshop

Date: August 29, 2006

Time: 9:00-5:40

Location: Building 401/A1100

Coordinators: Kenneth Evans, Jr., Francesco De Carlo, Pete Jemian, Jonathan Lang, Ulrich Lienert, John Maclean, Matt Newville, Brian James Tieman, Brian H. Toby, Michel A. Van Veenendaal

The purpose of this 2006 XSD Scientific Software Workshop on behalf of the X-ray Science Division at the APS is to determine our fundamental needs and opportunities in scientific software systems for x-ray data reduction, analysis, modeling and simulation.

Specifically, the workshop report is to address the following questions:

1. What is the current status of scientific software availability at APS beamlines? What scientific opportunities are addressed by the current software?
2. How would optimal scientific software and analysis systems improve the scientific impact of APS? Can we prioritize APS data analysis software needs? What new analysis tools will be needed in the future?
3. What is the best way to satisfy the demand for improved scientific software? What is the optimum path for software development efforts within XSD to achieve the objectives?

The APS management has stated that "Attaining our goal of maximizing the scientific productivity and impact will demand not only changes in beamline configuration but also improved detectors and software for data reduction and analysis.... Providing robust data reduction, data analysis, modeling and simulation software to our users is an important enabler to increase the volume of high-impact APS results. This program has very high priority, and will be pursued simultaneously with the highest priority beam line upgrades."

The results of this workshop will help formulate such a software program.

A list server has been set up for XRAYS: X-Ray Analysis Software. Information about the list, including how to suscribe, is available at http://www.aps.anl.gov/mailman/listinfo/xrays, and the archives are available at http://www.aps.anl.gov/Mailman/archives/public/xrays/2006-June/date.html.

If you would like to attend the workshop, please click on the "Registration for Planning Meetings" link on the left.

The Presentations

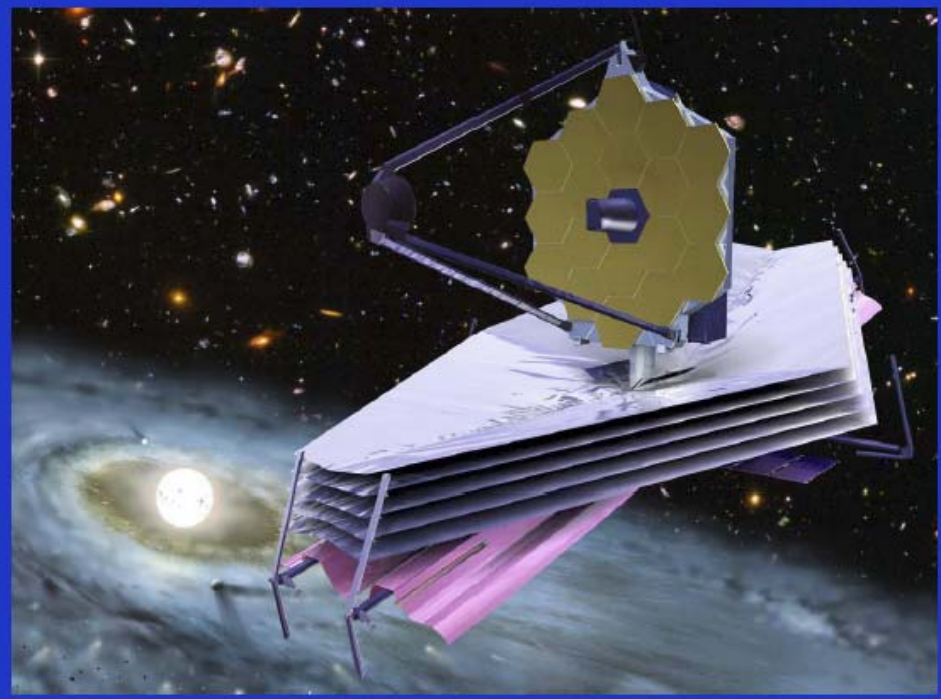
- The presentations will be on the workshop page
  - After the usual legal authorizations
- One slide from each presentation will be shown here
  - Chosen more for graphic impact than content
  - To give a flavor of the workshop
  - To shamelessly serve my own purposes

Data Archive and Science Software Tools in Ground-Based and Space Astronomy

Knox Long
Space Telescope Science Institute

Conclusions from astronomy for this workshop

- **Standardize data formats across instruments and facilities**
- **If archival analysis is important, then must**
  - Standardize data taking modes
  - Ensure sufficient metadata to describe the observations
  - Standardize analysis
- **If common analysis procedures are important**
  - Adopt a user environment that has a very large user base
    - Python, or something similar
- **No matter how optimal the architecture, scientists will not use it unless it provides functionality that is needed**
- **Webb plans**
  - FITS-compatible formats
  - VO-ready products
  - Pyraf
  - Pipelines and other heavy duty applications in c



James Webb Space Telescope (1-28 μ) 2013

A Data Analysis Framework for the Neutron Community

Michael McKerns
Caltech, Project Manager of DANSE

What is DANSE?

