An Infrastructure for Remote Applications for Macromolecular Crystallography at SSRL

NOBUGS 2004

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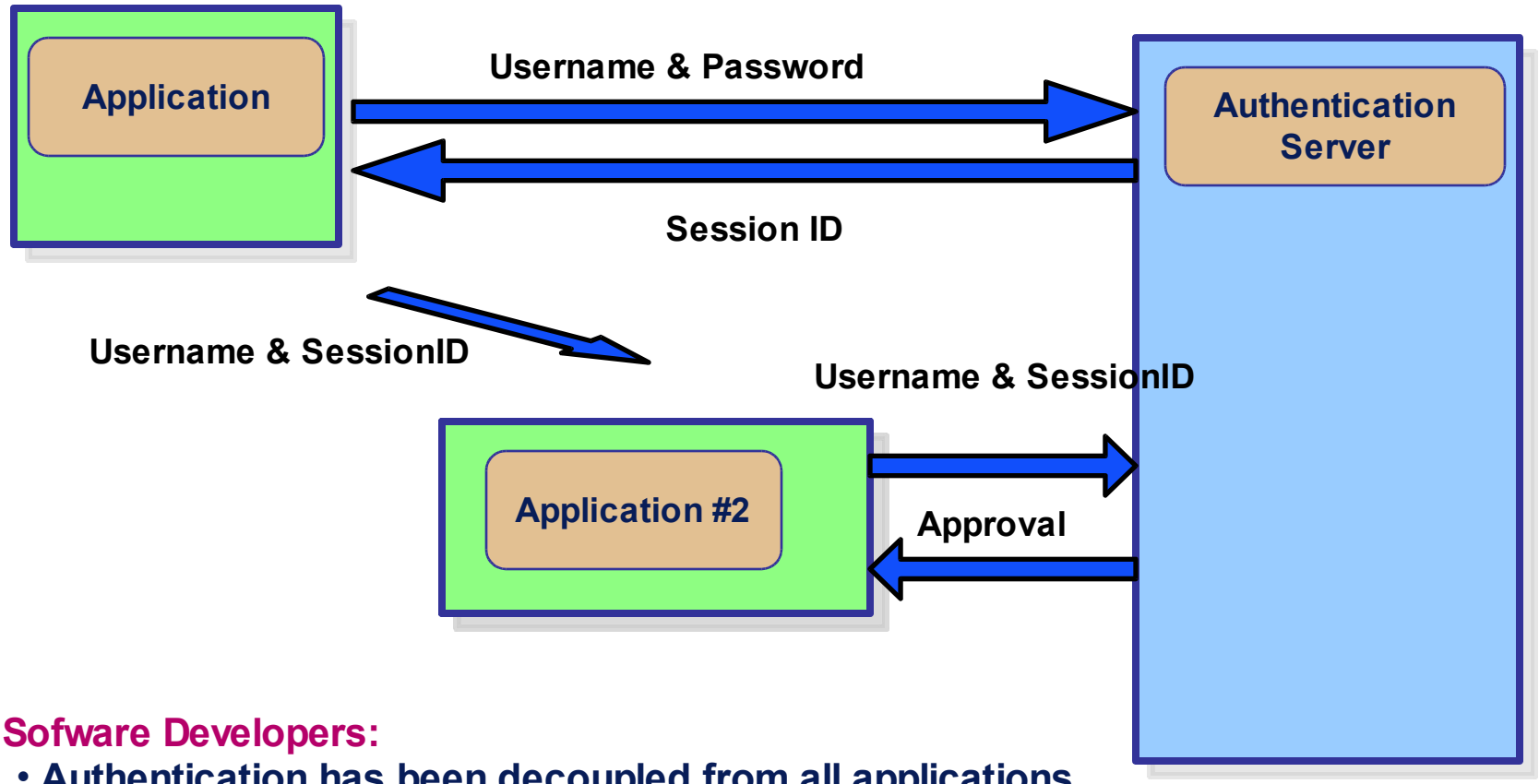
Why a Common Applications Infrastructure is Needed

- 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.

Authentication Server

- 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 Sofware Developers:

- Authentication has been decoupled from all applications.

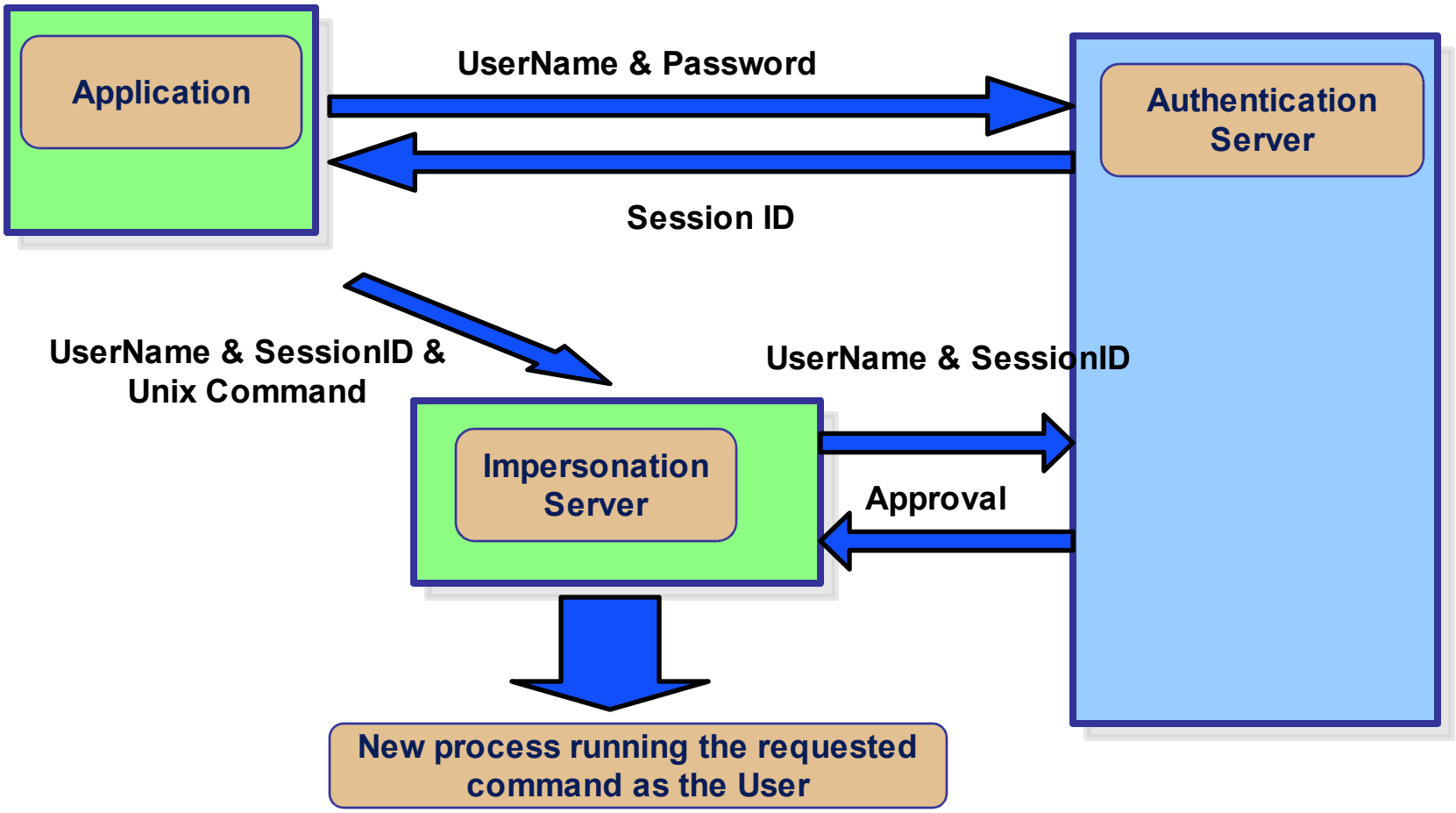
For Users:

- 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.

