

# **An Infrastructure for Remote Applications for Macromolecular Crystallography at SSRL**

**NOBUGS 2004**

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## Why a Common Applications Infrastructure is Needed

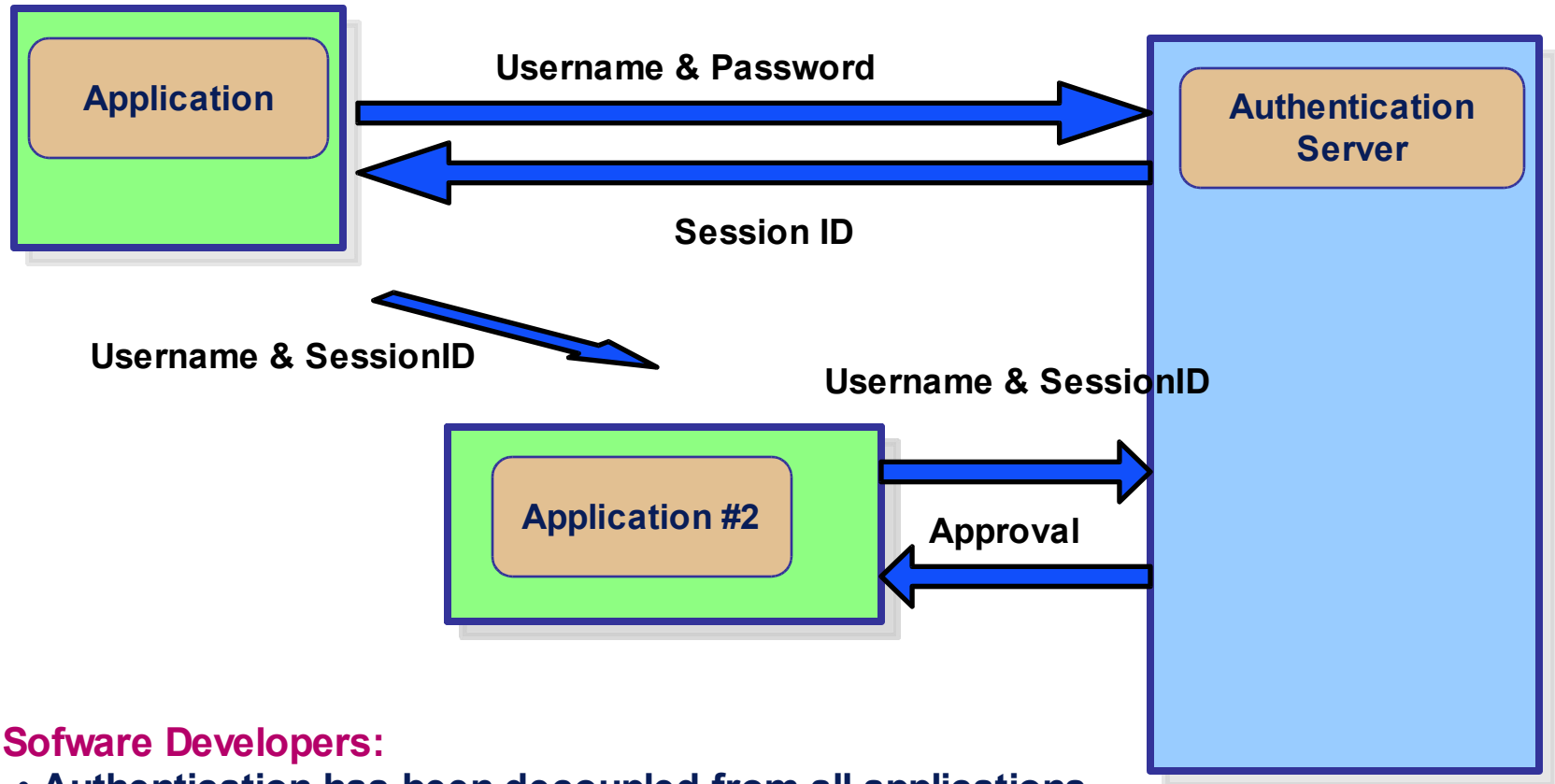
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- **Several browser-based applications have been developed or are in the process of being developed: Video System, Archive System, Crystal Screening, User Resource Management, and Web-Ice.**
- **Applications need a common means to securely authenticate users, identify active beam lines, and store information on the web server as a “session”.**
- **Applications must be able to share a session so that user’s need not log in separately for each application.**
- **Non browser-based applications (such as Blu-Ice) must also be able to create and share sessions with web apps.**
- **Applications running on behalf of a remote user must be able to access user’s computing resources at SSRL in order to run scripts and access directories and files.**

- **Java servlets provide a common HTTP authentication protocol for all web-based and stand-alone applications.**
- **Multiple authentication methods supported.**
- **User information stored in server session accessed via 128-bit SecureRandom SessionID.**
- **All web-based applications securely authenticate with this server via SSL.**
- **Users navigate seamlessly between applications by passing SessionID in a cookie or URL parameter.**
- **Access to beam line systems is based on the beam port schedule. Access to other resources (data directories, etc.) available 24/7.**
- **Requests (other than login page) limited to known application servers.**

