

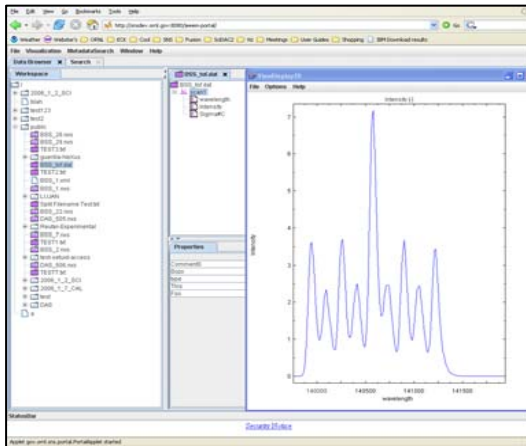
The SNS Science Portal: Web-Based Visualization, Analysis and Simulation



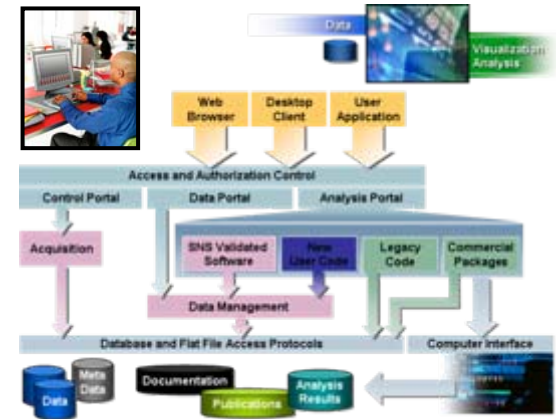
James “Jeeembo” Kohl

Computer Science and Mathematics

Oak Ridge National Laboratory



DANSE Meeting
Tuesday, January 23, 2007



Cast of ~~Thousands~~ Dozens!



SNS Scientific Computing Group

CSMD: James Kohl, Sudharshan Vazhkudai,
Jens Schwidder, Al Geist

SNS: Pete Peterson, Michael Reuter, Shelly Ren,
Jean-Christophe Bilheux, Steve Miller

CCS/TeraGrid: Vickie Lynch, John Cobb

CS/UTK: Tom Swain



Science Portal: One-stop shopping at SNS



- SNS manages
 - Multiple instruments, multiple users (2000/year)
 - Multiple services:
 - Data, acquisition, analysis, simulation, and visualization
- Portal is a common “gateway” to a complex set of services:
 - Software analysis tools and applications for neutron science data
 - Instruments and data **acquisition**
 - **Data** repositories, file systems, and archives
 - Databases with **metadata** and provenance
 - High-performance **computing** resources — analysis and simulation
 - Collaborative services — interactive **visualization**, information sharing
- Several access modes: web-based, desktop-applications...
- **Zero user cost:** Just a web browser, no client-side installation!

SNS Software Organization

Interfaces provide extensibility and integration;
they don't tie users to one framework



Software users run on their own computers using data downloaded from SNS

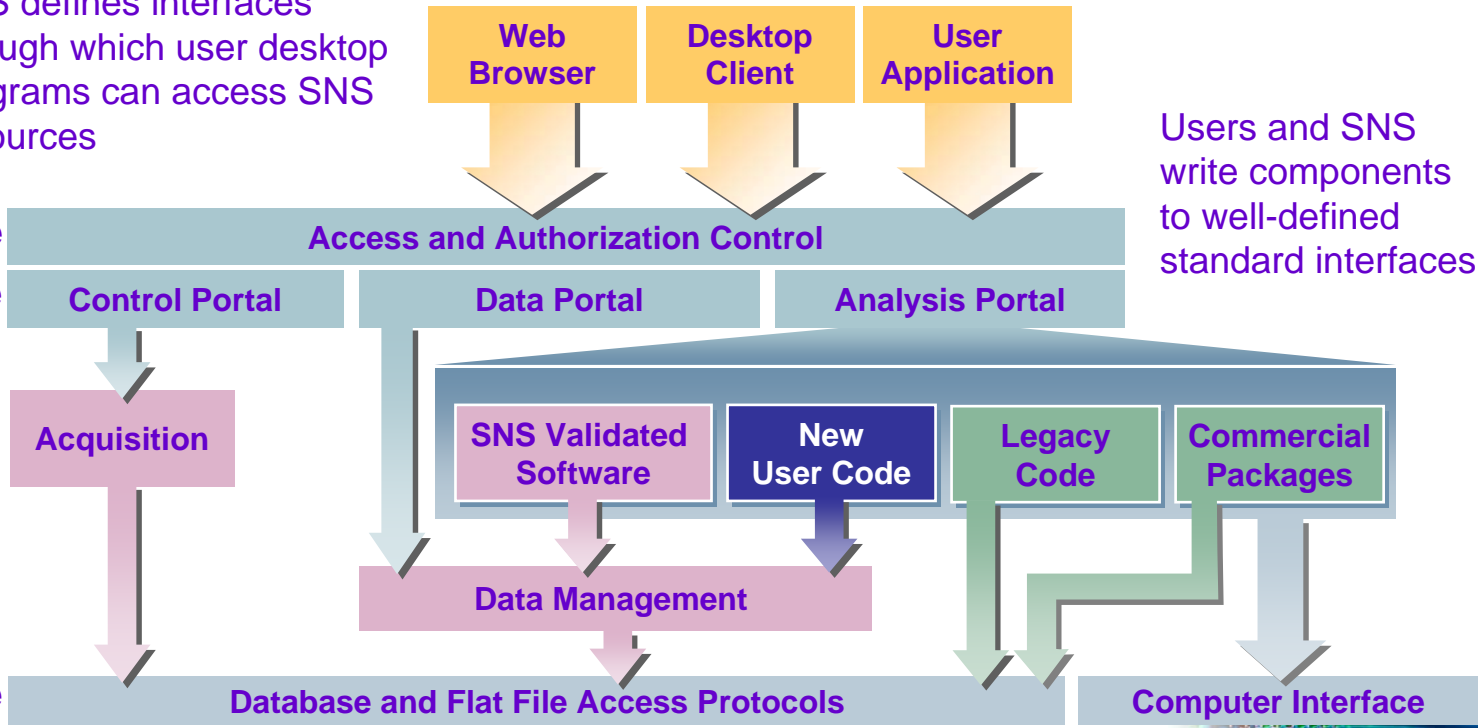
SNS defines interfaces through which user desktop programs can access SNS resources