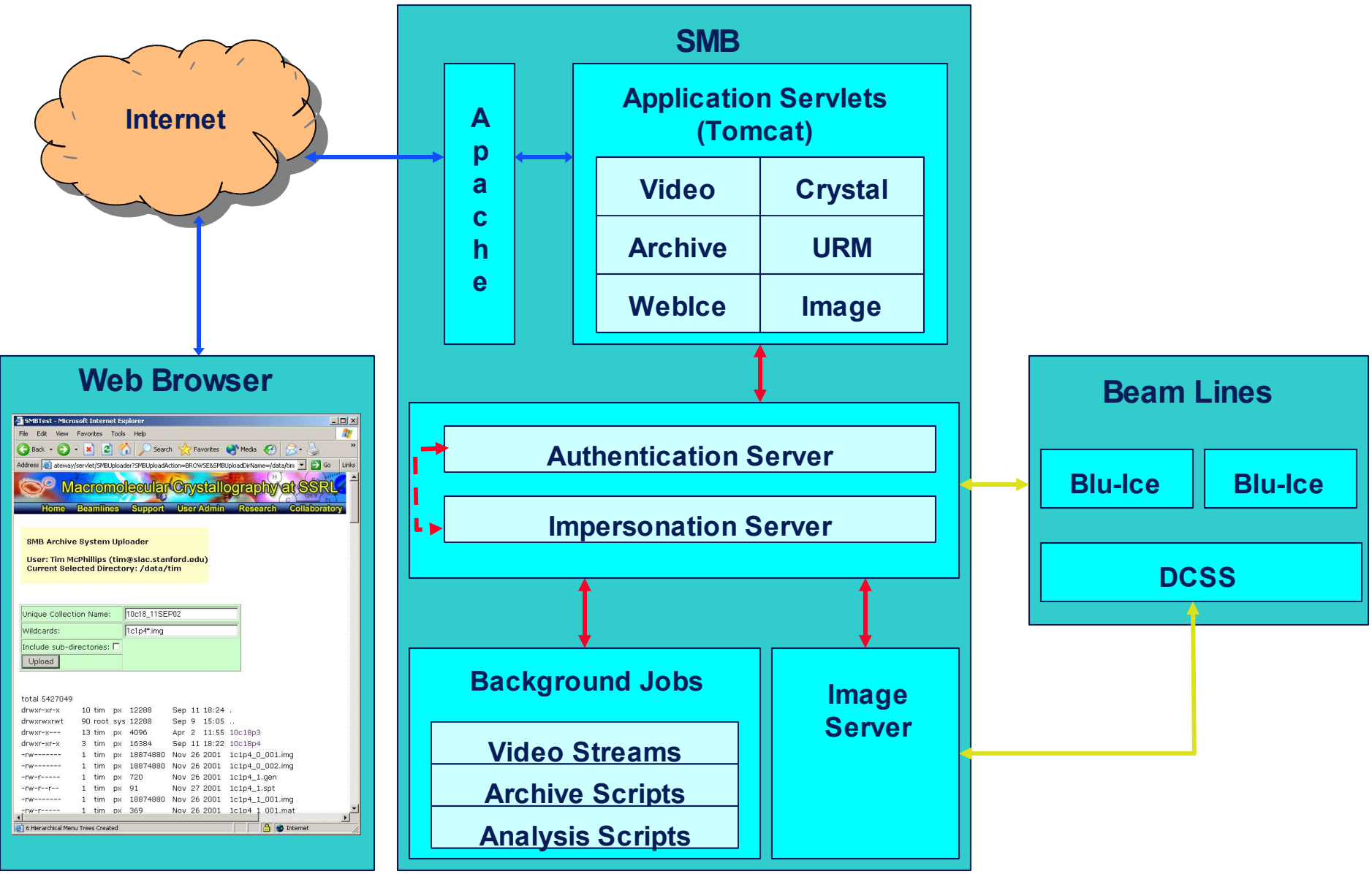
Impersonation Server

- 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.