- a 12M$ five-year NSF IMR-MIP software construction project
- a collaborative effort between software professionals, neutron scattering scientists, and facilities

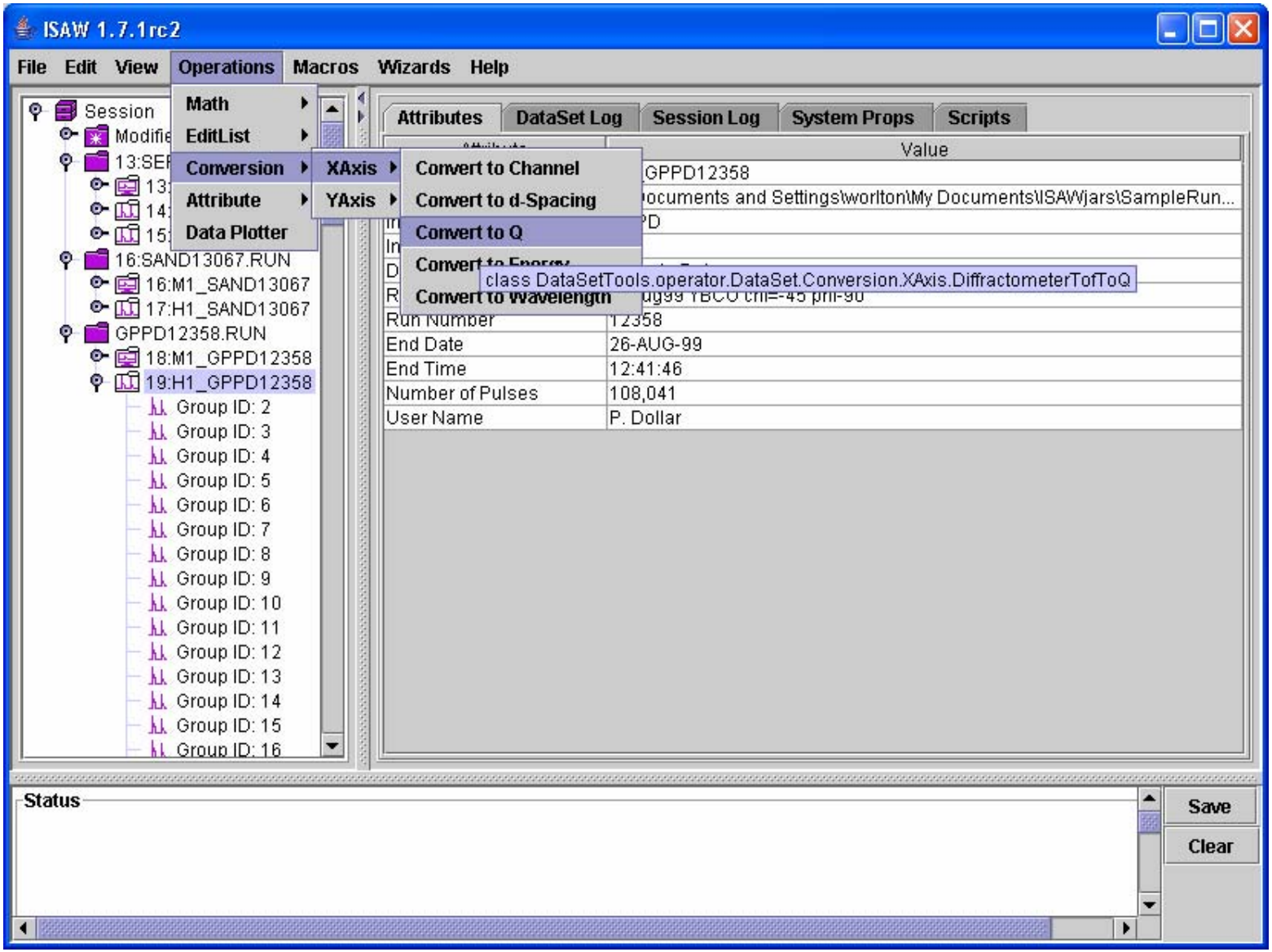
- a software engineering effort
  - open-source development environment
  - framework for the interoperability of modular components
  - integration of legacy codes and community-standard software
  - connectivity to facility databases and software repositories
- a scientific endeavor
  - to develop software modules for different subfields of neutron scattering
  - to enhance neutron scattering research and facilitate new science
  - to build tools for education, collaboration, and plausibility assessment

- an integration framework for building data analysis, visualization, modeling, and instrument simulation tools for all areas of neutron scattering