Data



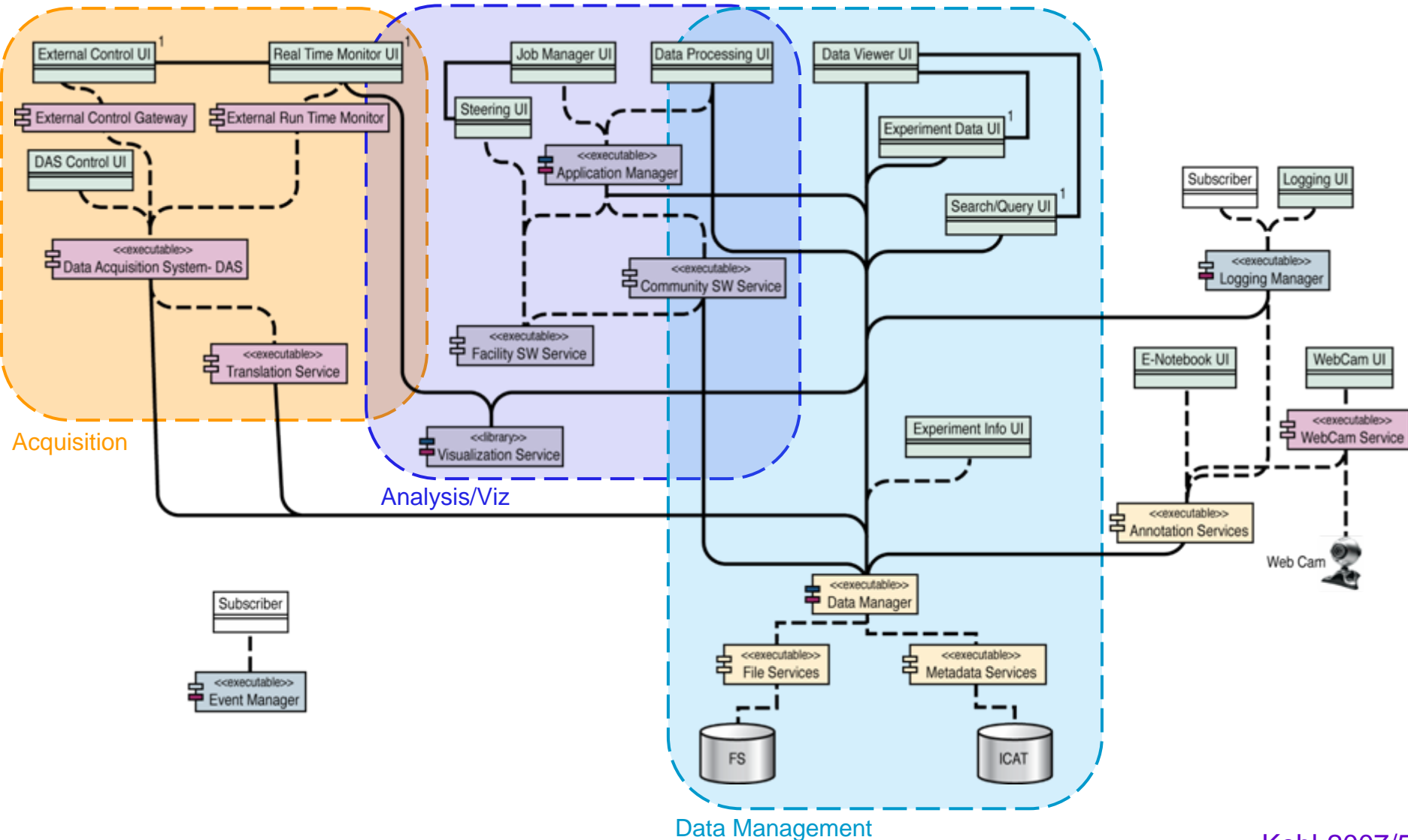
Visualization & Analysis

Security Interface
Function Interface



Users and SNS write components to well-defined standard interfaces

Backend SNS Software Architecture (interface specification / dependencies)



Data Management Hierarchy

/facility /instrument /ExperimentID /experiment /nexus_files
 /extra_metadata
 /submitted_analysis
 /shared

ICAT metadata catalog
Oracle DB

/facility /users /john /workspace (read/write)
 /ExperimentID (read only)
 /ExperimentID (read only)
 /public (read only)

/public /ExperimentID
 /ExperimentID *(Nightly update of /public...)*

Metadata Search

sample_name	create_time	instrument	file_name	experiment_number	formula	investigator_name
???	2006-05-03 11:57:42.0	BSS	BSS_1.ms	2006_1_2_SCI		
???	2006-05-03 11:57:42.0	BSS	BSS_1.ms	2006_1_2_SCI		
???	2006-04-28 14:46:09.0	MCA	MCA_1.ms	2006_1_7_SCI		
???	2006-05-03 11:57:42.0	BSS	BSS_1.ms	2006_1_2_SCI		
???	2006-04-28 14:46:09.0	MCA	MCA_1.ms	2006_1_7_SCI		
???	2006-04-28 14:46:09.0	MCA	MCA_1.ms	2006_1_7_SCI		

Optional Search Fields

ICAT Schema for SNS, Attribute search...

Workspaces created/updated when proposal accepted
Group permissions enforce facility authorization policy

(Note: Grayed names are symbolic links within the data hierarchy.)