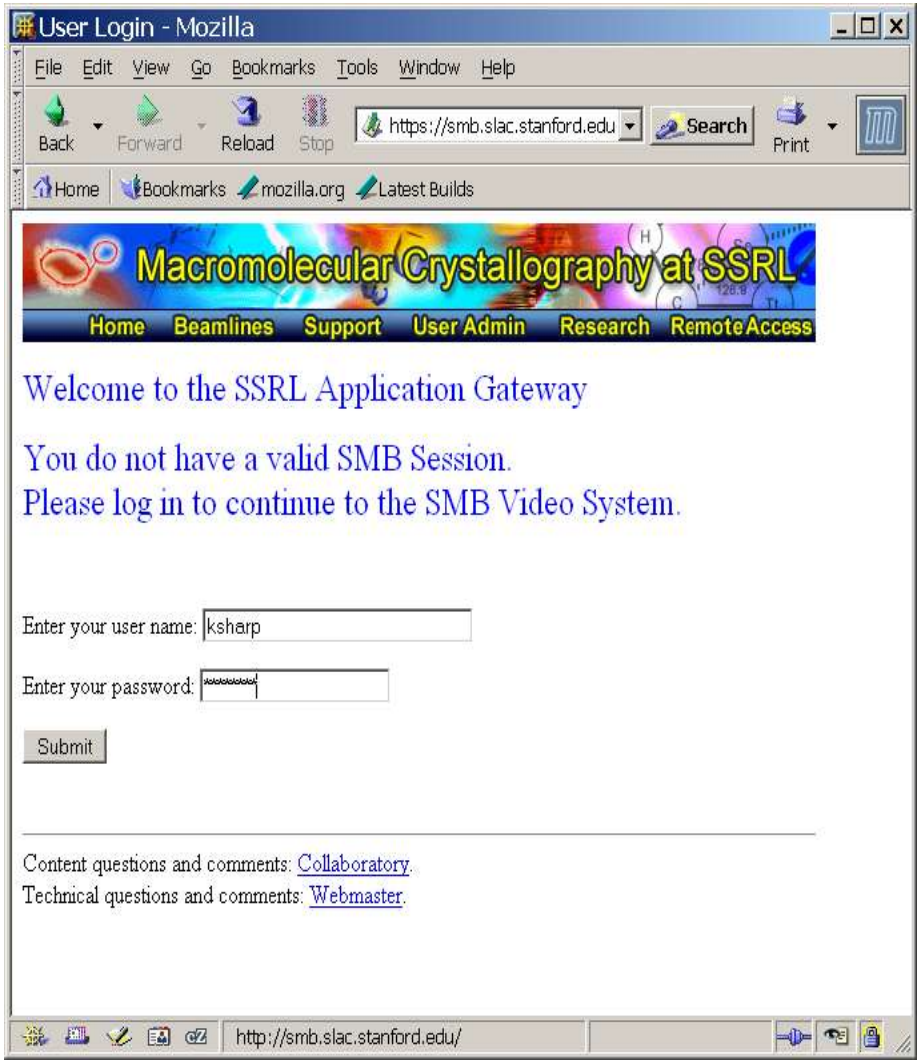
The Impersonation Process



Application Architecture



Authentication Servlets



- **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.**

Impersonation Server Interface

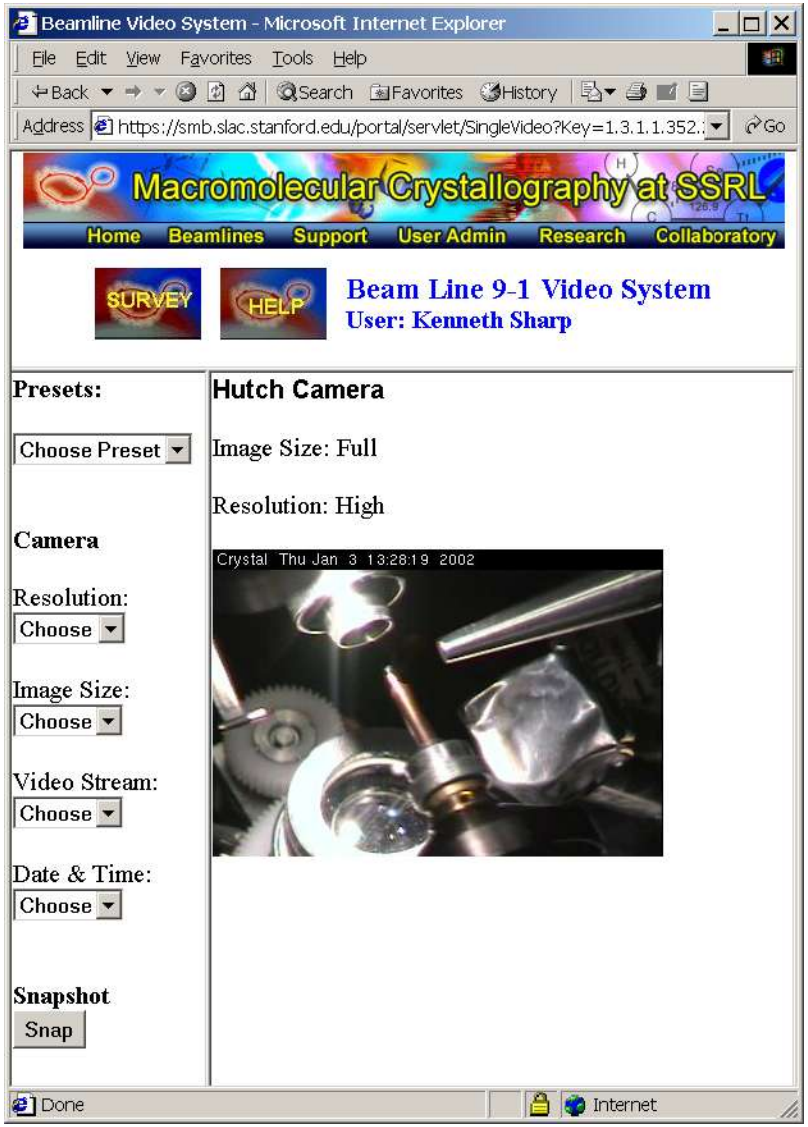
- HTTP Interface
- Request URI includes UserID and SessionID (checked against Authentication Server), Command, and Parameters (which may include a file or directory path and permissions or the name of a script or executable to run).
- Scripts run on same system as the Impersonation Server as if run locally 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

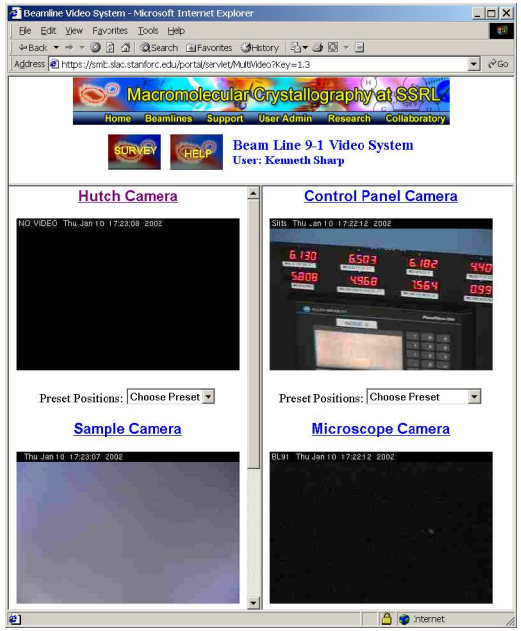
Beam Line Video System

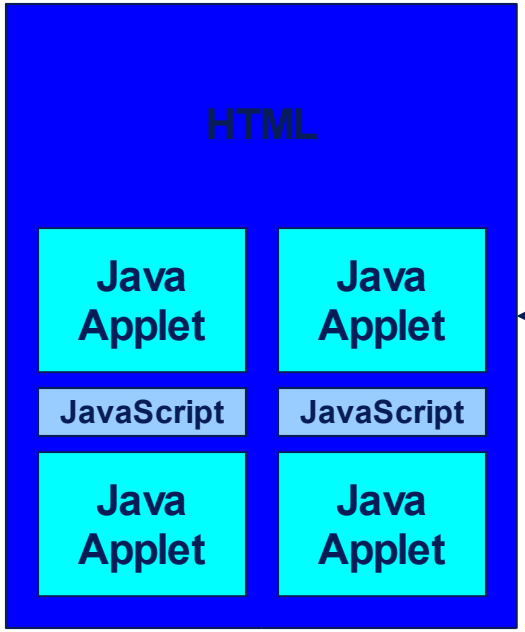


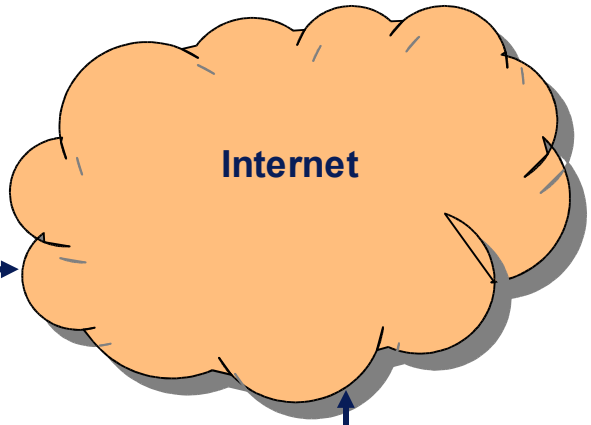
Goals and Challenges

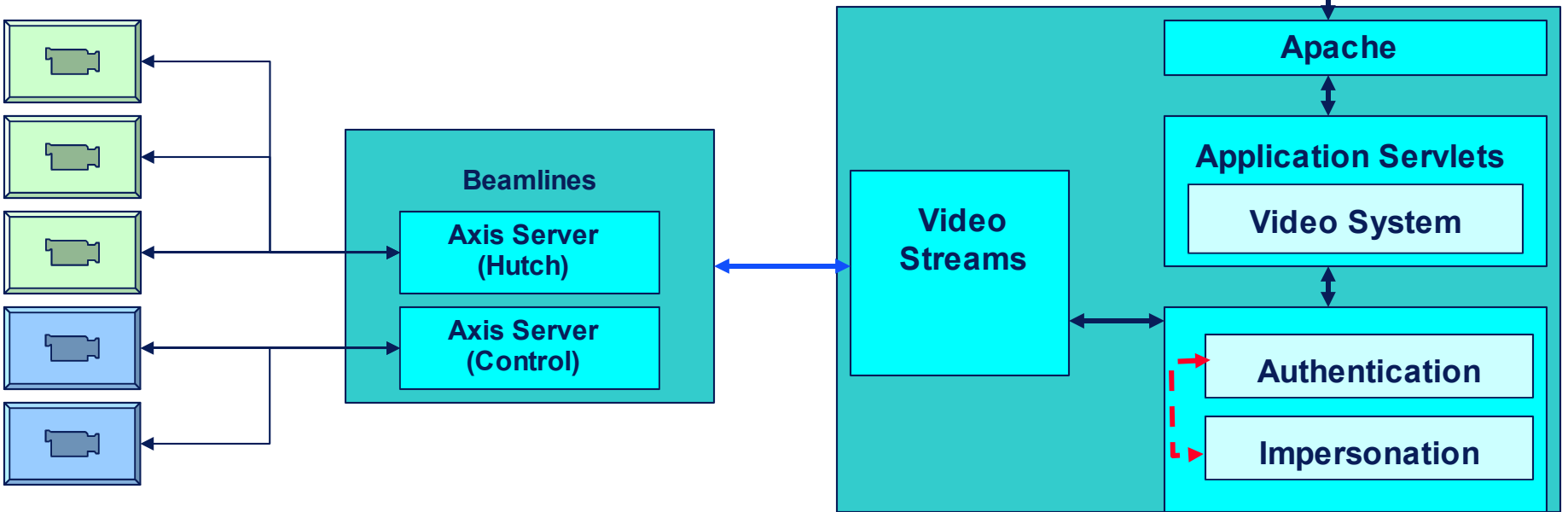
- Browser interface – no additional software for user to install.
- Use Authentication Server to determine which beam lines user may access.
- Display selected views from multiple camera servers.
- Limited JPEG streams available from each camera server.
- Hide camera server CGI calls to change camera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