# The Authentication Process



## For Software Developers:

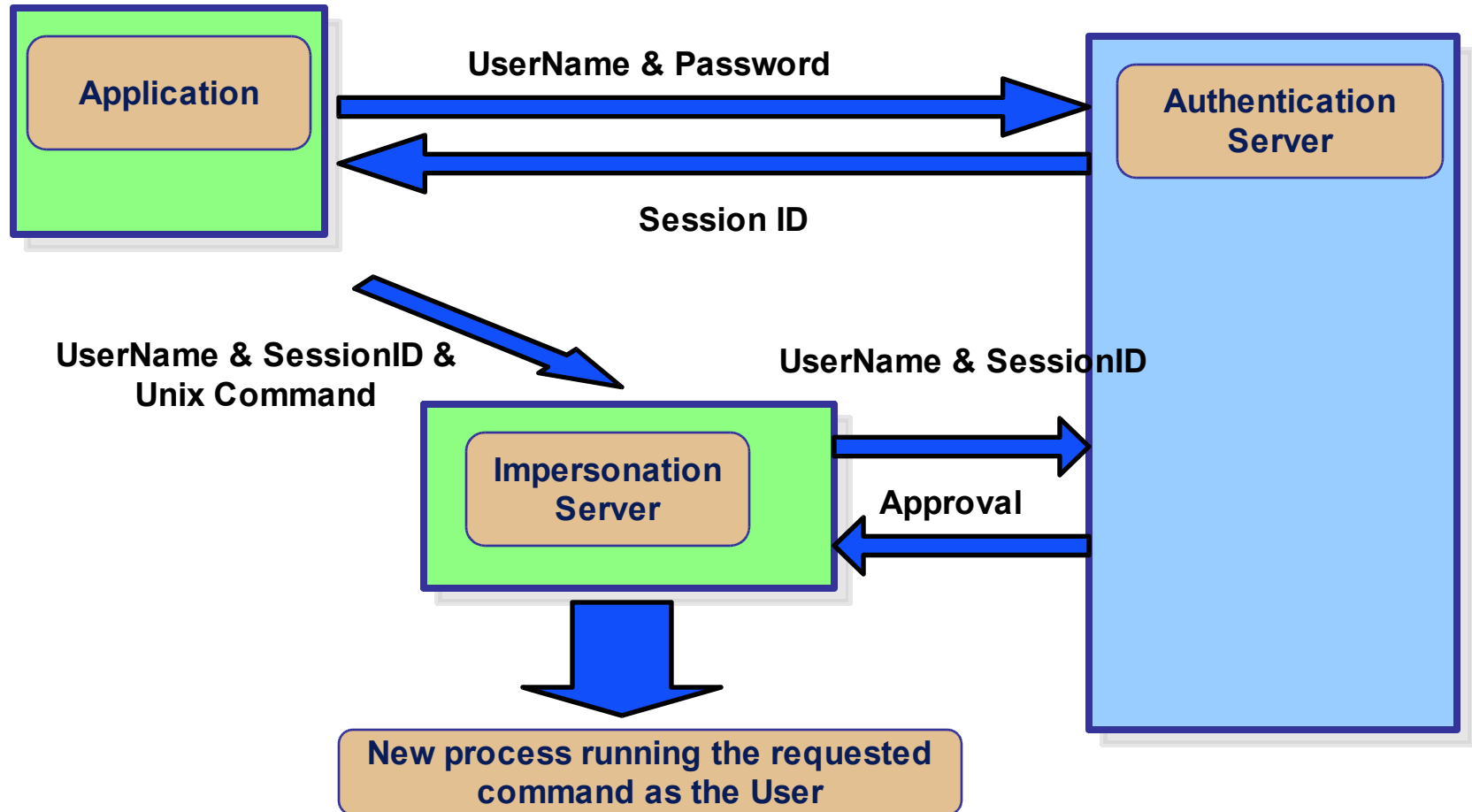
- Authentication has been decoupled from all applications.

## For Users:

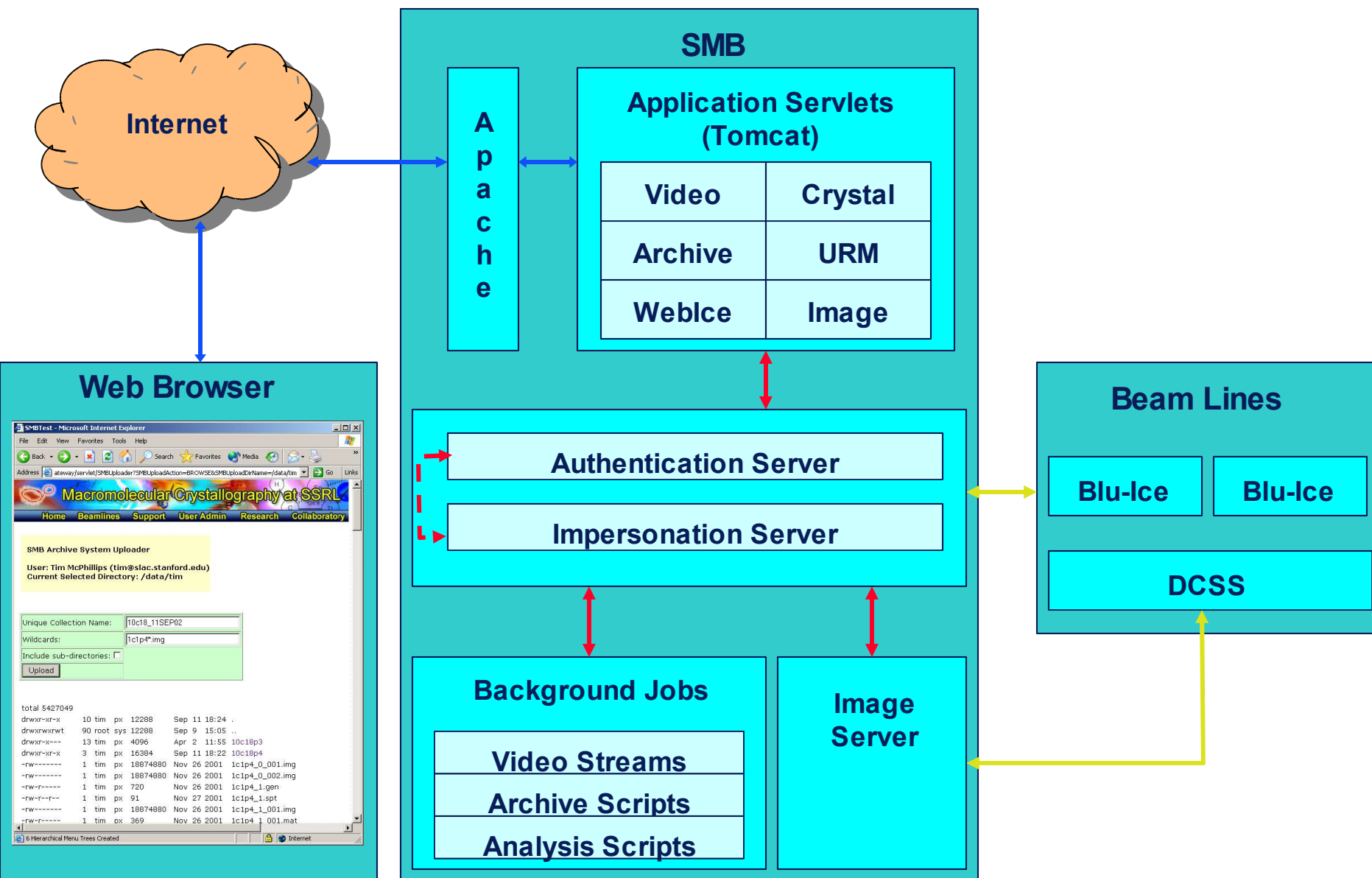
- Users log in once for all applications.
- Applications can have buttons to spawn authenticated web pages.
- User can log out after system has a session Id.

