


User Guide for SS Import and FOXMAS Processing

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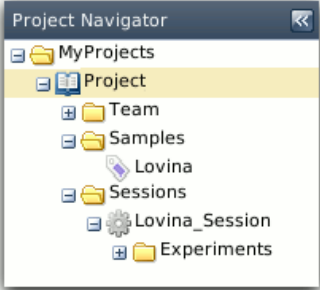
1. Import a Scan Into ScienceStudio

1.1 Browse to <http://sciencestudioproject.com/>



The Science Studio logo features a stylized atom with a central nucleus of yellow and blue spheres, surrounded by black and blue elliptical orbits. The word "Science" is in black and "Studio" is in blue, both in a bold, sans-serif font.

Home Sign In Learn Register Simulation

Downloads <ul style="list-style-type: none">Science StudioPeakabooFOXMASOther Tools	<p>Science Studio is a web portal providing remote access to synchrotron user office, beamline and data storage facilities. It allows scientists to manage:</p> <ul style="list-style-type: none">▶ Beamtime▶ Samples▶ Experimental Data▶ Teams	 <p>The Project Navigator window shows a hierarchical tree structure under "MyProjects". The "Project" folder is expanded, showing sub-folders: "Team", "Samples", "Sessions", "Lovina_Session" (containing a gear icon), and "Experiments".</p>
Facilities <ul style="list-style-type: none">VESPERSNanoFab	<p>Science Studio's aim is to provide end-to-end coverage of the experimental process. Beginning with the initial stages of an experiment such as proposals and team creation, Science Studio will provide a unified working environment all the way through to the analysis and retrieval of experimental data.</p>	
More Information <ul style="list-style-type: none">Summary ReportProject DetailsUser GuidesPublicationsPartnersBackgroundArchitecture	<p>Initially targeted at the VESPERS beamline, Science Studio will be used to various degrees on other beamlines at the Canadian Light Source.</p> <p>Science Studio is an open source project, and is free for anyone to use, modify, and redistribute. Science Studio is released under the Revised BSD License</p>	

Click on “Sign In” if you have a Science Studio account, otherwise, click on “Register” to get an account.

1.2 Choose an Authentication Service to Log Into Science Studio

Once you click on “Sign In” after you register a Science Studio account, there are two Central Authentication Services (CAS), select the “University of Western Ontario” (UWO) CAS.



Experiment remotely using scientific instruments.



Organize your samples and experimental data.



Share experimental data with your research team.

Select a Central Authentication Service

[University of Western Ontario](#)
London, Ontario, Canada

[Canadian Light Source](#)
Saskatoon, Saskatchewan, Canada



[Firefox \(3.6+\)](#) is recommended.

Other standards-compliant browsers are known to work, however only Firefox is thoroughly tested and supported.

Input the user ID and password and log into Science Studio.

The image shows a screenshot of the Science Studio login interface. At the top is the Science Studio logo. Below it is a form titled "Enter your NetID and Password". The form contains two input fields: "NetID:" and "Password:". Below these fields is a checkbox labeled "Warn me before logging me into other sites." At the bottom of the form are two buttons: "LOGIN" and "clear".

1.3 For New Users

Only administrators can import existing scan data into a project. The data set to be imported should be located at one of the machines at ALS that has the Science Studio file transfer service enabled. Once this data has been imported, regular users belonging to the same project (ie. project team members) can process that data with FOXMAS.

The following sections will describe the steps for an administrator to import data sets into Science Studio.

1.4 Select or Create a Project for Import Data (Administrators)

Clicking on "Projects" in the Project Navigator panel will bring you to the "View"

panel for your Projects. You can either select an existing project, or create a new

The screenshot shows the Science Studio interface. On the left is the Project Navigator with a tree view containing 'Projects', 'UWO Project 1', and 'UWO Project 2'. The 'View' button is highlighted in red. The main area displays a table of projects:

GD	Name	Start	End	Status
UWO1P	UWO Project 1	2011-12-22	2012-02-29	ACTIVE
UWO2P	UWO Project2	2012-01-10	2012-01-31	ACTIVE

Below the table is an 'Add Project' form with fields for Name and Description. The 'Add Project' button is highlighted in red. At the bottom, there are navigation controls including 'Find: 9', 'Next', 'Previous', 'Highlight all', and 'Match case'.

one.