Data Browsing in the Portal

- Workspace Tree Display

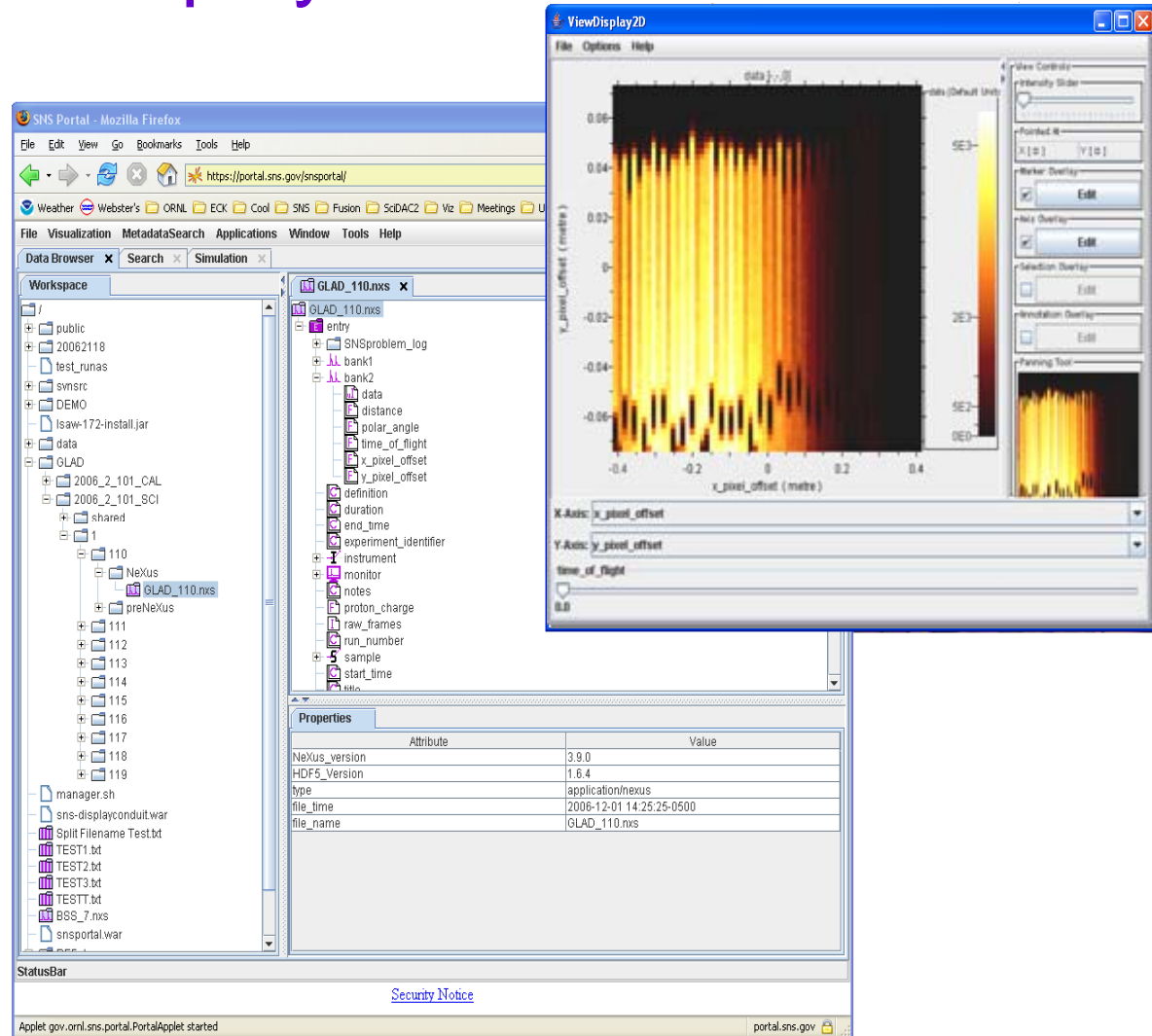
- NeXus Files
 - HDF & XML
- 3-Col ASCII (SPEC)
- XML Files
- Text Files

- Internal Struct

- Scans, Banks

- File Properties

- Basic File Ops

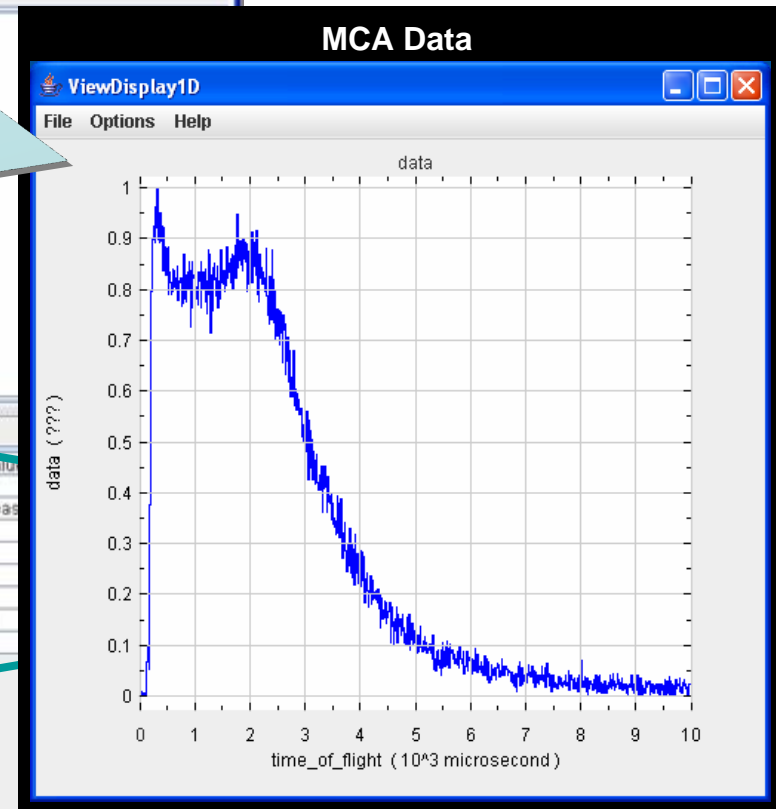


Browsing CD-4 data with SNS portal...

The screenshot shows the SNS Data Browser interface in Microsoft Internet Explorer. The address bar displays <https://snsportal.ornl.gov/snsportal/>. The workspace shows a file tree with folders like '23576', '2006_1_7_CAL', and '1'. Under '1', there are 'NeXus' and 'preNeXus' folders, with 'MCA_1.nxs' selected. A callout box labeled 'NeXus Files' points to this folder. The 'entry' section lists various attributes, with 'monitor2237' and 'monitor2238' highlighted. A callout box labeled 'NeXus Tags' points to these entries. The 'Properties' section at the bottom contains a table of metadata.