Video System Architecture

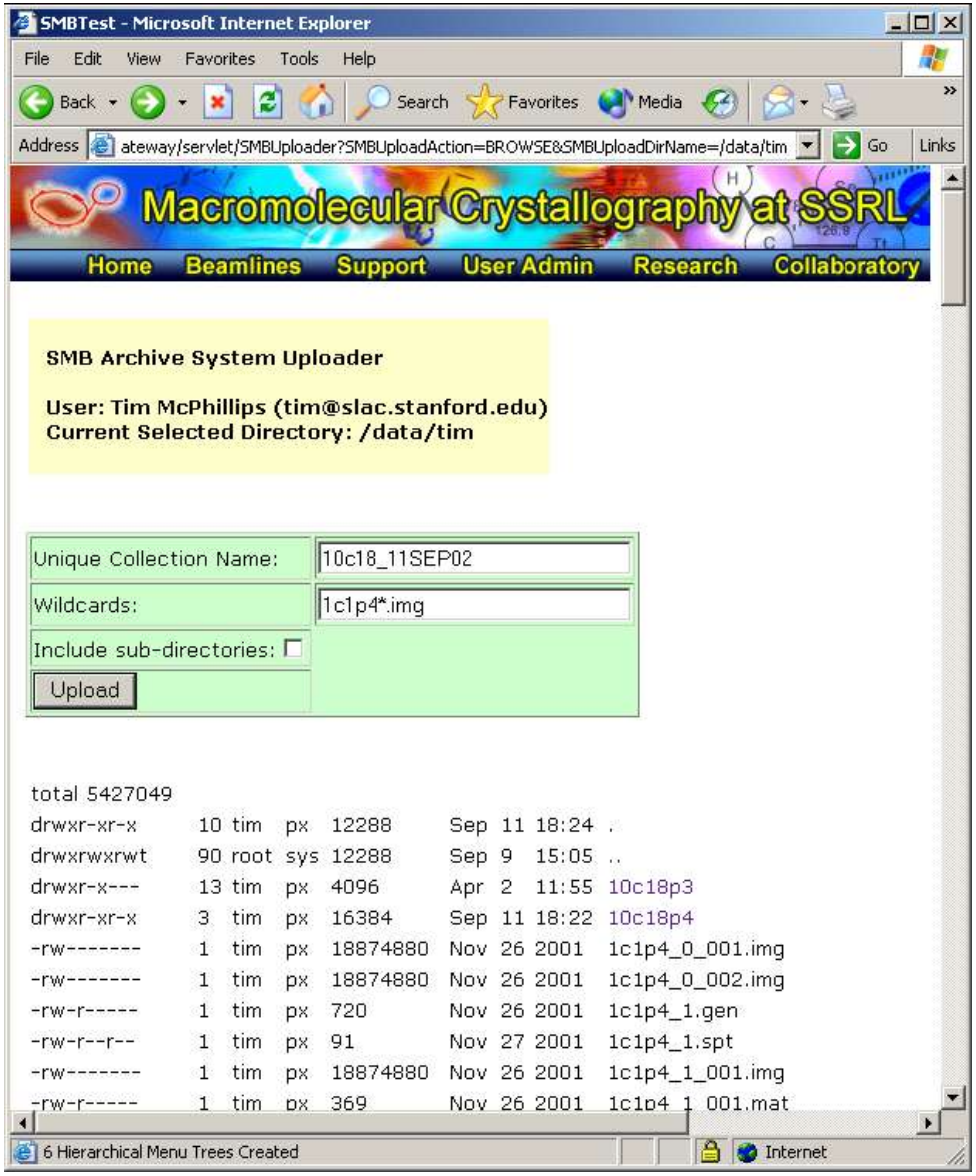








SMB Archive System



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.

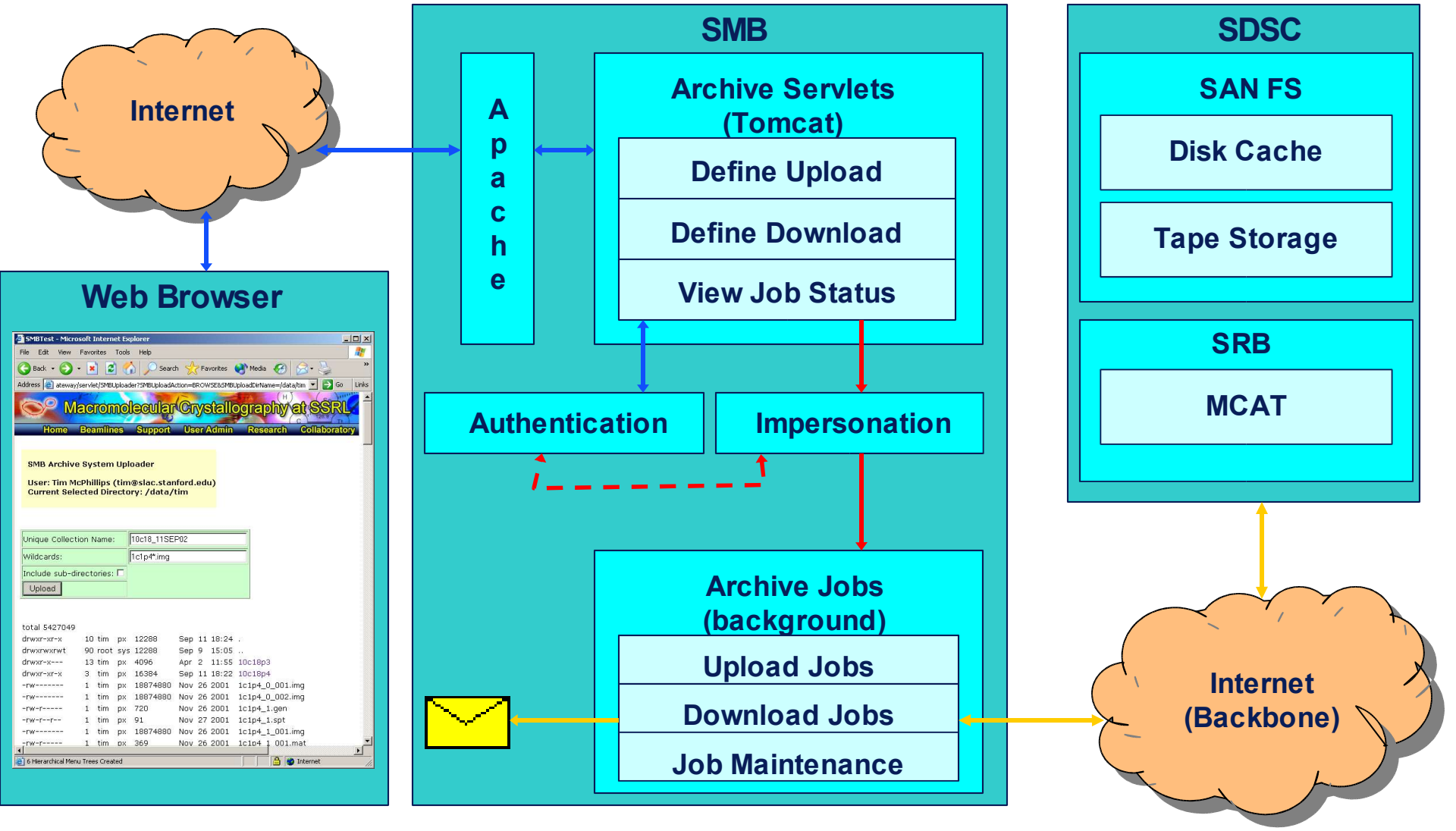
Simple archive job definition

- 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.)