- **Unix daemon that can run any non-interactive program on behalf of any Unix user.**
- **Enables web applications to display user directories and files for selection in a web browser.**
- **Enables web applications to run background jobs for a user with the actual rights of the Unix user account.**
- **Accepts commands via the HTTP protocol.**
- **Verifies authentication information with the Authentication Server.**

# The Impersonation Process



# Application Architecture



# Authentication Servlets



User Login - Mozilla

File Edit View Go Bookmarks Tools Window Help

Back Forward Reload Stop <https://smb.slac.stanford.edu> Search Print

Home Bookmarks mozilla.org Latest Builds

**Macromolecular Crystallography at SSRL**

Home Beamlines Support User Admin Research RemoteAccess

Welcome to the SSRL Application Gateway

You do not have a valid SMB Session.  
Please log in to continue to the SMB Video System.

Enter your user name:

Enter your password:

Content questions and comments: [Collaboratory](#).  
Technical questions and comments: [Webmaster](#).

<http://smb.slac.stanford.edu/>

- **WEBLOGIN** – Redirects browser to login page; redirects back to application after authentication.
- **APPLOGIN** – Non-browser application creates a session by passing userid and password.
- **SessionStatus** – Returns information about user (beam line access, display name, etc.) and whether session is still active.
- **EndSession** – Logs out the user.
- **Utility Beans and Classes** – adds a layer above HTTP for easier programming.



- **HTTP Interface**
- **Request URI includes UserID and SessionID (checked against Authentication Server), Command, and Parameters (which may include a file or directory path and permissions or the name of a script or executable to run).**
- **Scripts run on same system as the Impersonation Server as if run locally by the user.**
- **Response Code indicates success or failure. Response data contained in HTTP Headers and Body.**
- **Process Commands include: runScript and runExecutable.**
- **File and Directory Management Commands include:**
  - listDirectory, createDirectory, deleteDirectory, copyDirectory**
  - getFileStatus, getFilePermissions, isFileReadable**
  - readFile, writeFile, deleteFile, renameFile, copyFile**

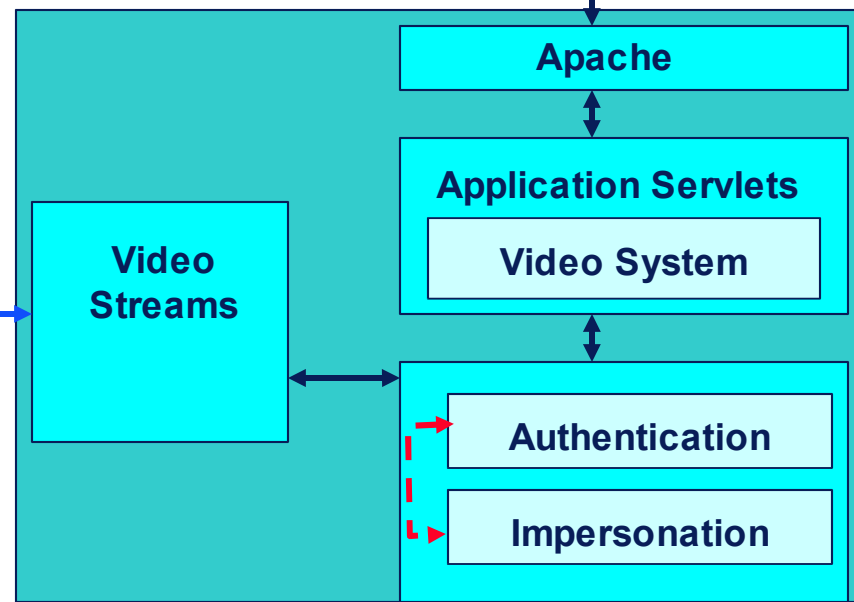
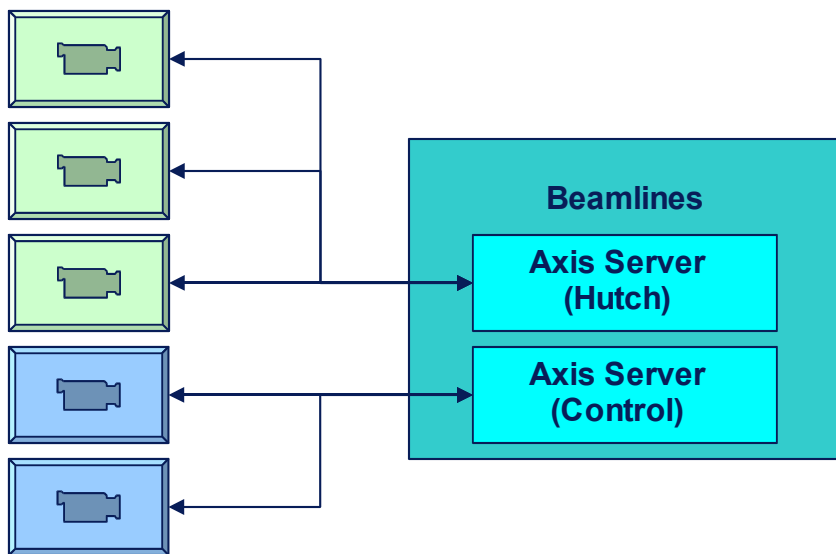
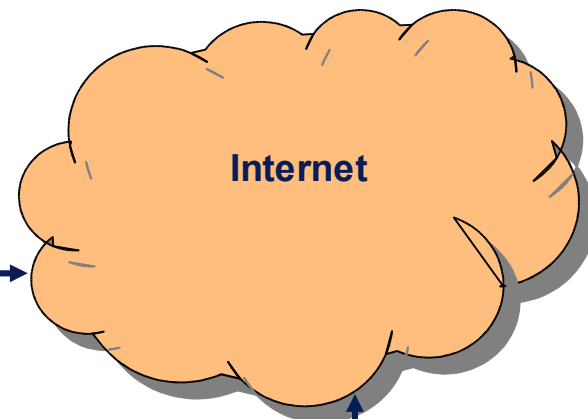
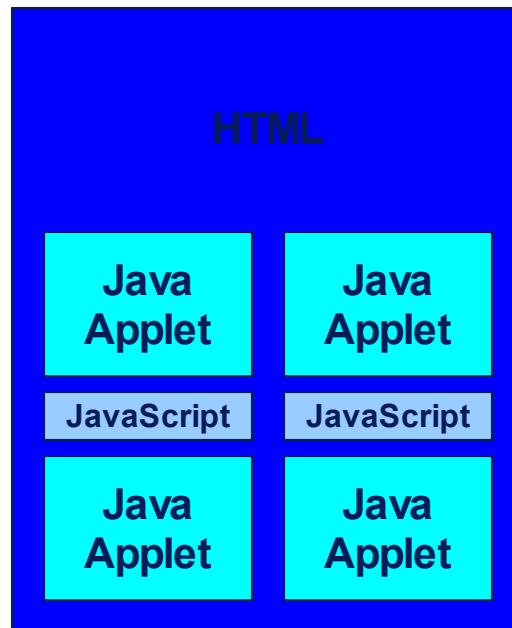
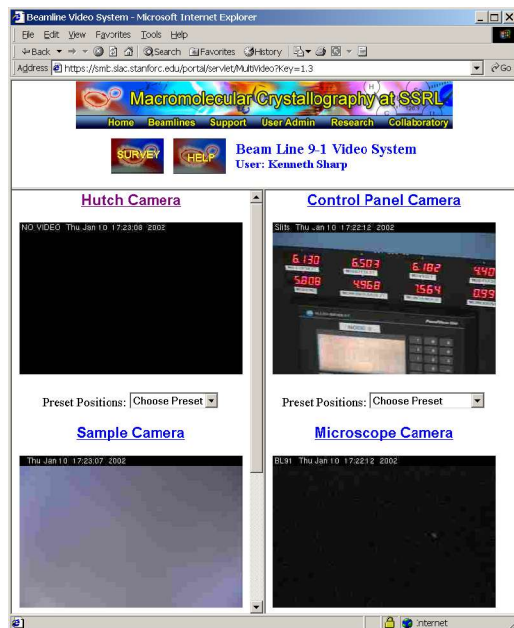
# Beam Line Video System