Attribute	Value
NeXus_version	3.0.0
HDF_version	NCSA HDF Version 4.2 Release
nexusPlottable	true
value	
type	NXmonitor
nexusViewable	false
file_time	2006-05-01 09:33:00-0500
file_name	./NeXus/MCA_1.nxs

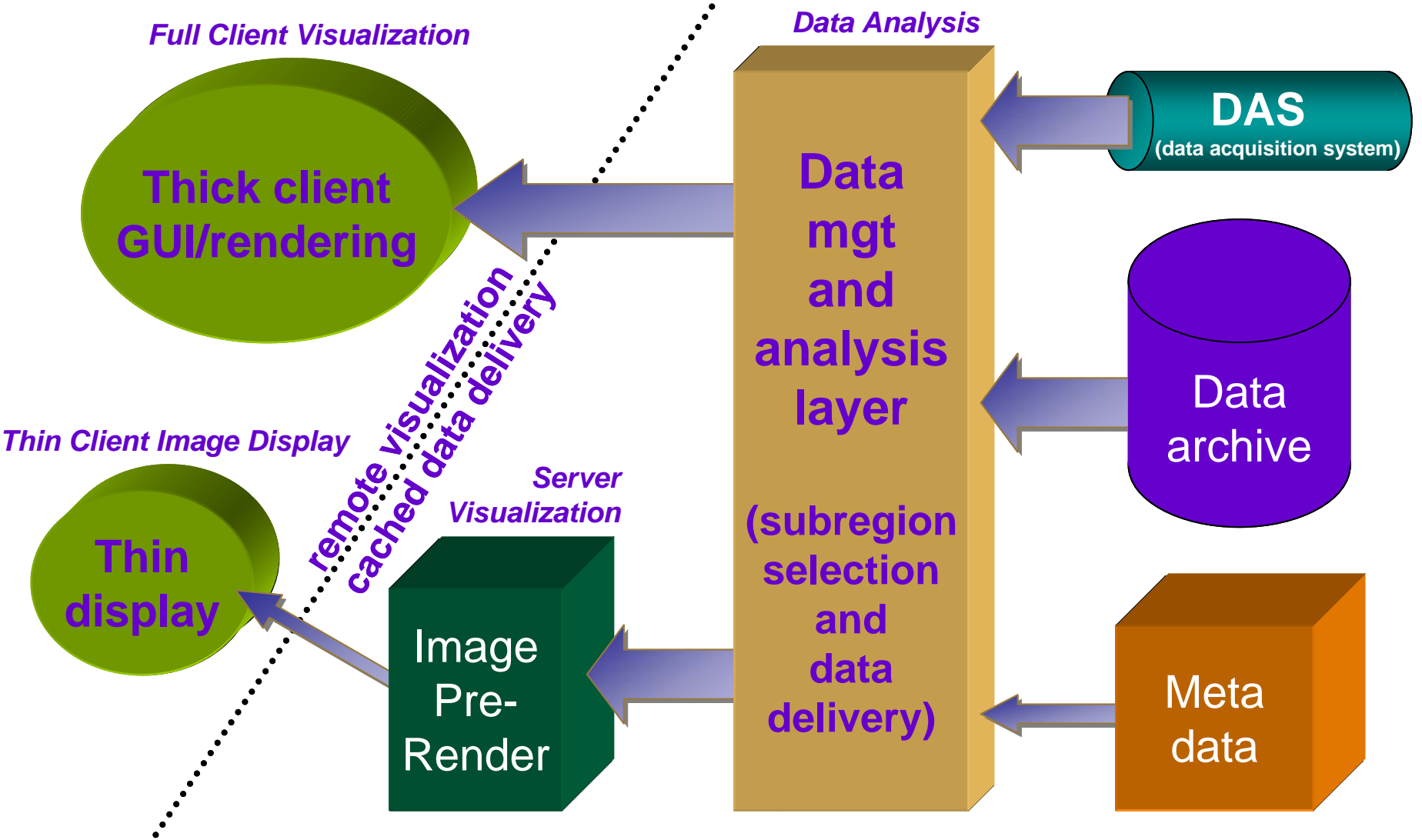
Callouts include 'NeXus Files', 'NeXus Tags', and 'Meta Data' (pointing to the Properties table). A large arrow labeled 'ISAW Plot' points from the 'nexusPlottable' attribute to the 'MCA Data' plot window.