Visualization and Analysis with ISAW

Tom Worlton
Argonne, Group Leader for Controls and Computing at IPNS

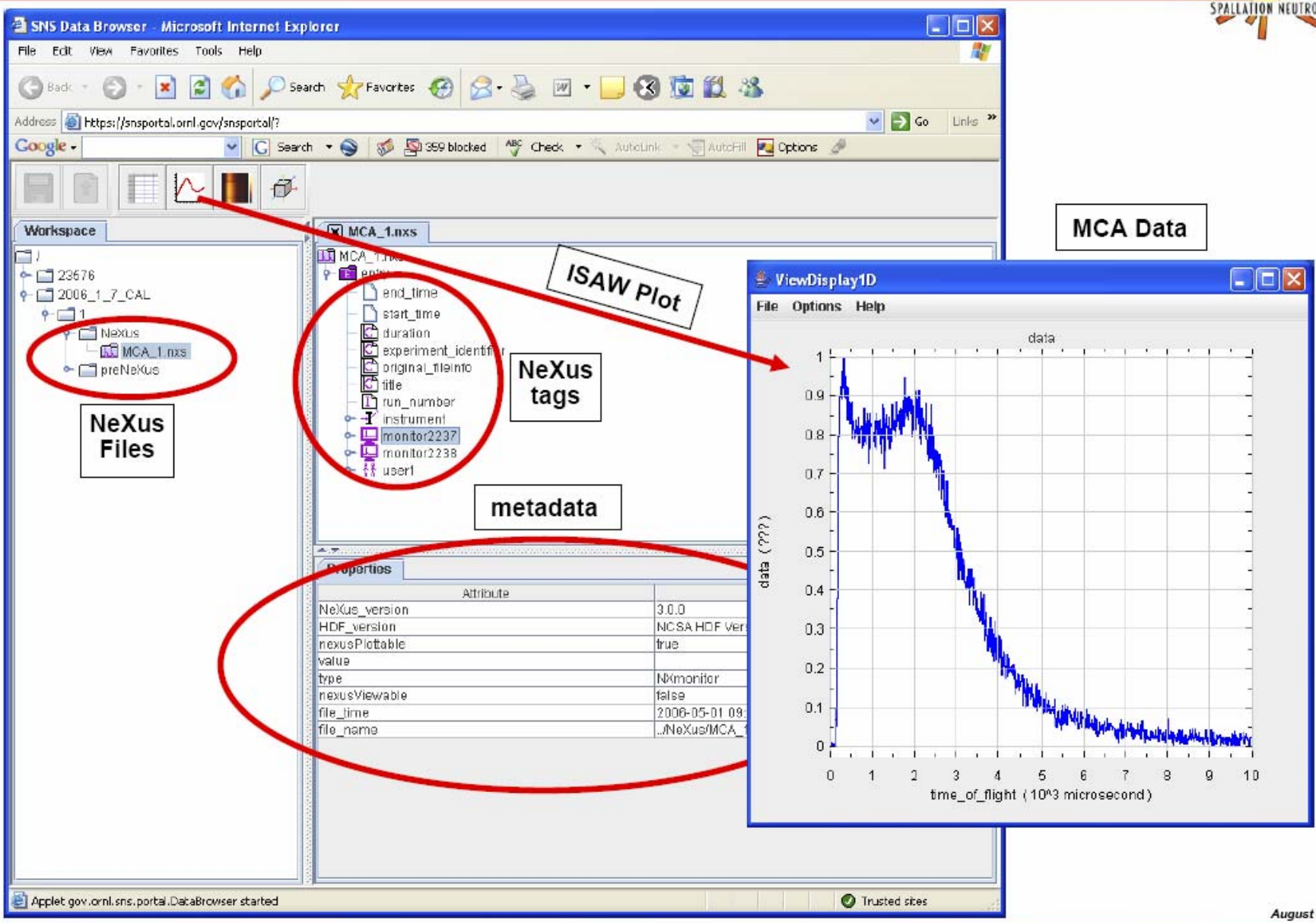
ISAW DataSet operations



Software Development at SNS

Steve Miller
Oak Ridge, Analysis Software Team Leader for the SNS

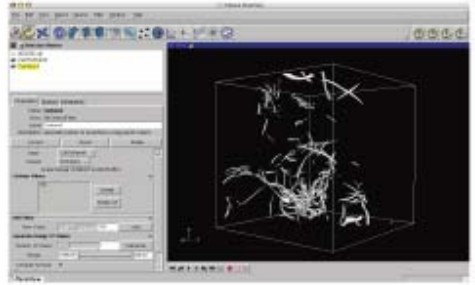
Visualizing Data via the Portal



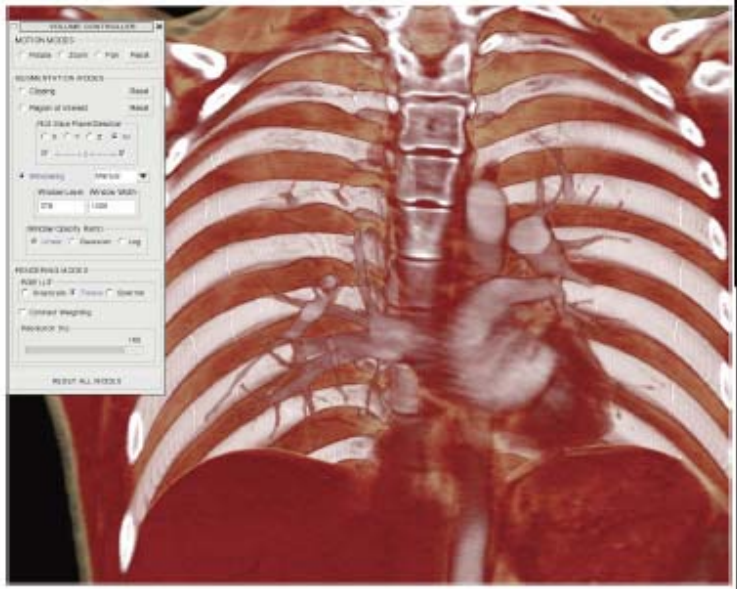
Visualization, Collaboration, and the Grid

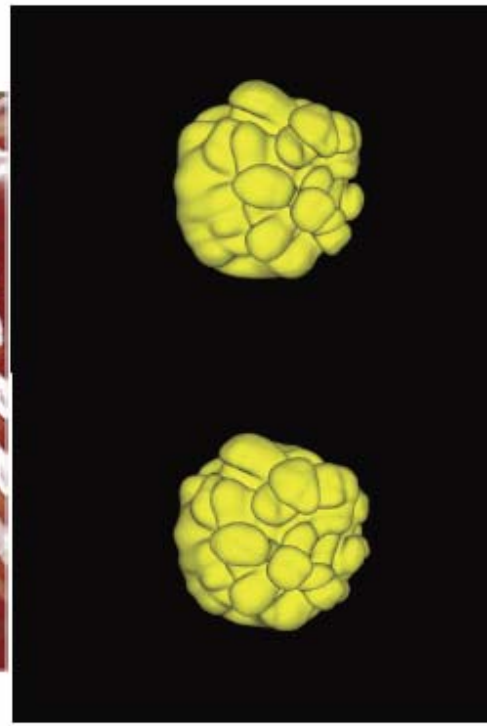
Michael E. Papka
Argonne, Mathematics and Computer Science