## Goals and Challenges

- **Browser interface** – no additional software for user to install.
- **Use Authentication Server** to determine which beam lines user may access.
- **Display selected views** from multiple camera servers.
- **Limited JPEG streams** available from each camera server.
- **Hide camera server CGI calls** to change camera presets and image sizes.

# Video System Architecture



# SMB Archive System



SMBTest - Microsoft Internet Explorer

File Edit View Favorites Tools Help

Address: ateway/servlet/SMBUploader?SMBUploadAction=BROWSE&SMBUploadDirName=/data/tim

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Home Beamlines Support User Admin Research Collaboratory

**SMB Archive System Uploader**

User: Tim McPhillips (tim@slac.stanford.edu)  
Current Selected Directory: /data/tim

Unique Collection Name: 10c18\_11SEP02

Wildcards: 1c1p4\*.img

Include sub-directories: ☐

Upload

total 5427049

drwxr-xr-x	10	tim	px	12288	Sep 11 18:24	.
drwxrwxrwt	90	root	sys	12288	Sep 9 15:05	..
drwxr-x---	13	tim	px	4096	Apr 2 11:55	10c18p3
drwxr-xr-x	3	tim	px	16384	Sep 11 18:22	10c18p4
-rw-----	1	tim	px	18874880	Nov 26 2001	1c1p4_0_001.img
-rw-----	1	tim	px	18874880	Nov 26 2001	1c1p4_0_002.img
-rw-r----	1	tim	px	720	Nov 26 2001	1c1p4_1.gen
-rw-r--r--	1	tim	px	91	Nov 27 2001	1c1p4_1.spt
-rw-----	1	tim	px	18874880	Nov 26 2001	1c1p4_1_001.img
-rw-r----	1	tim	px	369	Nov 26 2001	1c1p4_1_001.mat

6 Hierarchical Menu Trees Created

## Goals and challenges:

- Need replacement for tapes.
- Large-area CCD detectors quickly produce large amounts of data.
- Automated beam lines and large sample sets require a metadata store.
- Users may define archive jobs over the web using any common browser.