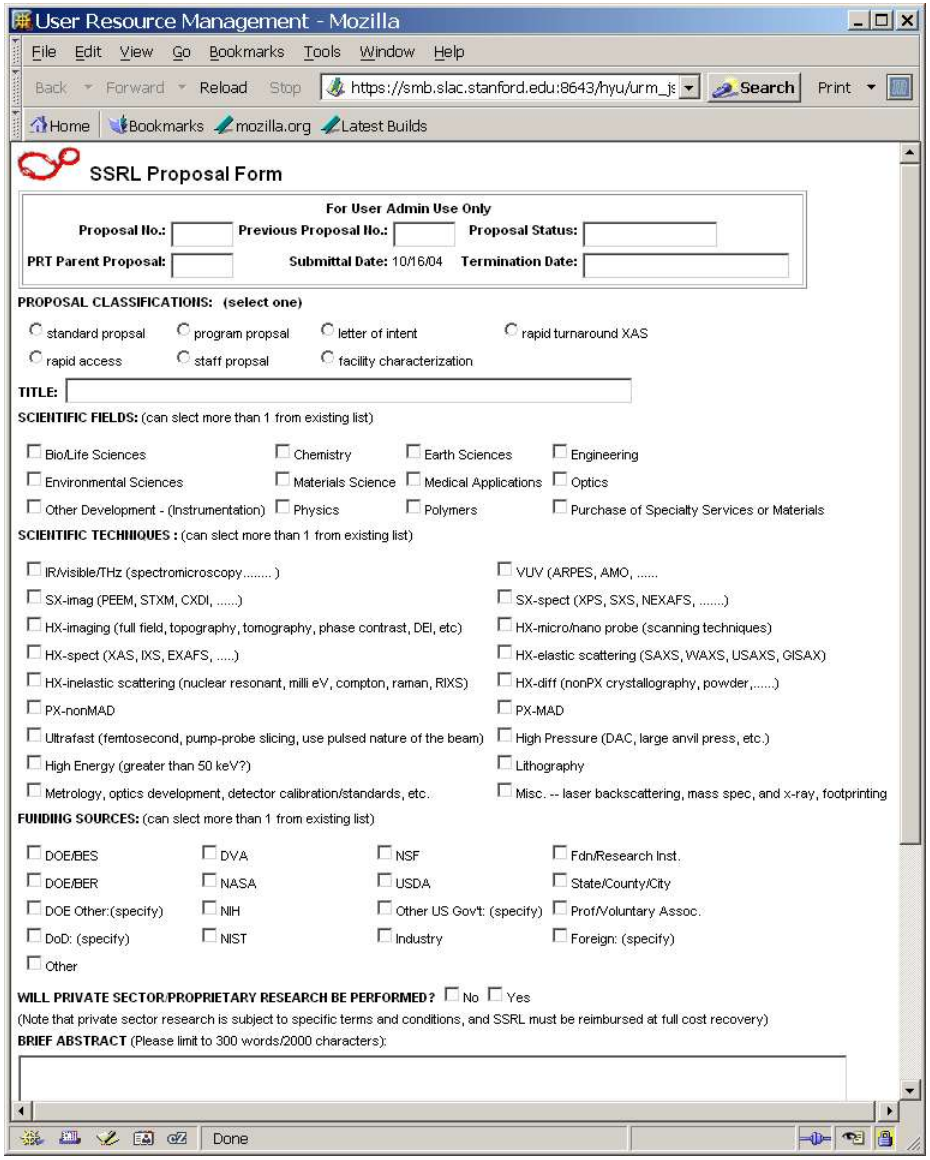
New Archive System Developments

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

Archive System Web Architecture

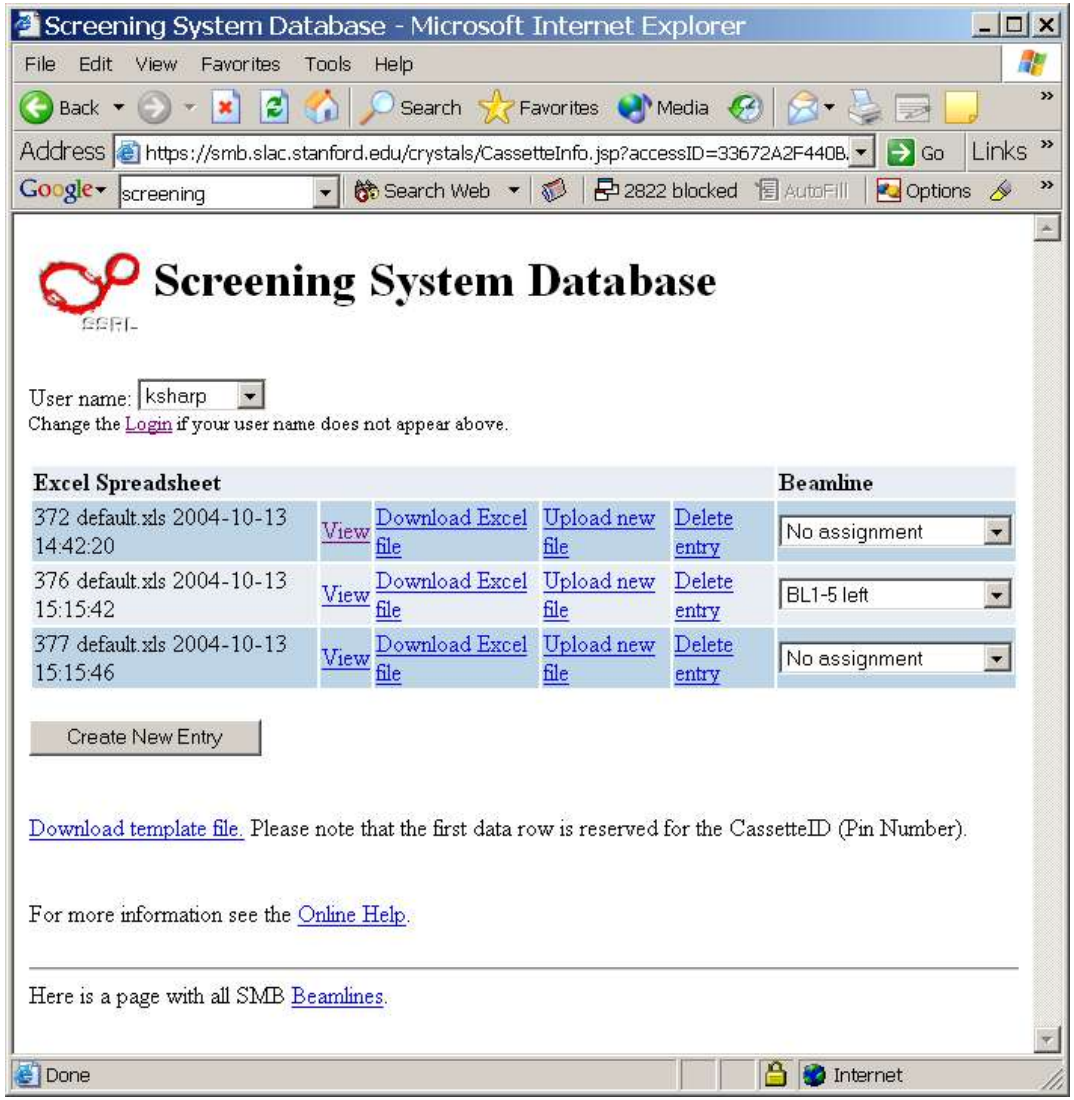


User Resource Management System



- **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

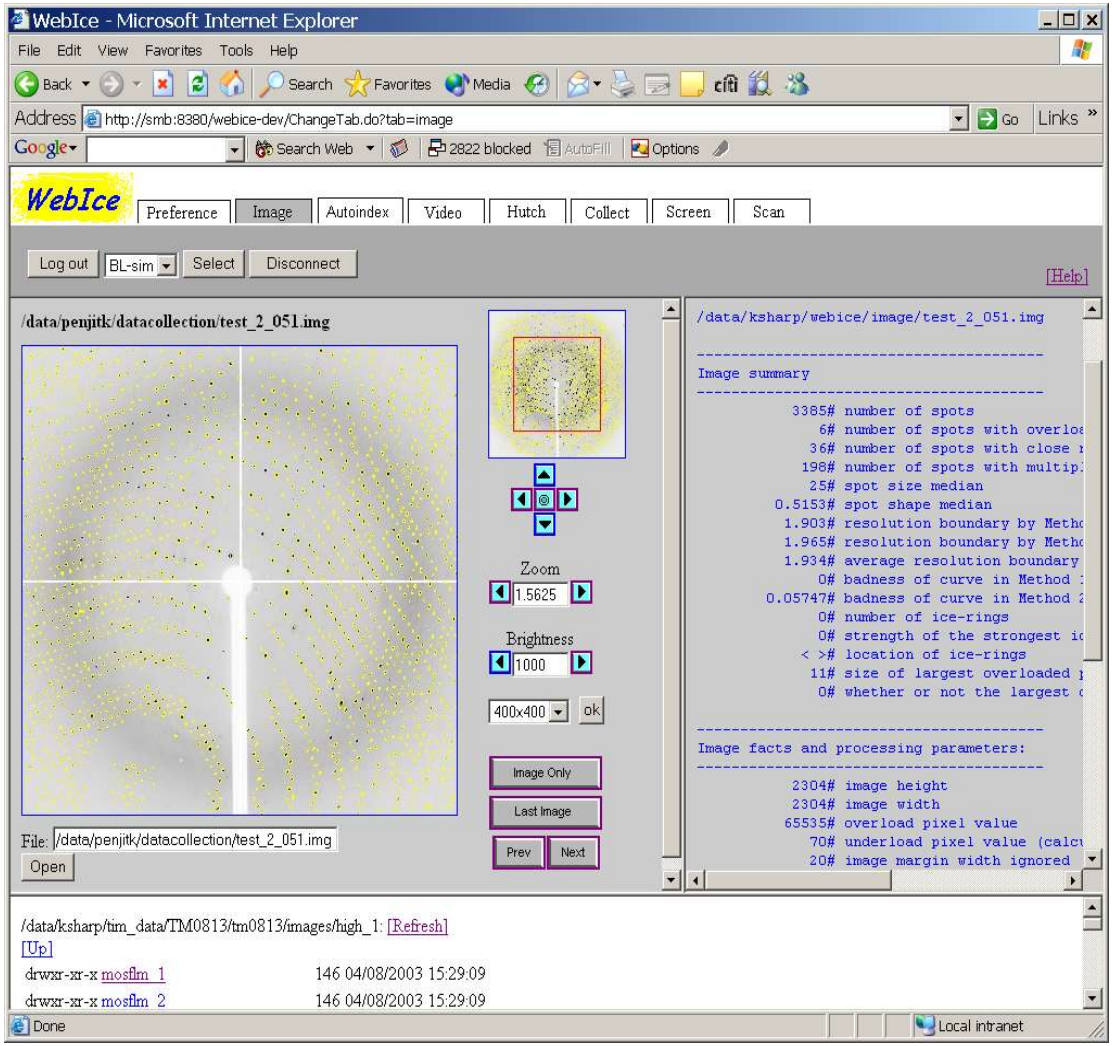


The High-Throughput Screening System (HTSS) allows for the