Visualization



- Gaming cards bring unprecedented graphics capabilities
  - 1 GB Memory (512 MB per GPU) — 512^3 volume in memory of card
  - > 500 million triangles per second — complex polygonal models in real-time
- High level abstractions for development
  - OpenGL 2.0
  - OpenGL Shader Language
  - Visualization Toolkit
  - ParaView



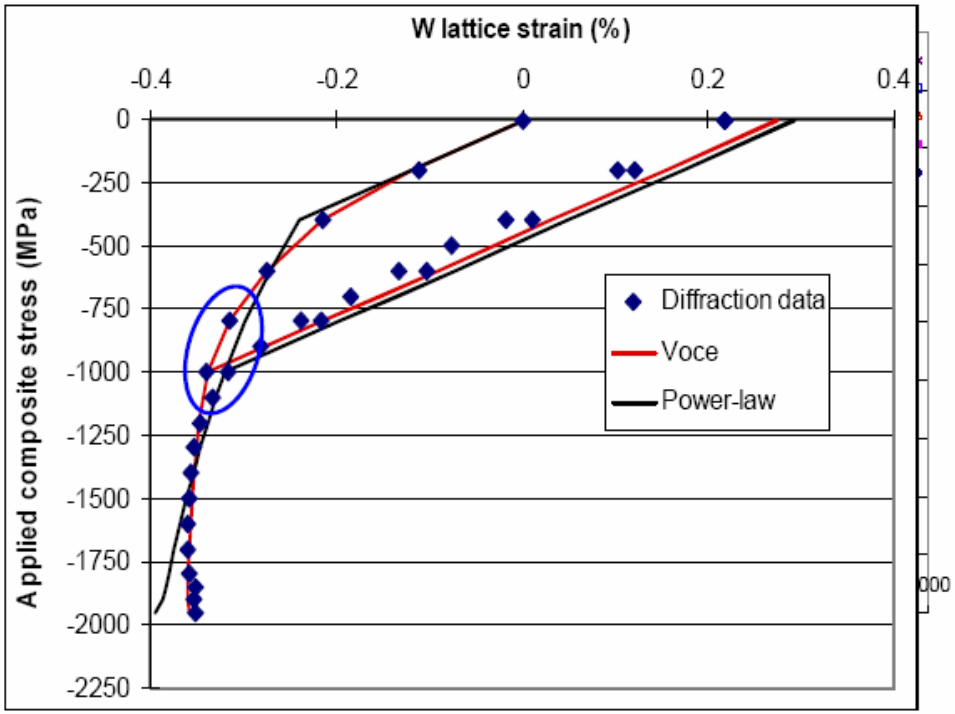


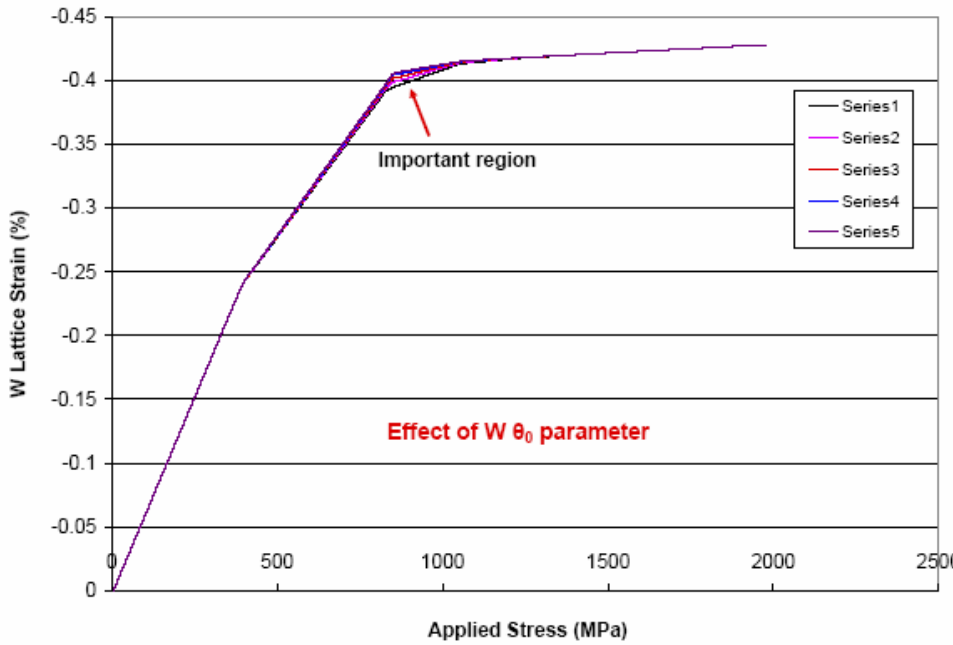
A User's Perspective on Software: Lessons Learned from DANSE