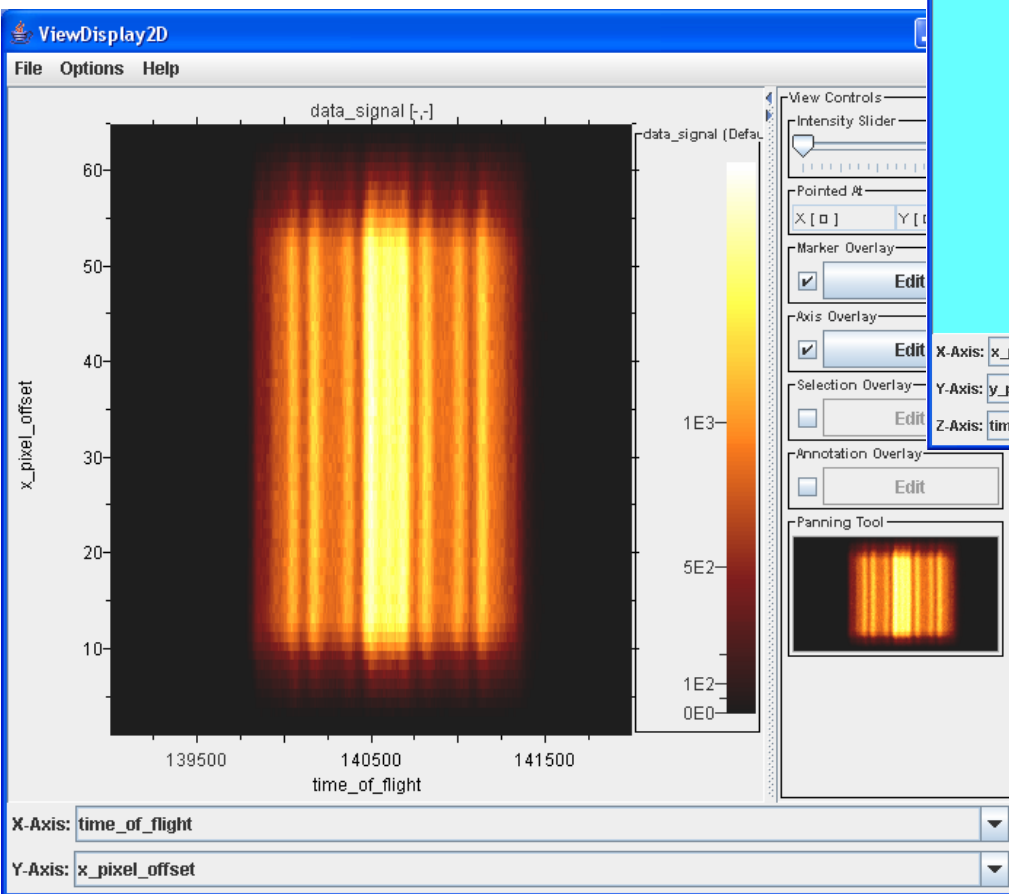
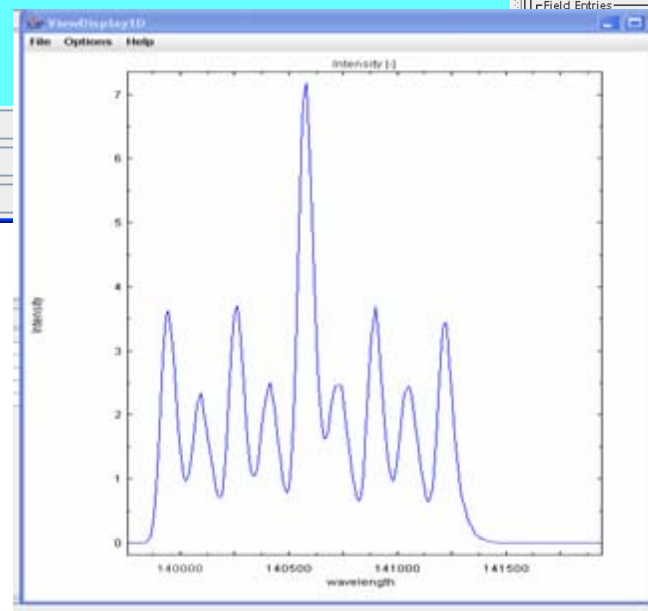
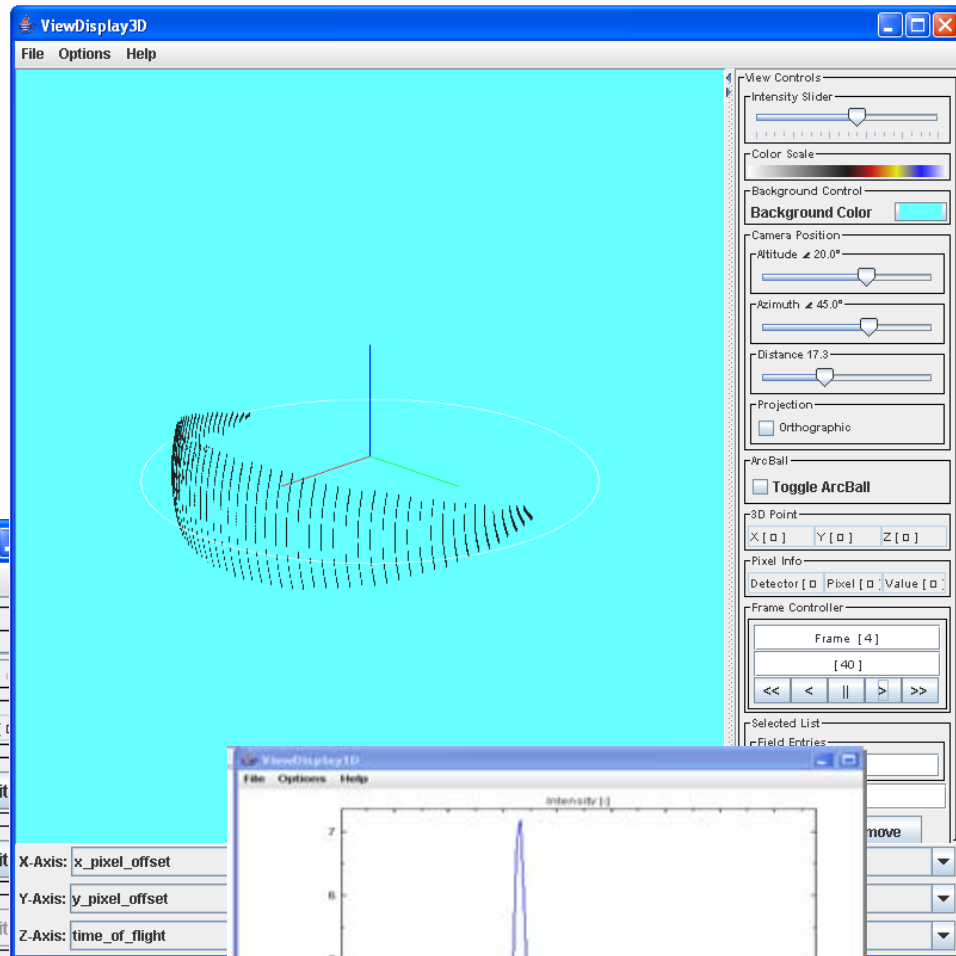
SNS Visualization Architecture *Revealed*