efficient screening of crystals through the use of automated sample mounting from special cassettes.

A web application allows users to upload spread-sheets containing crystal information.

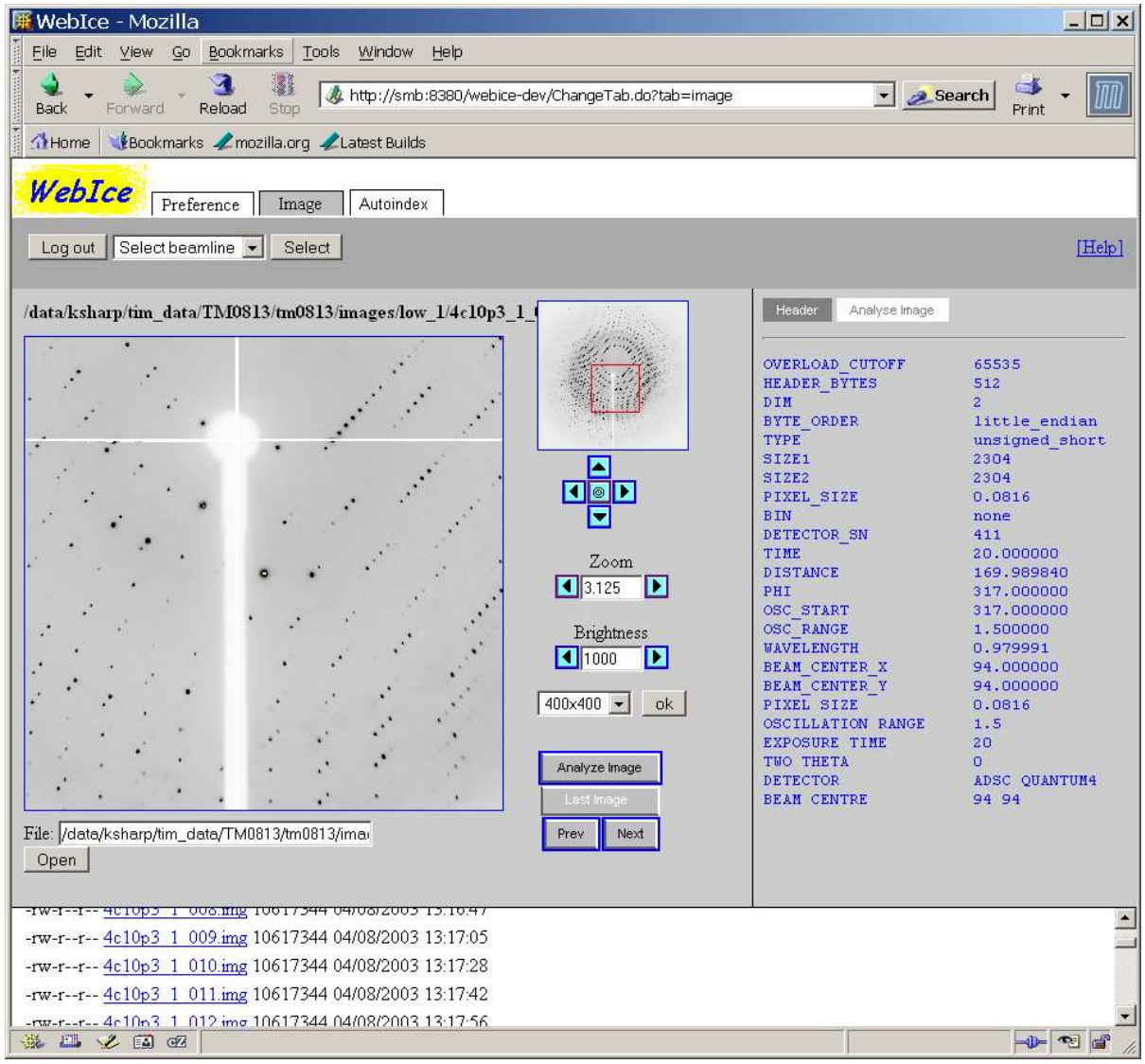
The Authentication Server allows users to access their crystal spreadsheets 24/7, but only allows them to associate a crystal cassette with a beam line when they have beam time.