Ersan Üstündag
Iowa State University

Neural Network Analysis

Sensitivity Studies





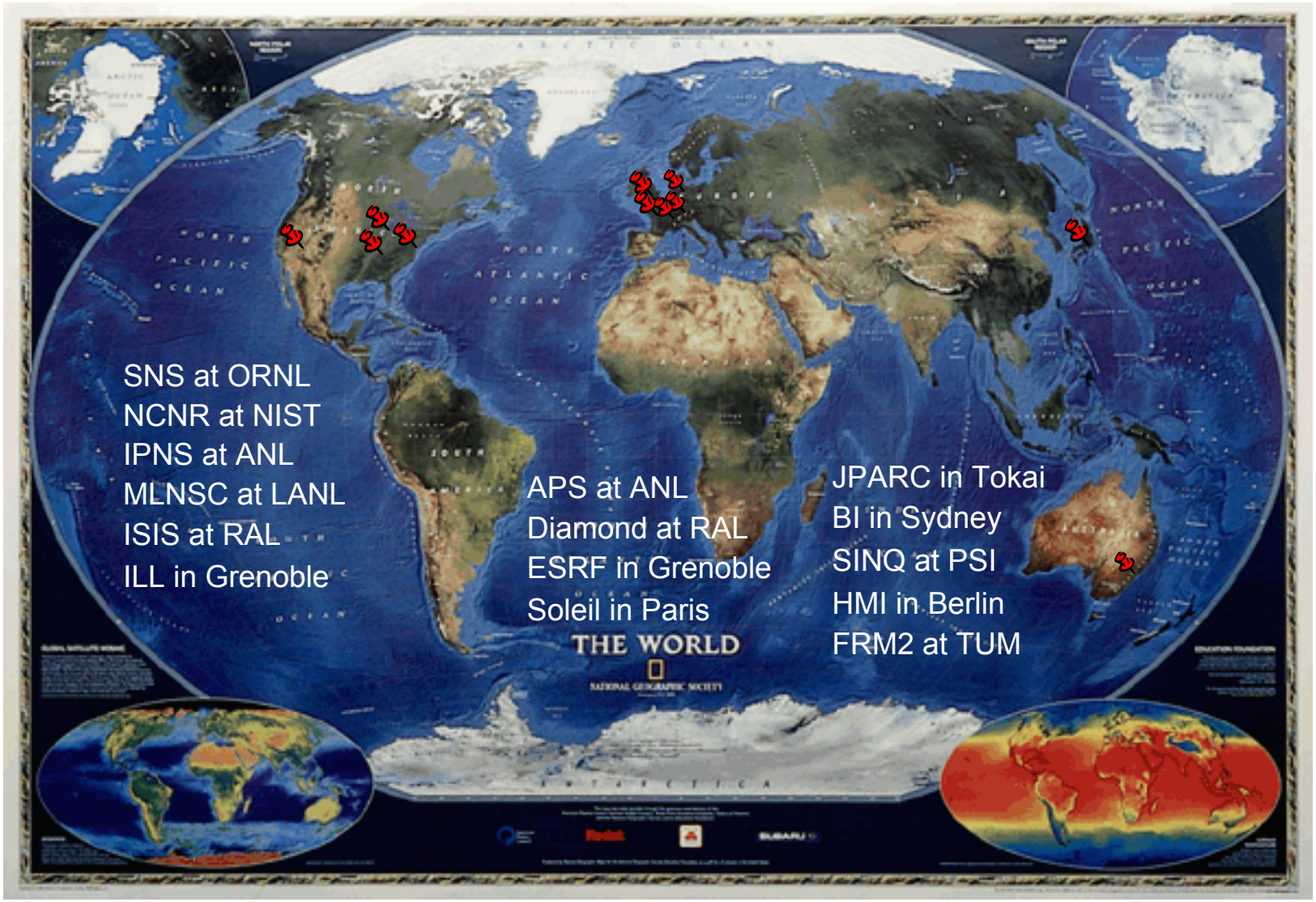
- **Strong influence by parameters:** $(\sigma_0)_{BMG}$, $(\sigma_0)_W$, $(\sigma_1)_W$ **and** $(\theta_0)_W$
- **Weak/no influence by parameters:** n_{BMG}, $(\theta_1)_W$ **and** ΔT
- ***Rigorous experiment planning to optimize data collection***