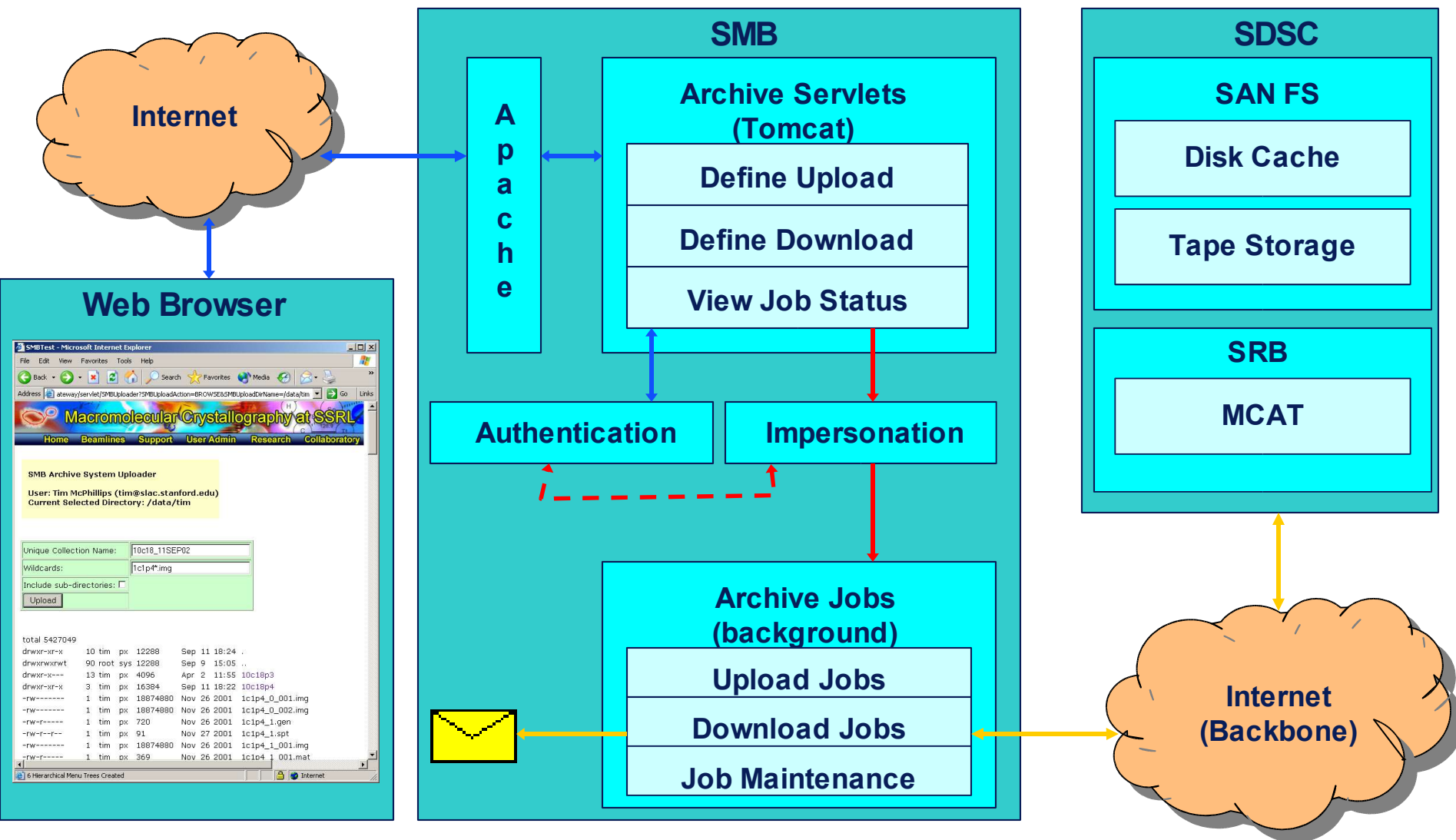
## Simple archive job definition

- Users may rapidly browse their /home and /data directories.
- Directories may be navigated by clicking on directory names.
- Files to be uploaded may be filtered according to a list of wildcards.
- Subdirectories may be archived recursively.
- User must be able to manage jobs (view job status, abort job, etc.)

## New Archive System Developments

- Identical interface to DVD Burner
- In-house implementation of SRB

# Archive System Web Architecture





# User Resource Management System



User Resource Management - Mozilla

File Edit View Go Bookmarks Tools Window Help

Back Forward Reload Stop [https://smb.slac.stanford.edu:8643/hyu/urm\\_js](https://smb.slac.stanford.edu:8643/hyu/urm_js) Search Print

Home Bookmarks mozilla.org Latest Builds

## SSRL Proposal Form

**For User Admin Use Only**

Proposal No.:  Previous Proposal No.:  Proposal Status:

PRT Parent Proposal:  Submittal Date: 10/16/04 Termination Date:

**PROPOSAL CLASSIFICATIONS: (select one)**

☐ standard proposal ☐ program proposal ☐ letter of intent ☐ rapid turnaround XAS

☐ rapid access ☐ staff proposal ☐ facility characterization

**TITLE:**

**SCIENTIFIC FIELDS: (can select more than 1 from existing list)**

☐ BioLife Sciences ☐ Chemistry ☐ Earth Sciences ☐ Engineering

☐ Environmental Sciences ☐ Materials Science ☐ Medical Applications ☐ Optics

☐ Other Development - (Instrumentation) ☐ Physics ☐ Polymers ☐ Purchase of Specialty Services or Materials

**SCIENTIFIC TECHNIQUES: (can select more than 1 from existing list)**

☐ IR/Visible/THz (spectromicroscopy,.....)

☐ SX-imag (PEEM, STXM, CXDI,.....)

☐ HX-imaging (full field, topography, tomography, phase contrast, DEI, etc)

☐ HX-spect (XAS, IKS, EXAFS,.....)

☐ HX-inelastic scattering (nuclear resonant, milli eV, compton, raman, RIXS)

☐ PX-nonMAD

☐ Ultrafast (femtosecond, pump-probe slicing, use pulsed nature of the beam)

☐ High Energy (greater than 50 keV?)

☐ Metrology, optics development, detector calibration/standards, etc.

☐ VUV (ARPES, AMO,.....)

☐ SX-spect (XPS, SXS, NEXAFS,.....)

☐ HX-micro/nano probe (scanning techniques)

☐ HX-elastic scattering (SAXS, WAXS, USAXS, GISAX)

☐ HX-diff (nonPX crystallography, powder,.....)

☐ PX-MAD

☐ High Pressure (DAC, large anvil press, etc.)

☐ Lithography

☐ Misc. -- laser backscattering, mass spec, and x-ray, footprinting

**FUNDING SOURCES: (can select more than 1 from existing list)**

☐ DOE/BES ☐ DVA ☐ NSF ☐ Fdn/Research Inst.

☐ DOE/BER ☐ NASA ☐ USDA ☐ State/County/City

☐ DOE Other: (specify) ☐ NIH ☐ Other US Gov't: (specify) ☐ Prof/Voluntary Assoc.

☐ DoD: (specify) ☐ NIST ☐ Industry ☐ Foreign: (specify)

☐ Other

**WILL PRIVATE SECTOR/PROPRIETARY RESEARCH BE PERFORMED?** ☐ No ☐ Yes

(Note that private sector research is subject to specific terms and conditions, and SSRL must be reimbursed at full cost recovery)

**BRIEF ABSTRACT (Please limit to 300 words/2000 characters):**

- Provide SSRL users with browser-based tools for submitting proposals and beam time requests; updating personal information; and viewing personalized beam time schedules.
- Facilitate communication with user administration and user support staff.
- Integrate with production SSRL database system, eliminate older user interfaces and reporting tools.
- Authenticates through SSRL database instead of SMB; Different authentication method than other applications.

# Crystal Screening System




Screening System Database - Microsoft Internet Explorer

File Edit View Favorites Tools Help

Back Forward Stop Home Search Favorites Media

Address <https://smb.slac.stanford.edu/crystals/CassetteInfo.jsp?accessID=33672A2F440B> Go Links

Google screening Search Web 2822 blocked AutoFill Options

 **Screening System Database**

User name:

Change the [Login](#) if your user name does not appear above.

Excel Spreadsheet				Beamline	
372 default.xls 2004-10-13 14:42:20	<a href="#">View</a>	<a href="#">Download Excel file</a>	<a href="#">Upload new file</a>	<a href="#">Delete entry</a>	<input type="text" value="No assignment"/>
376 default.xls 2004-10-13 15:15:42	<a href="#">View</a>	<a href="#">Download Excel file</a>	<a href="#">Upload new file</a>	<a href="#">Delete entry</a>	<input type="text" value="BL1-5 left"/>
377 default.xls 2004-10-13 15:15:46	<a href="#">View</a>	<a href="#">Download Excel file</a>	<a href="#">Upload new file</a>	<a href="#">Delete entry</a>	<input type="text" value="No assignment"/>

[Download template file](#). Please note that the first data row is reserved for the CassetteID (Pin Number).

For more information see the [Online Help](#).