WEB-ICE



- 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

Web-Ice Image Viewer



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

Analyze Last Collected Image

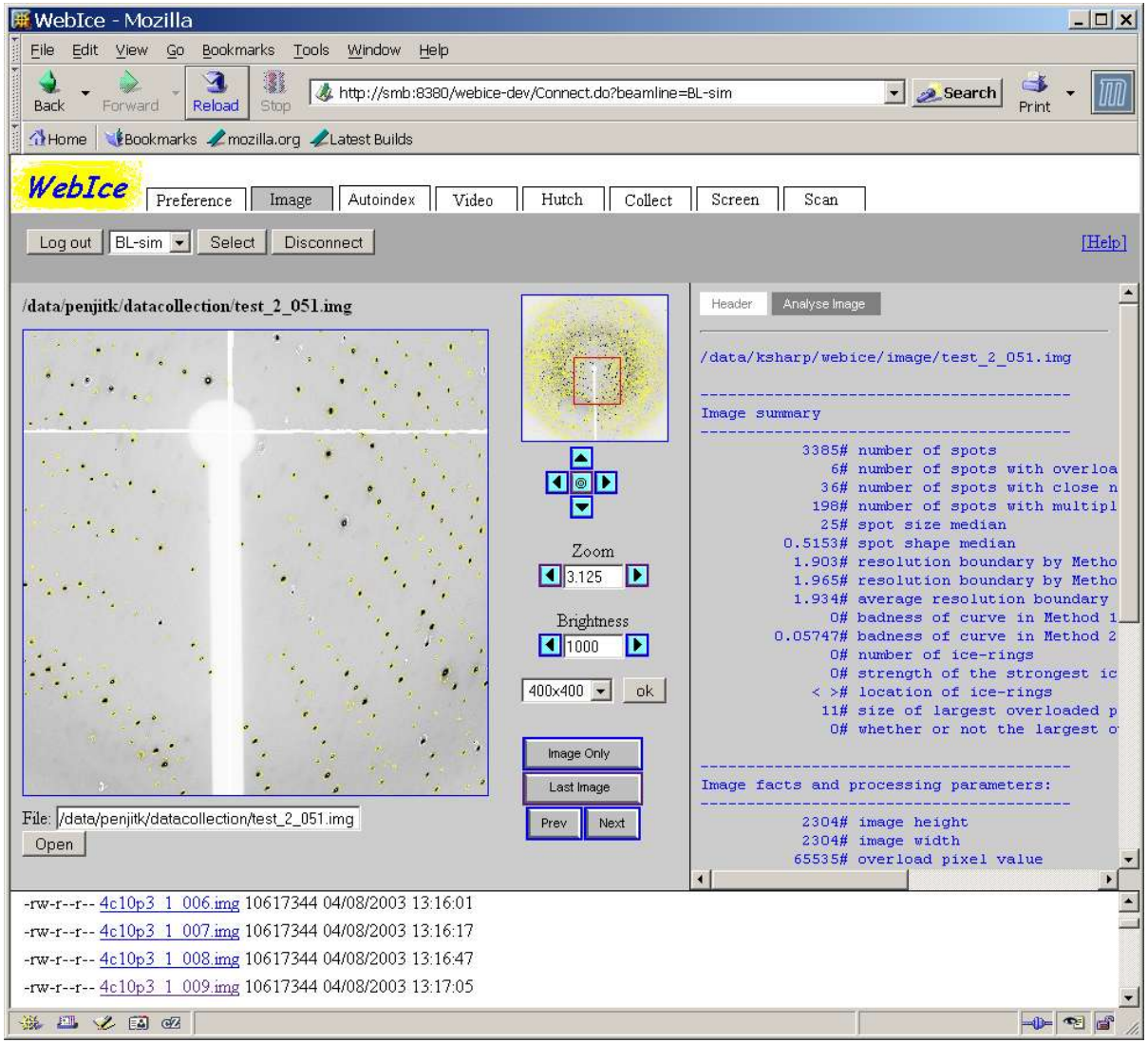
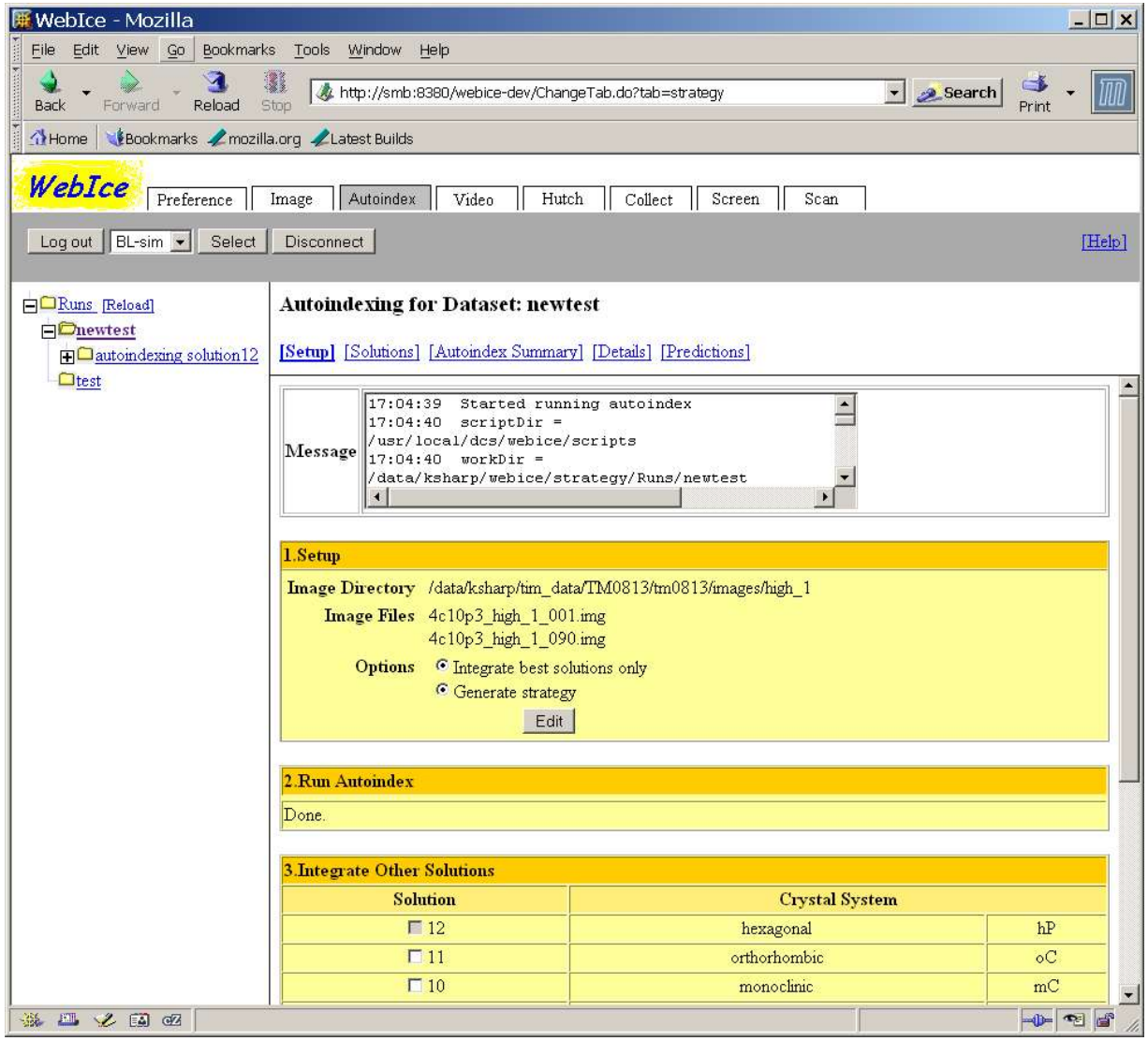