L. Li *et al.*

NeXus: The Advantages of a Common Data Format

Ray Osborne
Argonne, Materials Science Division

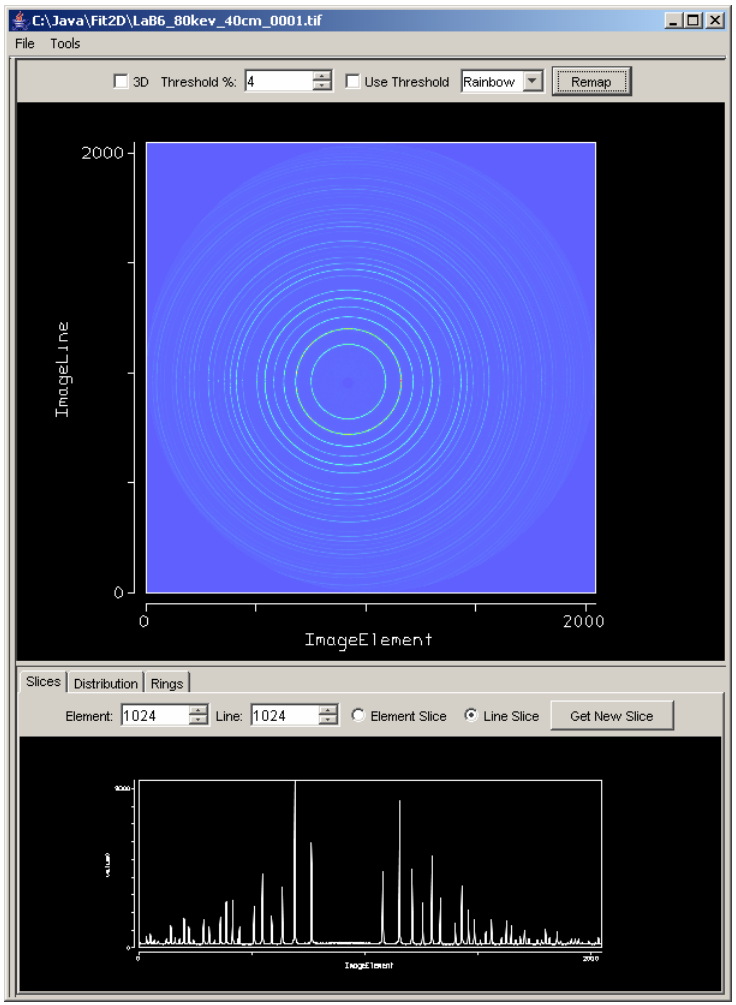
NeXus Community

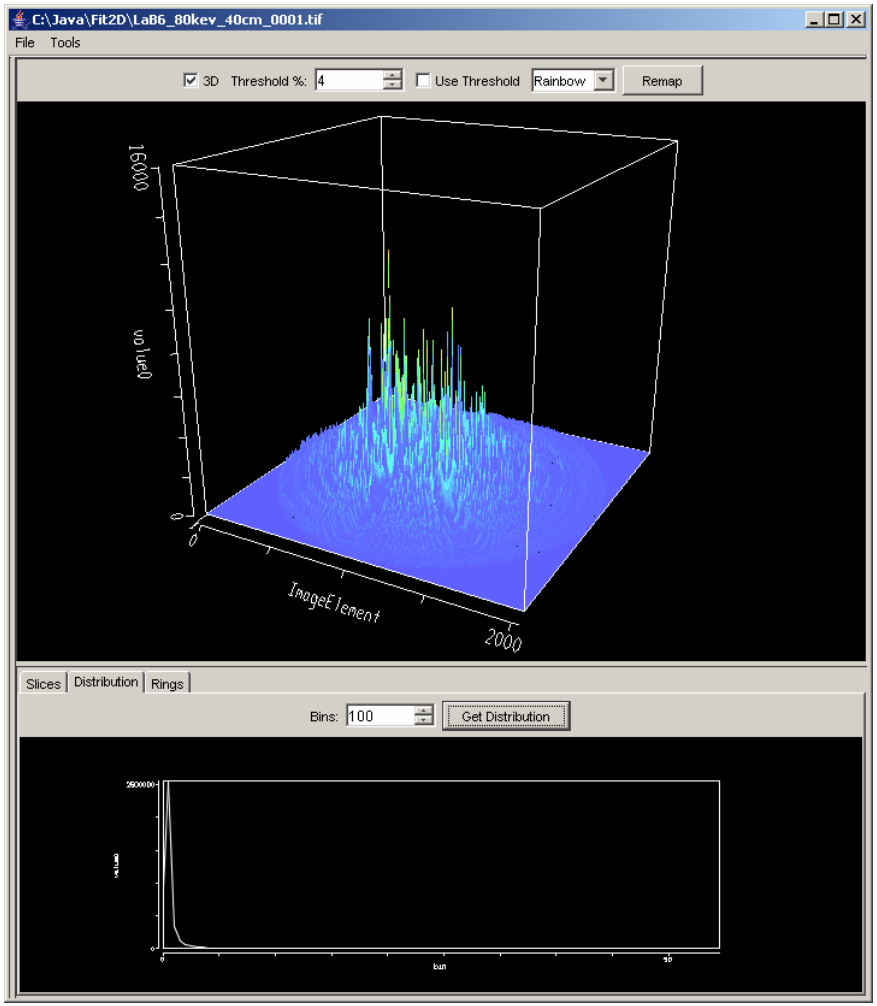


Workbenches, Toolboxes, and Frameworks

Ken Evans
Argonne, APS Controls Group

Prototype Image Analysis Tool using VisAD Graphics



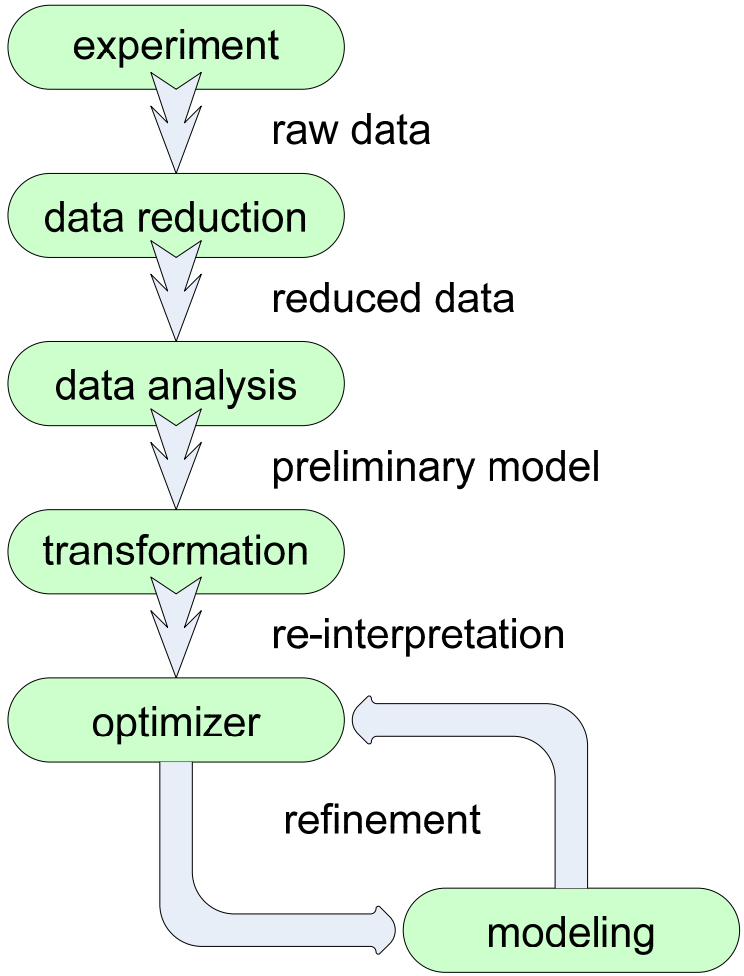


Workflow of the Data Analysis Process

Pete Jemian
Argonne, BCDA Group Leader

Typical Data Analysis Workflow

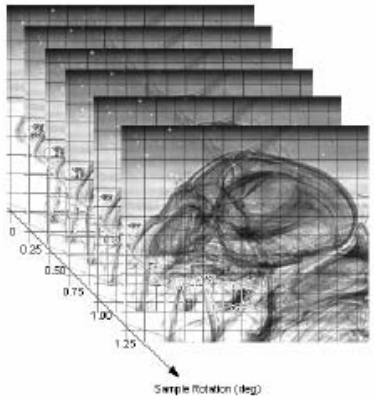
- Multi-step component processes
- Benefits from common data file format
- Data import/export mechanism is useful
- Needs visualization tools at each step
- Uses established software
- Uses custom software