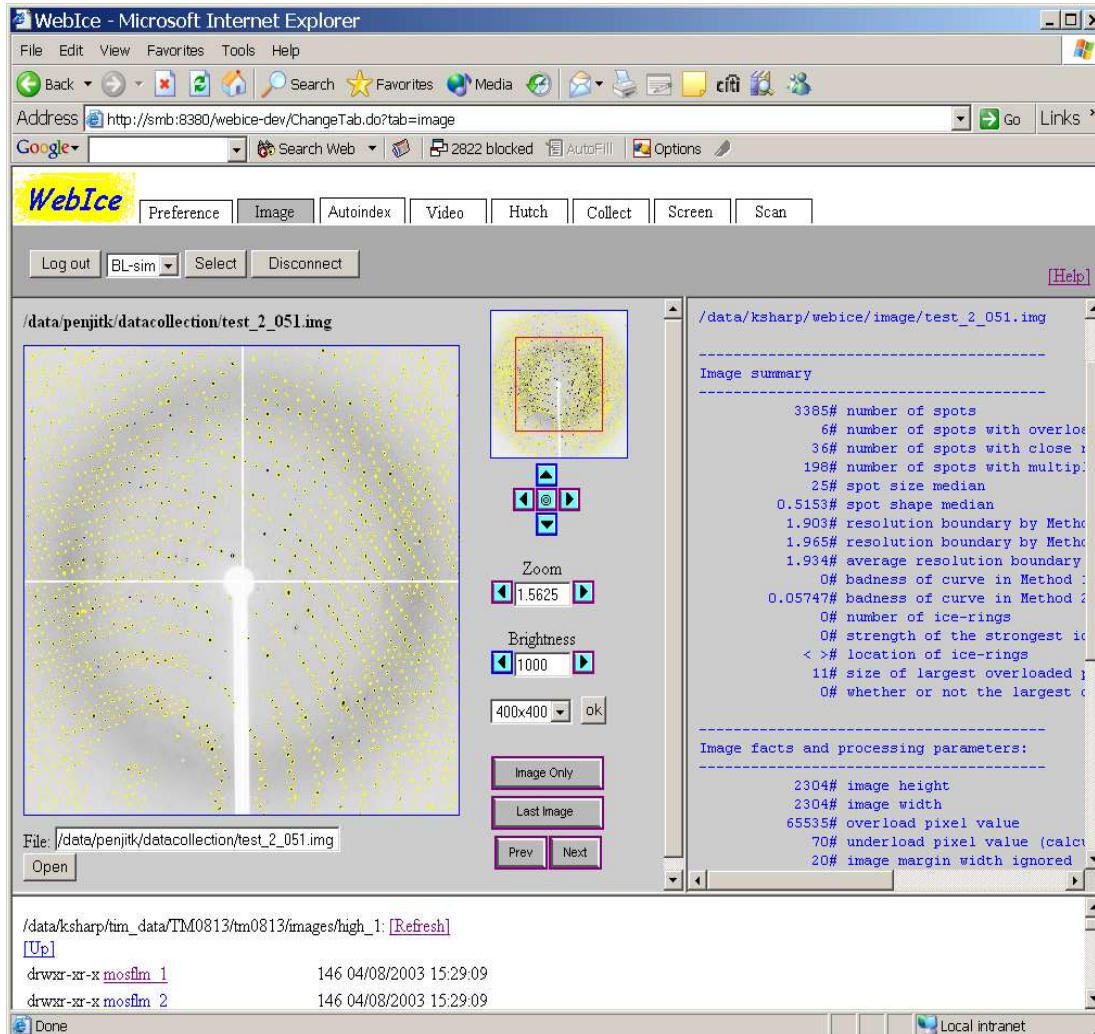
Here is a page with all SMB [Beamlines](#).

Done Internet

**The High-Throughput Screening System (HTSS) allows for the efficient screening of crystals through the use of automated sample mounting from special cassettes.**

**A web application allows users to upload spreadsheets containing crystal information.**

**The Authentication Server allows users to access their crystal spreadsheets 24/7, but only allows them to associate a crystal cassette with a beam line when they have beam time.**



•WebIce is part of our effort to develop tools to facilitate remote access to the beam lines and enable users to work with geographically dispersed collaborators.

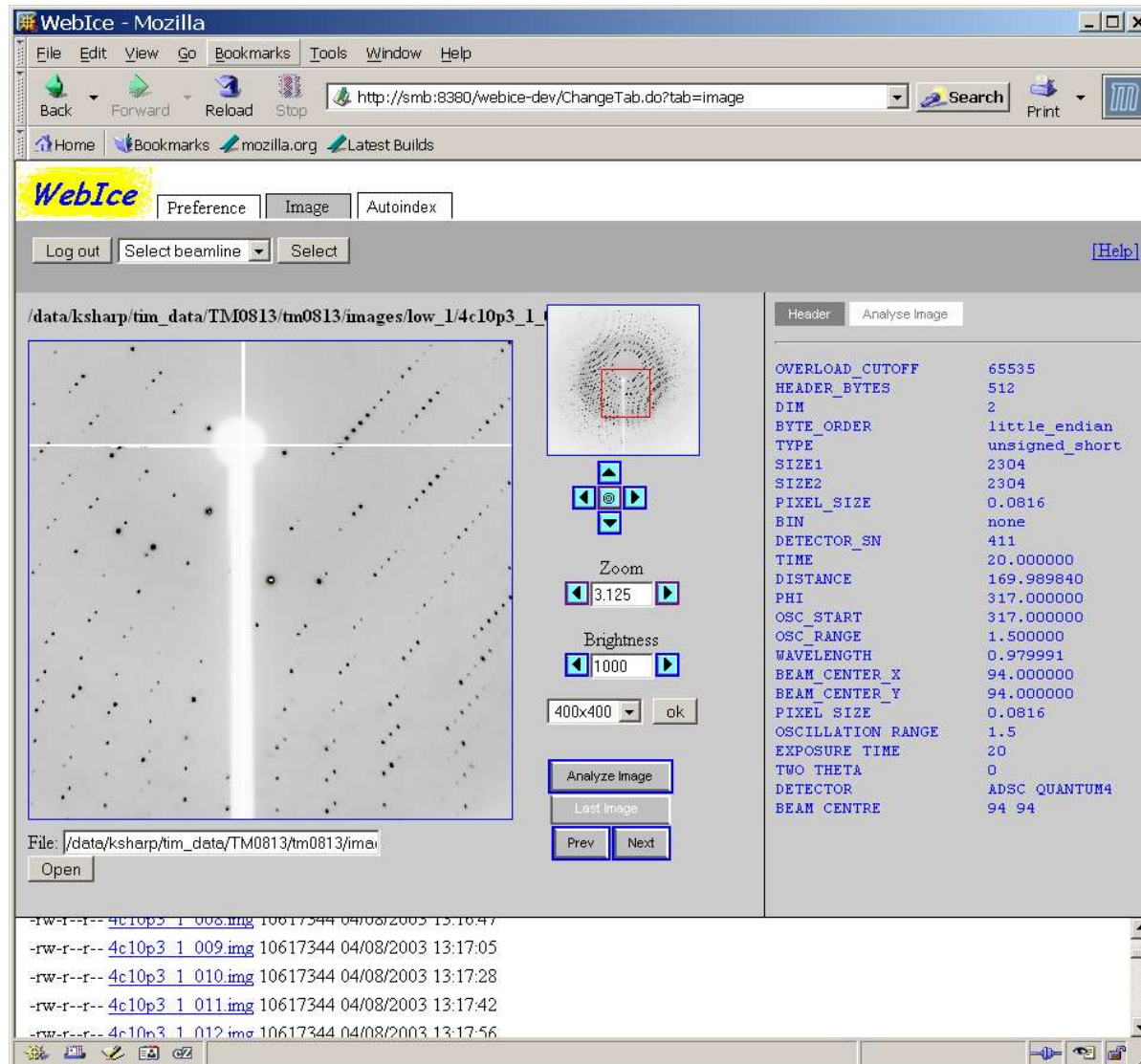
•In its first release, WebIce provides tools to view diffraction images, perform preliminary automated analyses of their diffraction patterns, and autoindex and calculate a collection strategy based on selected images.