Front-End Client Side

Back-End Server Side

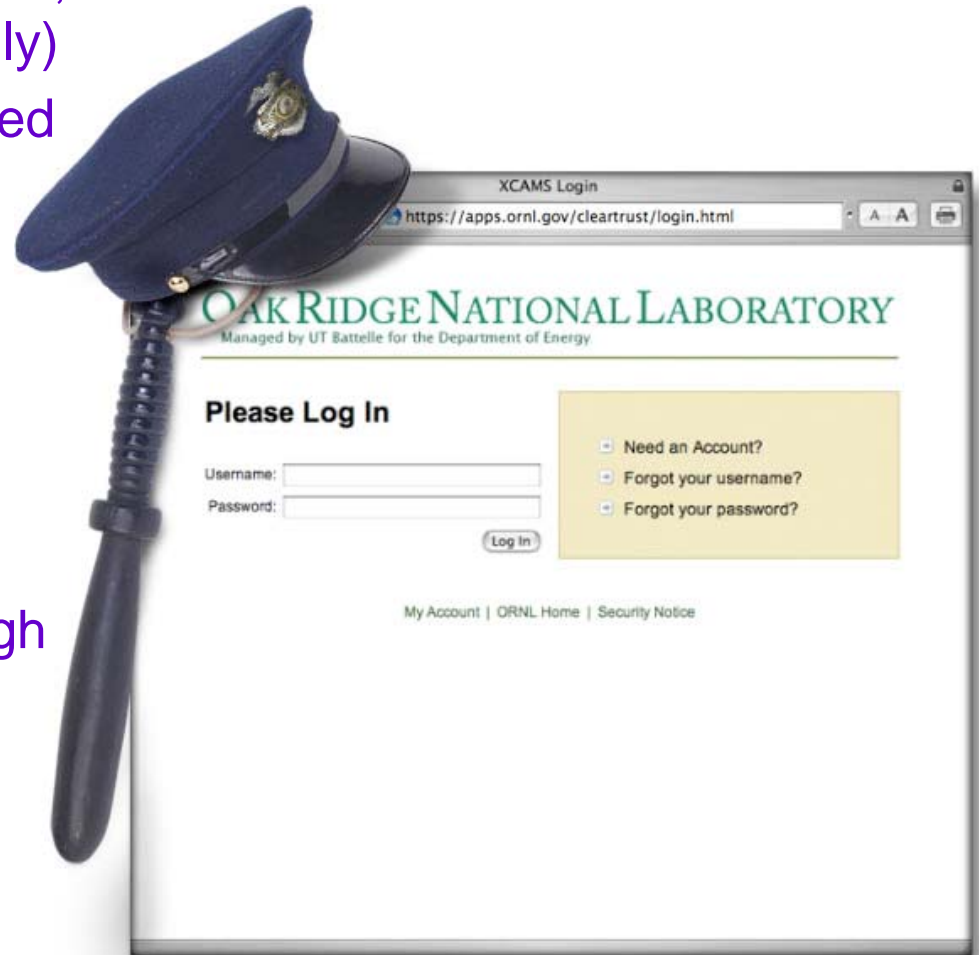


1-D, 2-D and 3-D Views (a la ISAW 😊)



Security/Authentication using XCAMS

- Portal authentication tied into ORNL XCAMS user authentication system, via ClearTrust (initial accounts only)
- Authenticated users are authorized to access resources:
 - Data management
 - Metadata/databases
 - Experiment proposals
 - High-performance Computing (HPC) systems/computing
- All portal transactions pass through authentication layer (i.e. “runas”)
- Future direction:
 - Support X.509 credentials to access other HPC resources



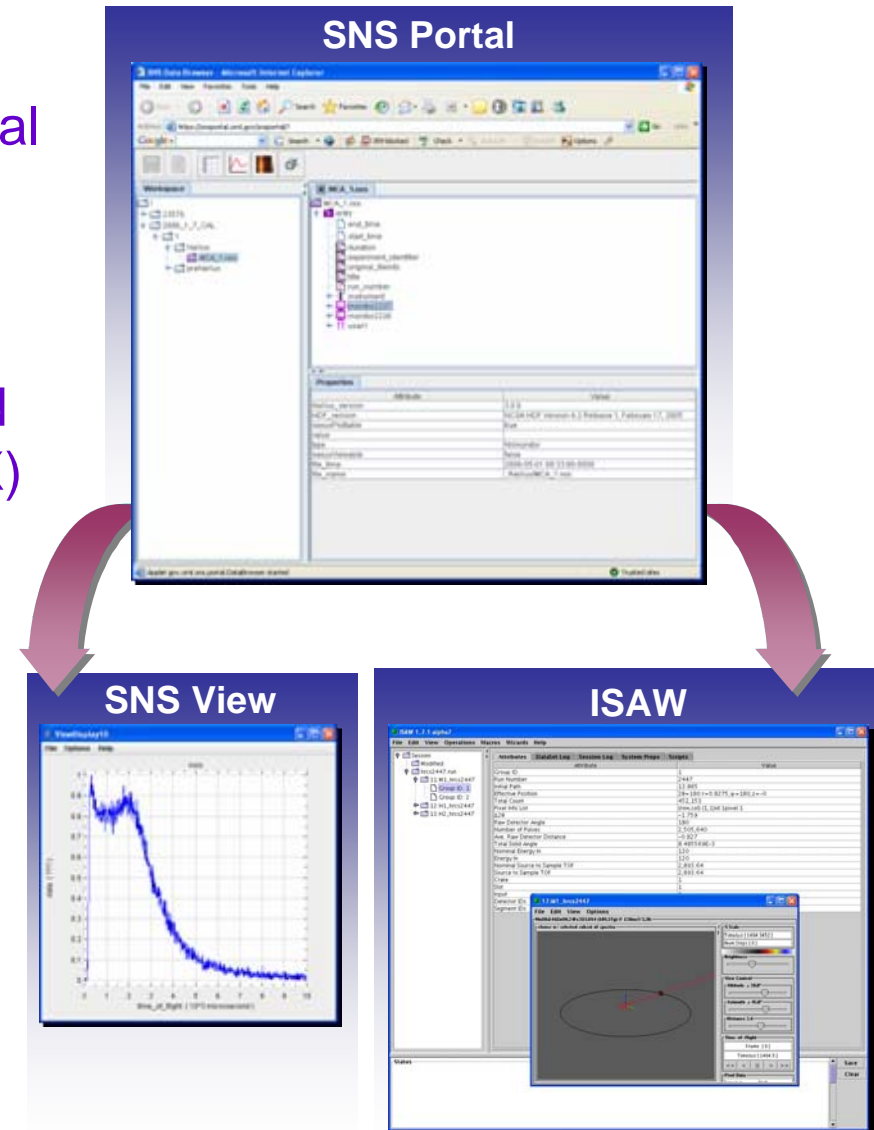
Portal Authorization & Access (a.k.a. “runas”)



- Access to Data via File/Group Permissions
 - Need to “setuid” to **become** the User...
 - Back-end Java server (no setuid!) must simultaneously handle multiple users...
 - Authorization moved into separate C program
 - All File Access of Any Kind Goes Through “runas”!
 - Read / Download, Raw Data (Viz), Tools, Simulations...
 - Ongoing struggle of Security vs. Accessibility
 - Root-squash filesystem mounts “protect” data...
 - No popping up “root” Xterms through the portal! :-o
 - Tricky to keep “runas” running...! ☺

Combining facility and community tools through the SNS Portal...