- Connections are software, too!
- Each component may require a single computer or a cluster, depending on the science and objective

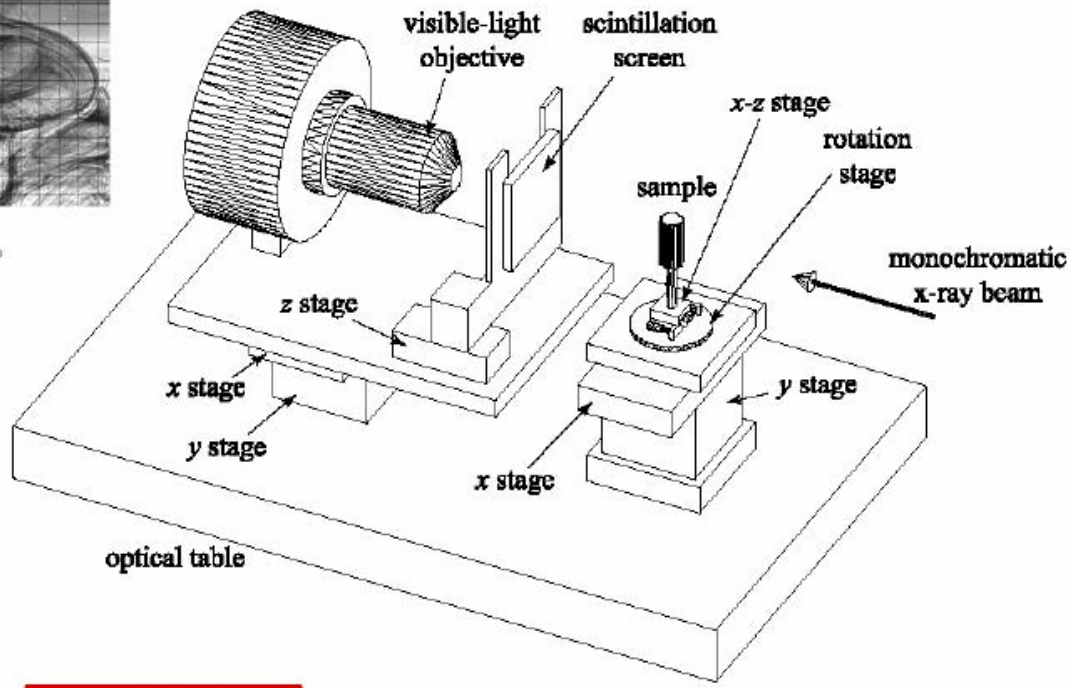


Software and Hardware Solution for the Tomography System at Sector 2

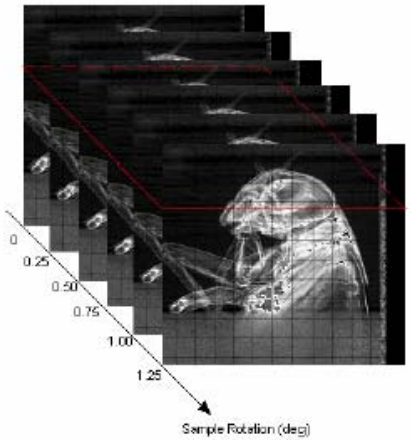
Francesco De Carlo
Argonne, Beamline Scientist, 2-BM

Tomography System

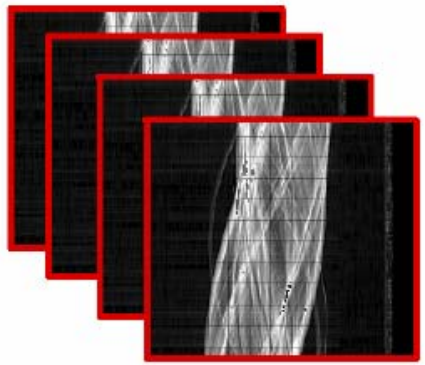




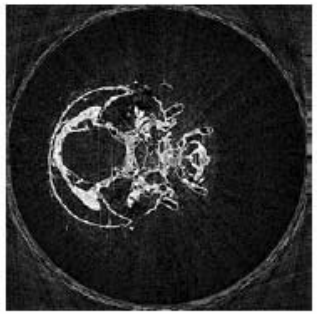
- NeXus/HDF
  - ImageJ plug-in
  - converters



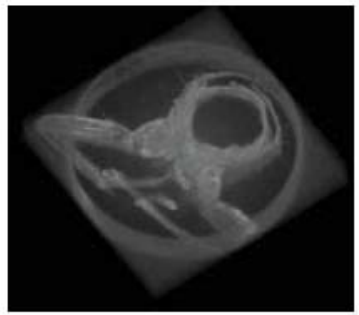
projections



sinograms



slices



3D rendering

Powder Diffraction Crystallography Software: the Present & Future

Brian Toby
Argonne, Materials Characterization Group Leader

How do we fit models to data?