•WebIce uses the Authentication Server to determine if the user has current beam line access, and Impersonation Server to run analysis scripts and manage autoindex strategy files. Some tabs do not require beamline access, such as Image Viewer and Autoindex.

•In future releases, WebIce will generate complete data collection strategies which can then be imported into beam line control software such as Blu-Ice, integrate beam line video into the application, and even allow beam line control from the web.

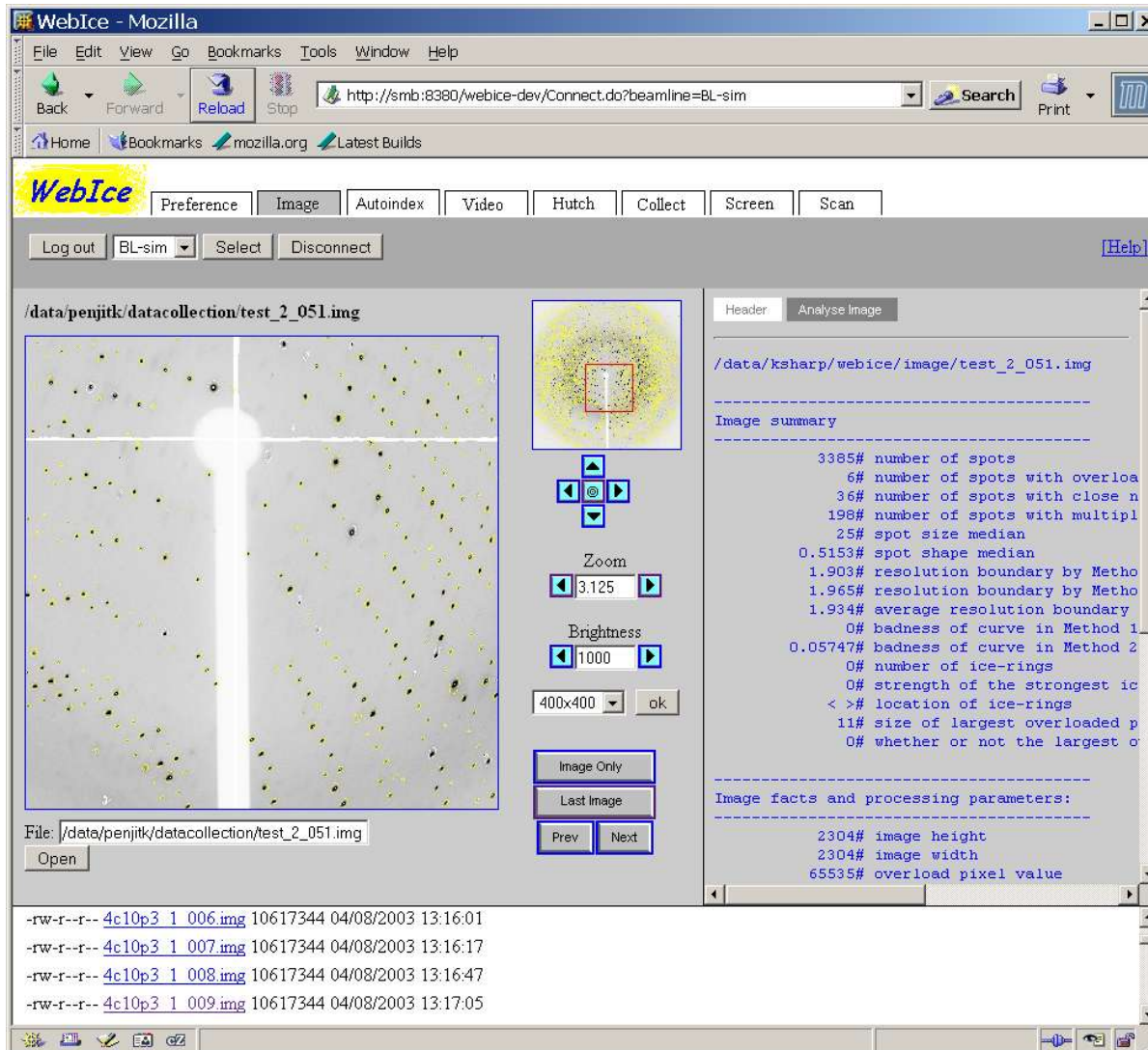


# Web-Ice Image Viewer



Web-Ice's Image Viewer replaces the Diffraction Image Viewer web application.

# Analyze Last Collected Image



**Image Viewer also enables the user to analyze last collected image from beam line with an in-house program called Spotfinder.**

# Autoindex Setup



WebIce - Mozilla

File Edit View Go Bookmarks Tools Window Help

Back Forward Reload Stop <http://smb:8380/webice-dev/ChangeTab.do?tab=strategy> Search Print

Home Bookmarks mozilla.org Latest Builds

**WebIce** Preference Image **Autoindex** Video Hutch Collect Screen Scan

Log out BL-sim Select Disconnect [Help]

Runs [Reload]  
newtest  
  autoindexing solution12  
  test

### Autoindexing for Dataset: newtest

[Setup] [Solutions] [Autoindex Summary] [Details] [Predictions]

**Message**

```
17:04:39 Started running autoindex  
17:04:40 scriptDir =  
/usr/local/dcs/webice/scripts  
17:04:40 workDir =  
/data/ksharp/webice/strategy/Runs/newtest
```

#### 1. Setup

**Image Directory** /data/ksharp/tim\_data/TM0813/tm0813/images/high\_1

**Image Files** 4c10p3\_high\_1\_001.img  
4c10p3\_high\_1\_090.img

**Options** ☒ Integrate best solutions only  
☒ Generate strategy

Edit

#### 2 Run Autoindex

Done.