- “**Facility**” tools — newly developed or modules tightly integrated into the portal
- “**Community**” tools — existing monolithic or commercial/independent software
 - Java applet-based X-emulation and forwarding (using WiredX/WeeerdX)
 - Application executes on portal server backend/clusters and feeds into SNS data management
- No installation on user desktop:
 - Rootless window executions
 - “Looks and feels” like local...
- Capitalize and combine existing and evolving neutron science analysis tools



The SNS Remote Display Conduit (a.k.a. “WeerdX” 😊)

- Goal: Run Stand-Alone Tools through Portal!
 - Tools installed on server, not on each client...!
- “Extending” existing Java X Windows Server
 - WiredX ~ JCraft.com, “Heavy” Licen\$ing... ☹️
 - WeirdX ~ “Free” (Old Buggy) Code Snapshot... 😊
 - Evolving into “WeerdX” to suit our purposes...!
- Better than VNC ~ Rootless Windows
 - Looks and Feels like running on *Local* Client!
 - Extra Java applet pops up from main Portal window...
- Challenge to cover full X extensions/features

WeeerdX

ISAW

SNS Remote Display Conduit

ISAW 1.7.2

Attribute	Value
Group ID	1
Run Number	6942
Initial Path	10.5
Effective Position	2θ=65.454;r=1.5285,φ=65.078,z=0.26
Total Count	75,149
Pixel Info List	(row,col):(1,1)id:5 pixel:5 (row,col):(1,1)id:6 pixel:6...
Δ2θ	
Raw Detector Angle	
Omega	
Number of Pulses	
Total Solid Angle	

3:H1_glad6942

File Edit View Options Help

background

-Loaded H1_glad6942-

X Scale

Time(us) [100:12500]

Num Steps [2480]

Brightness

Auto-Scale

Image Data

Time(us)	NaN
Counts	NaN
Col_Row	NaN
Channel	NaN
d-Spacing(Å)	NaN
Q(Inverse Å)	NaN
E(meV)	NaN
λ(Å)	NaN

Graph Data

Time(us)	NaN
Counts	NaN
Col_Row	NaN
Channel	NaN

Java Applet Window

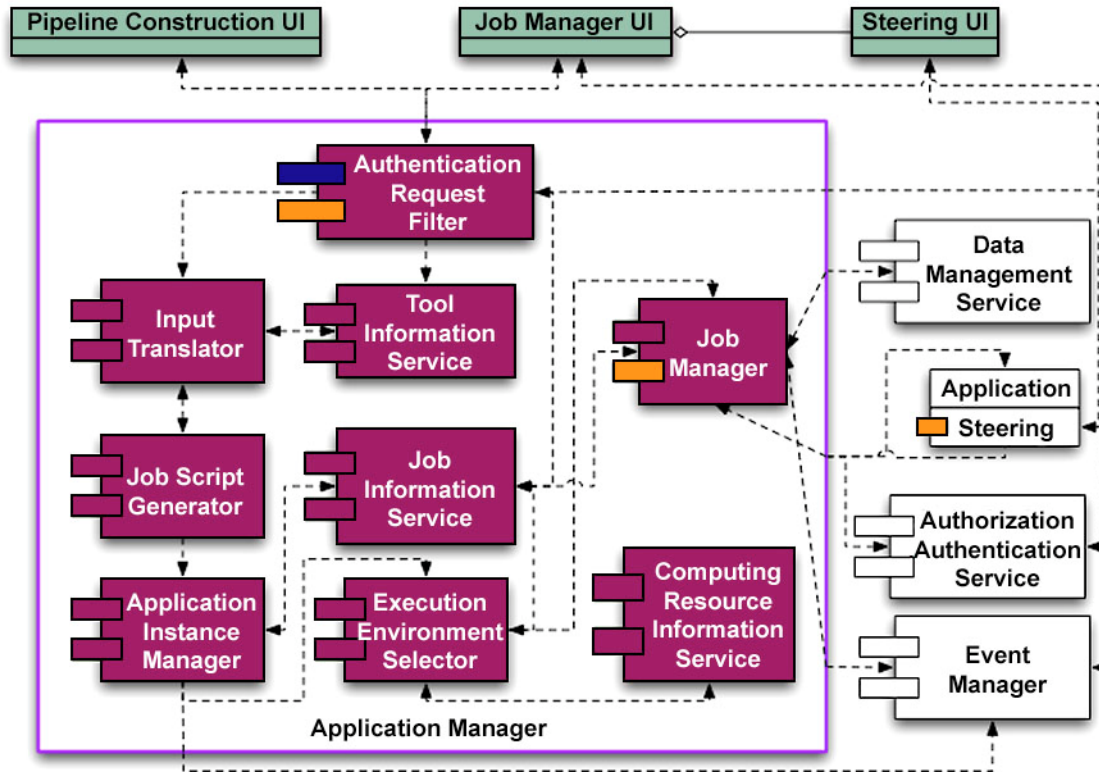
Applet gov.ornl.sns.portal.PortalApplet started