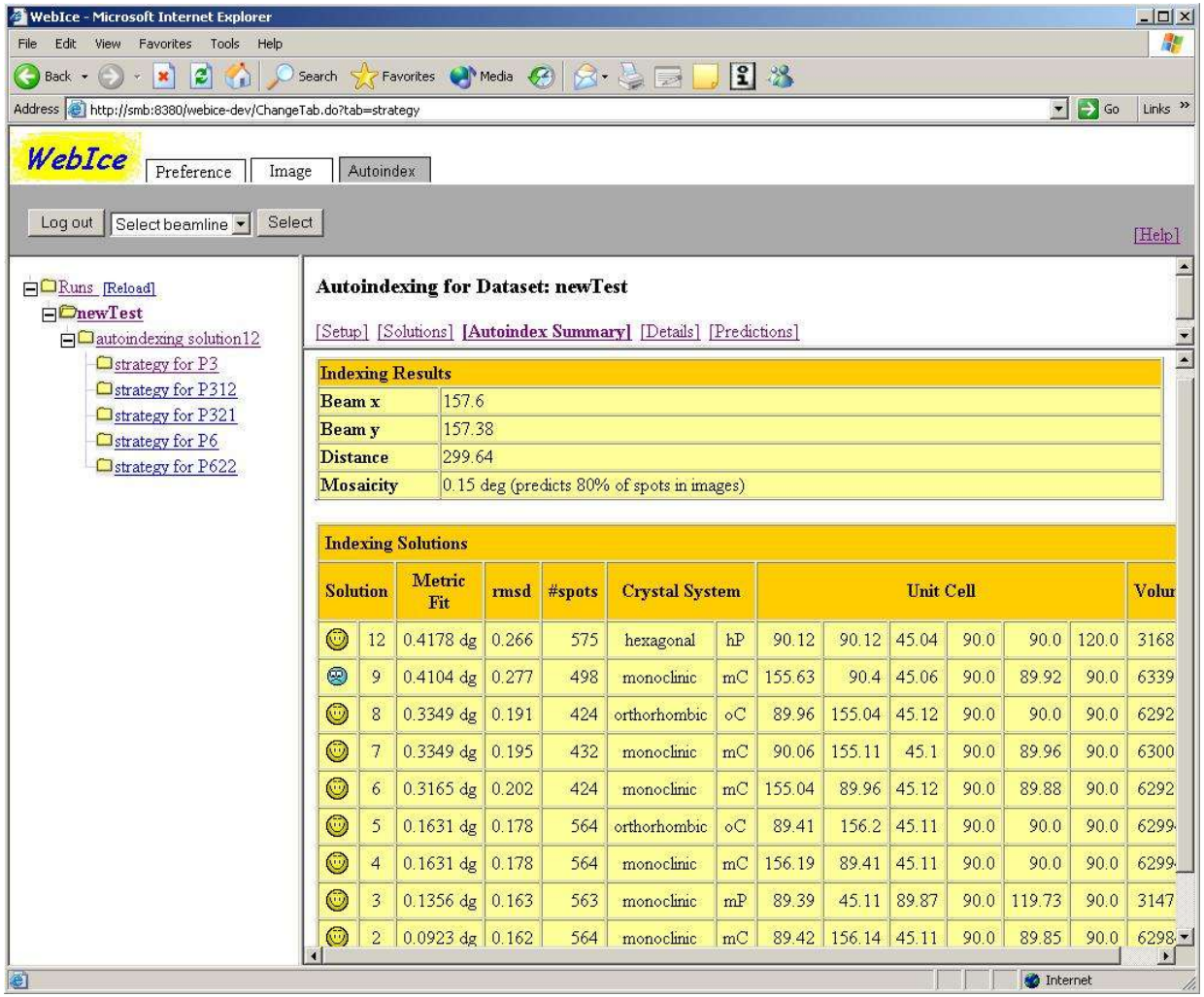
Image Viewer also enables the user to analyze last collected image from beam line with an in-house program called Spotfinder.

Autoindex Setup



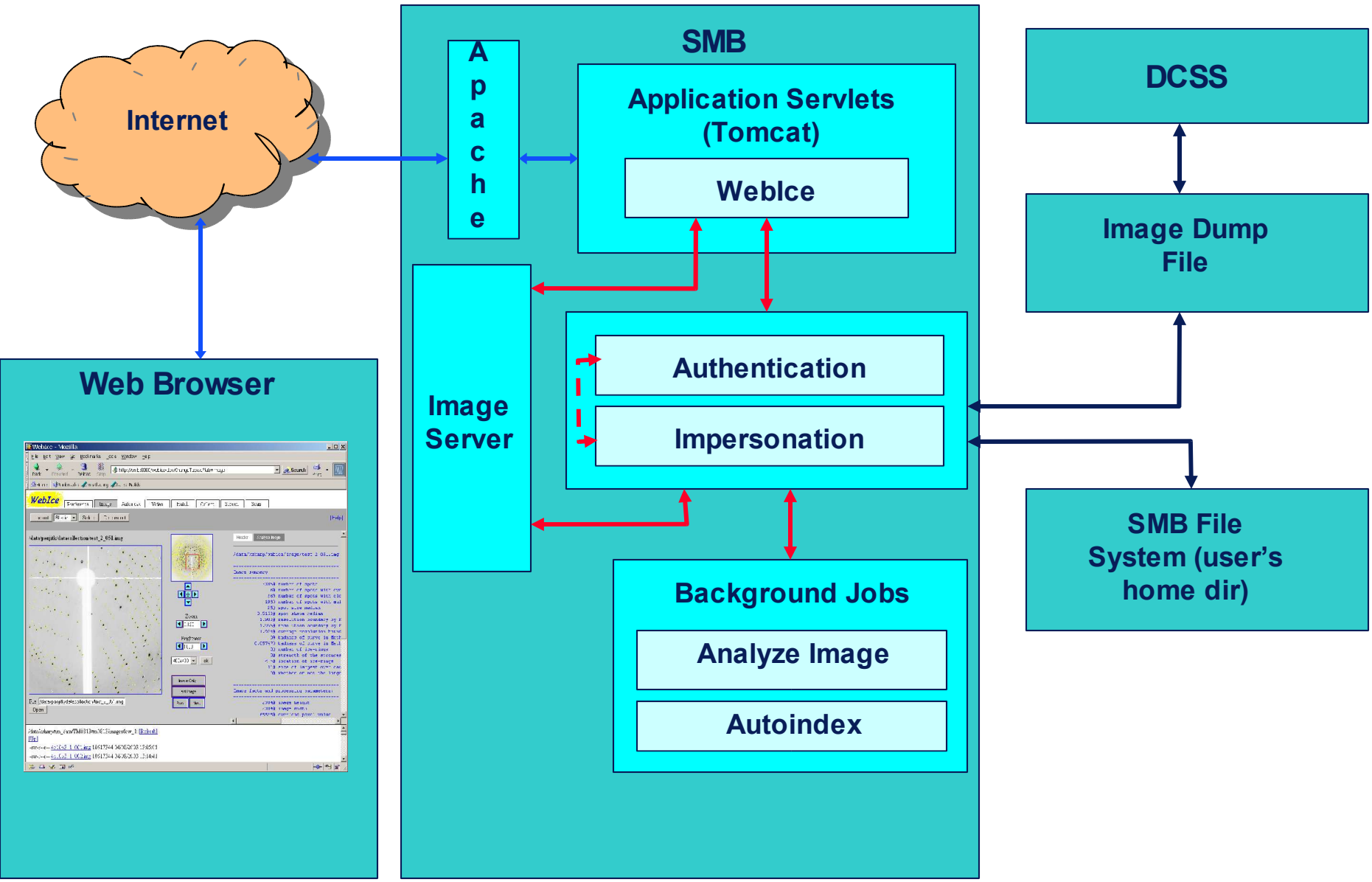
The Autoindex tab may be used to create data collection strategies.

Web-Ice AutoIndex Results



- **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

SSRL is funded by:

Department of Energy, Office of Basic Energy Sciences

The Structural Molecular Biology Program is supported by:

National Institutes of Health, National Center for Research Resources,Biomedical Technology Program

NIH, National Institute of General Medical Sciences

and by the

Department of Energy, Office of Biological and Environmental Research.

SSRL Director - Keith Hodgson
SMB Leader - Britt Hedman
MC Leader - Mike Soltis

Software Development and Support:

Scott McPhillips, Penjit Moorhead, Kenneth Sharp, Jinhu Song, Hilary Yu, Henry van den Bedem, Guenter Wolf, Thomas Eriksson, Leesa Yim