#### 3 Integrate Other Solutions

Solution	Crystal System
<input type="checkbox"/> 12	hexagonal hP
<input type="checkbox"/> 11	orthorhombic oC
<input type="checkbox"/> 10	monoclinic mC

The Autoindex tab may be used to create data collection strategies.

# Web-Ice AutoIndex Results



WebIce - Microsoft Internet Explorer

Address: http://smb:8380/webice-dev/ChangeTab.do?tab=strategy

WebIce Preference Image Autoindex

Log out Select beamline Select [Help]

**Autoindexing for Dataset: newTest**

[Setup] [Solutions] [Autoindex Summary] [Details] [Predictions]

**Indexing Results**

Beam x	157.6
Beam y	157.38
Distance	299.64
Mosaicity	0.15 deg (predicts 80% of spots in images)

**Indexing Solutions**

Solution	Metric Fit	rmsd	#spots	Crystal System	Unit Cell	Volur
12	0.4178 dg	0.266	575	hexagonal hP	90.12 90.12 45.04 90.0 90.0 120.0	3168
9	0.4104 dg	0.277	498	monoclinic mC	155.63 90.4 45.06 90.0 89.92 90.0	6339
8	0.3349 dg	0.191	424	orthorhombic oC	89.96 155.04 45.12 90.0 90.0 90.0	6292
7	0.3349 dg	0.195	432	monoclinic mC	90.06 155.11 45.1 90.0 89.96 90.0	6300
6	0.3165 dg	0.202	424	monoclinic mC	155.04 89.96 45.12 90.0 89.88 90.0	6292
5	0.1631 dg	0.178	564	orthorhombic oC	89.41 156.2 45.11 90.0 90.0 90.0	6299
4	0.1631 dg	0.178	564	monoclinic mC	156.19 89.41 45.11 90.0 90.0 90.0	6299
3	0.1356 dg	0.163	563	monoclinic mP	89.39 45.11 89.87 90.0 119.73 90.0	3147
2	0.0923 dg	0.162	564	monoclinic mC	89.42 156.14 45.11 90.0 89.85 90.0	6298

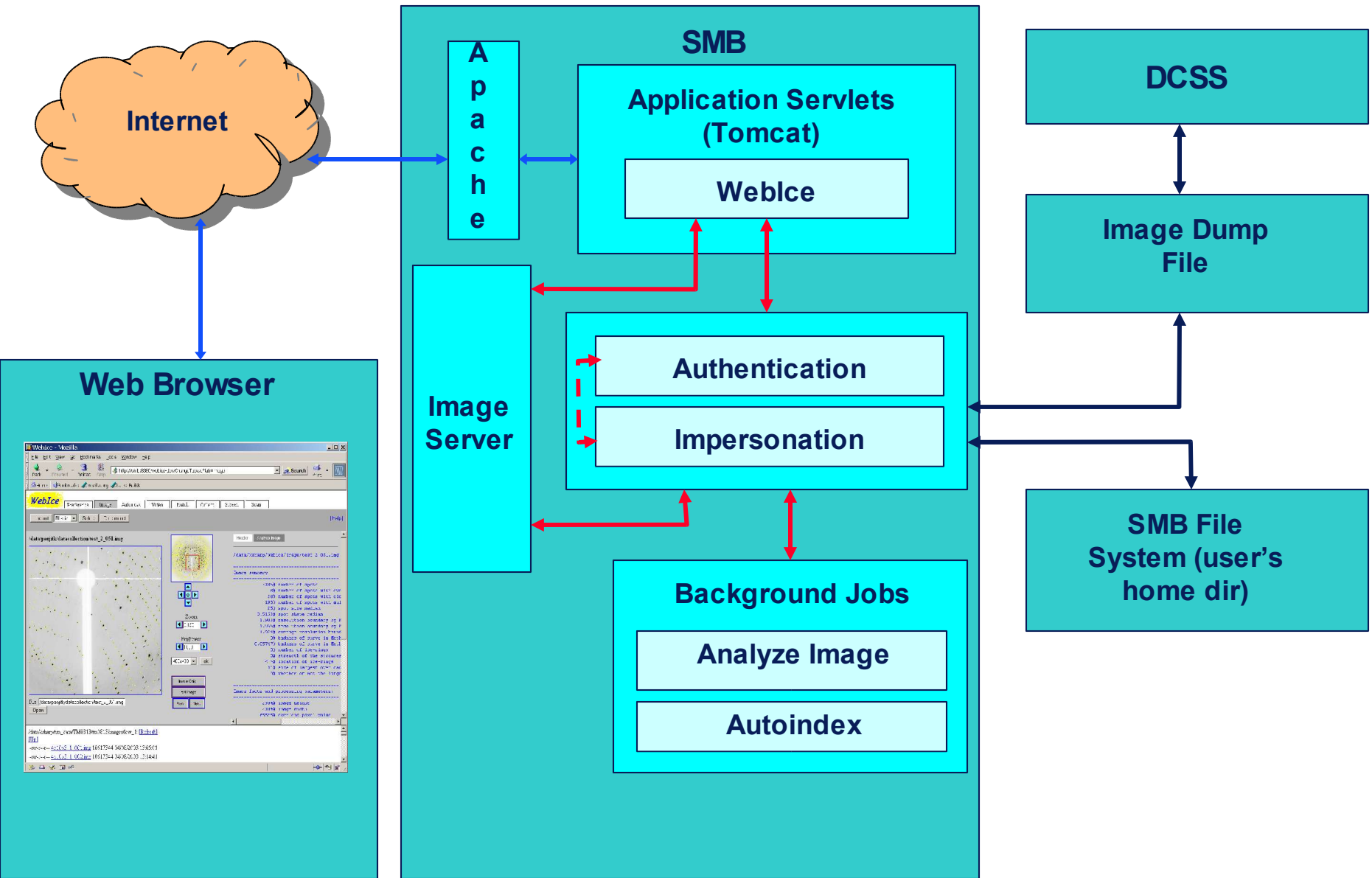
- WebIce uses the Impersonation Server to run autoindexing scripts in the background.

- The scripts generate data collection strategies and stores this information in the user's webice directory.

- Users may then view these strategies in the web browser.



# Web-Ice Architecture



# The Macromolecular Crystallography Group



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MC Leader - Mike Soltis**

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