Optimize a set of p parameters (coordinates, etc.) for an atomistic model.

- We have observations y_i with uncertainty $\sigma(y_i)$ at setting q_i
- The experimental observations are predicted by computing $M(p,q_i)$
- Fitting means that we want to minimize $\Sigma[M(p,q_i) - y_i]^2/\sigma^2(y_i)$

- This is achieved by solving $A^TWAp = A^TWy$
  - Where y is a vector of y_i values,
  - W is a weight matrix (diagonal for raw data)
  - $A_{ij} = \partial M(p,q_i) / \partial p_j$ (Design Matrix)

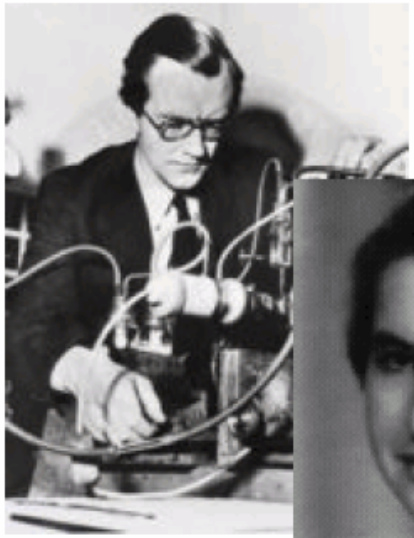
- Non-linear least squares: approximate $\partial M(p,q_i) / \partial p_j$ with a Taylor expansion and simplify to get $\delta = H^{-1}b$
  - $H = A^TWA$ (Hessian)
  - δ_j are shifts to apply to improve our initial p_j
  - $b_j = \Sigma_i[y_i - M(p,q_i)\ ]\ [\partial M/\partial p_j]\ /\sigma^2(y_i)$

Theory and Modeling

Michel van Veenendaal
Northern Illinois University and APS Synchrotron-Related Theory Group

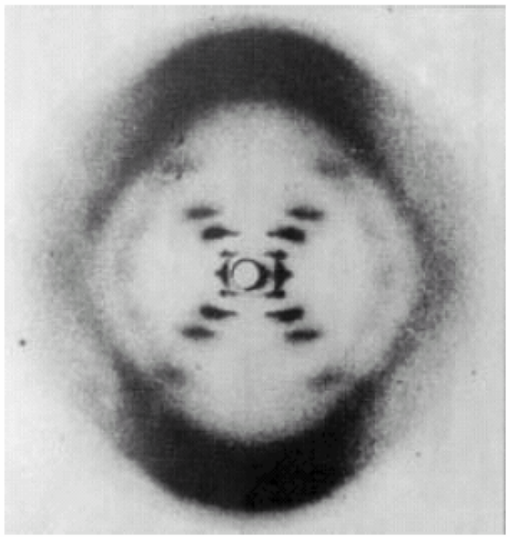
Data analysis was not always that straightforward:

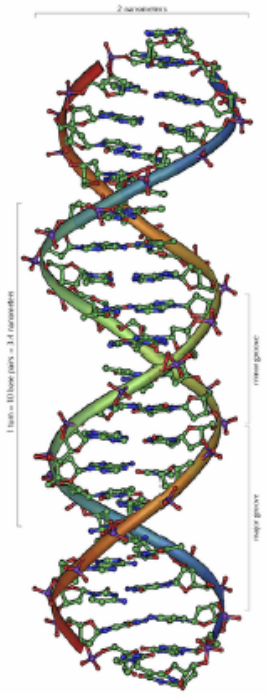
The Experimentalists:

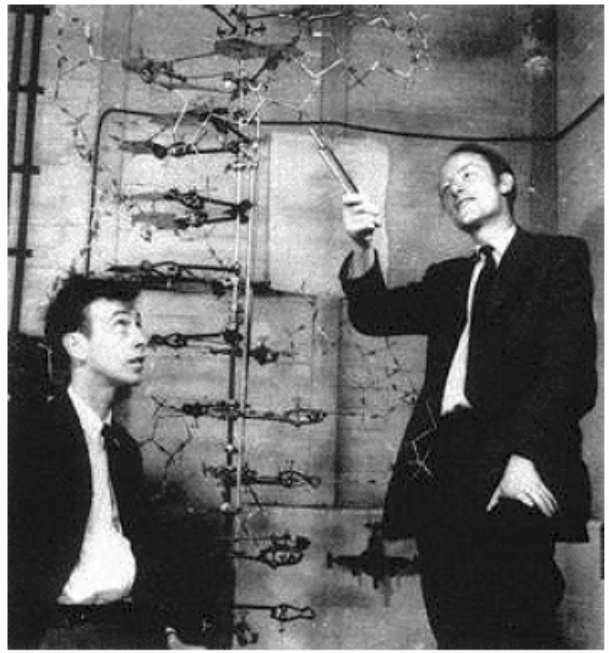


Rosalind Franklin

Maurice Wilkins







James Watson

Francis Crick

The Scientific Software Developers?

Software for XAFS Modeling and Analysis

Matt Newville
University of Chicago

What can the APS do?

For the XAFS community:

- Do we **need** a Framework? Probably not.
- We already have "at the beamline" and "take home on your laptop" analysis codes.
- Would we **use** a Framework if it existed? Maybe . . . .

Our main needs will not be met by more software engineering.

We need to focus on the Science and getting that science into software.

Thank You

This has been an

APS Scientific Software Presentation

Thank You

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