Applet com.jcraft.weirdx.WeirdX started

portal.sns.gov

Application Management

For staging, execution and monitoring/access

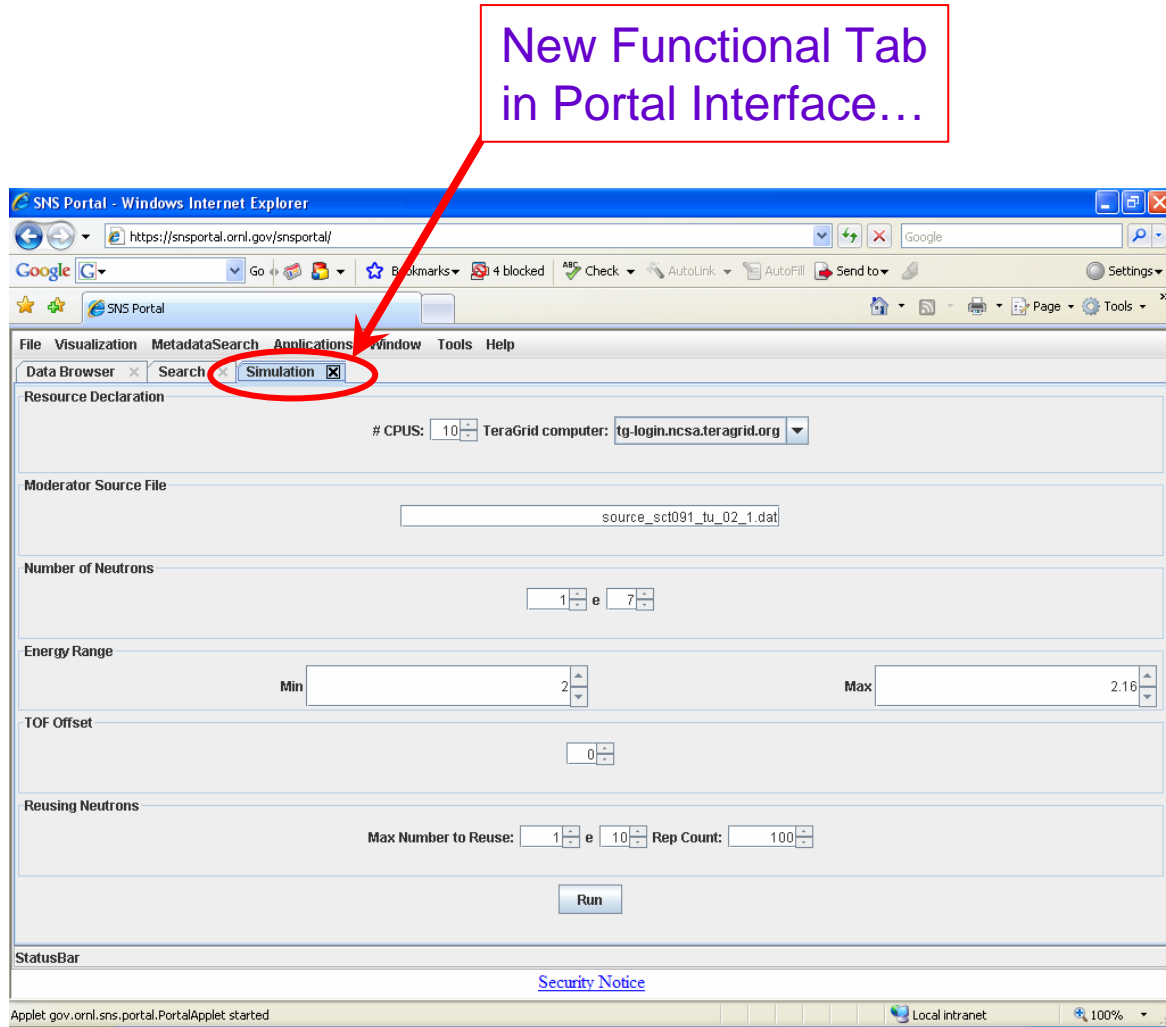


The application manager “realizes” the abstract data analysis pipeline specified by the user

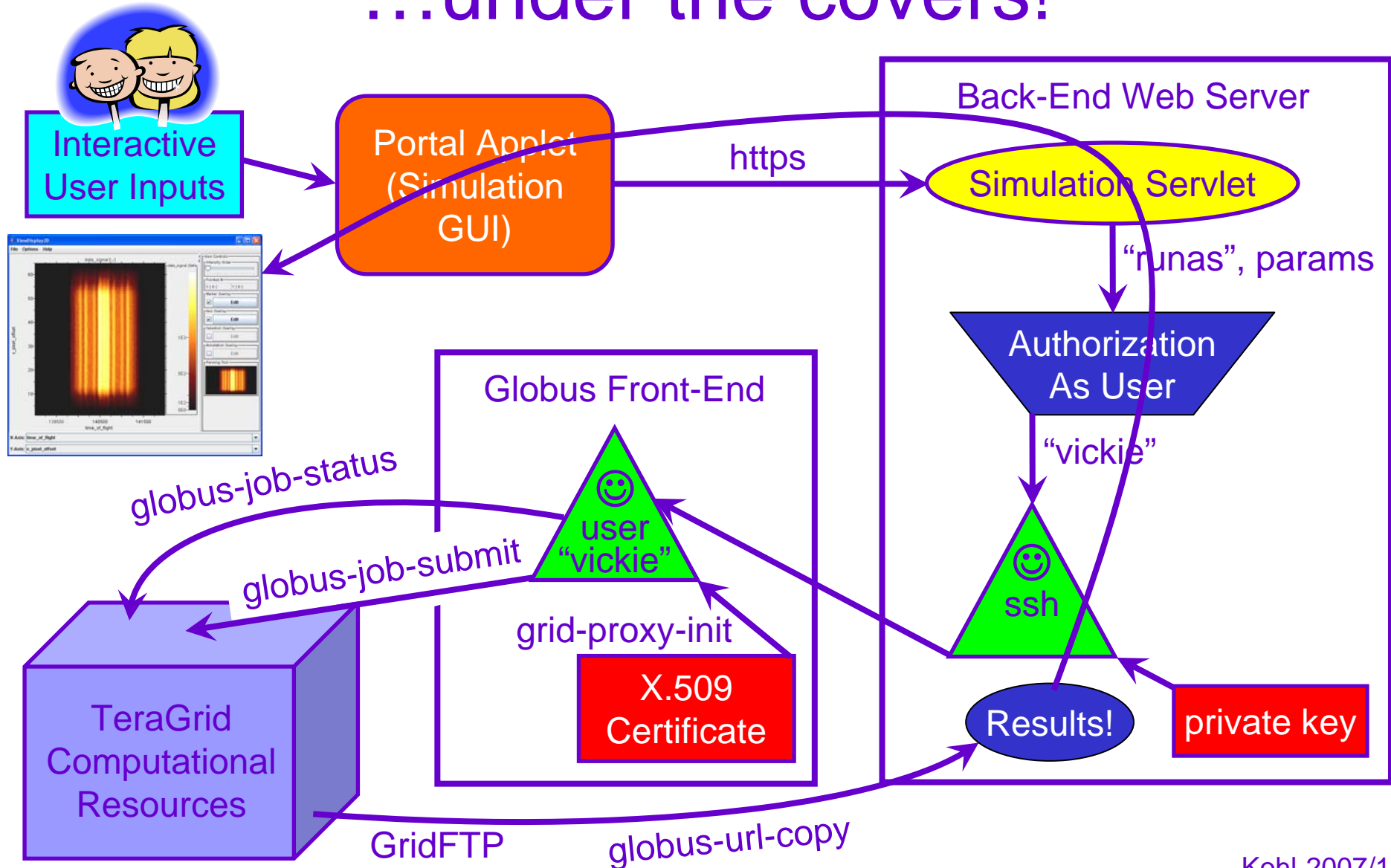
- Converts logical pipeline definition into functional scripts
- Coordinates scheduling, data staging, execution monitoring
- Interfaces to *both* facility and community software tools

Simulation Portal Development

- McStas simulation available via portal, for simulating backscattering experiments
- Java input panel
 - Pull-down menu for selecting TeraGrid resources...
 - Set min/max/step input parameters
 - Select source file



Portal-Initiated Simulations... ...under the covers!



SNS Science Portal Summary



- Secure access to key services:
 - Acquisition, analysis, visualization, simulation...
 - Data repositories, file systems and archives
 - Meta-data and provenance databases
 - High-performance computing resources
- Software analysis tools for neutron science
 - Web-based and programmatic desktop access
 - *Integration* of facility and community tools
- Extensible software architecture
 - Powerful data and application management