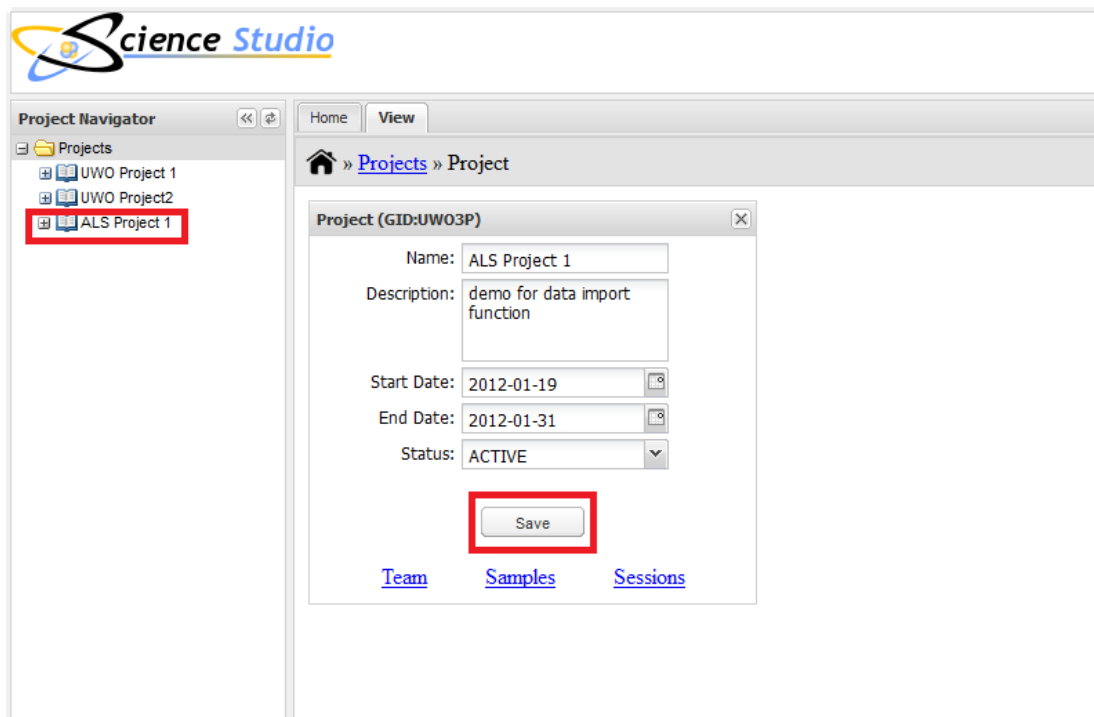
To create a new project, simply fill in the contents of the table “Add Project” at the bottom of the “View” for the new project to be added, then click “Add”

The 'Add Project' form is shown with the following fields filled out:

- Name: ALS Project 1
- Description: demo for data import function
- Start Date: 2012-01-19
- End Date: 2012-01-31
- Status: ACTIVE

The 'Add' button at the bottom is highlighted in red.

The new project “ALS Project 1” will then be added to the list of the “Projects” on the “Project Navigator” panel on the left. Click on “Save” to save the new project in Science Studio.



A project is the container of a *team*, the *samples* to be studied in the project, and all the activities that the team carried out with the samples. A session is the allocated *laboratory* time for the team to do *experiments*. An experiment can have several *scans*. A scan can be created by data acquisition in a laboratory, or by *importing* it from an existing source on a properly configured server. Some laboratories have a configured data source that supports importing (such as ALS BL 12.2.3), and some do not.

To import a data set to a *project*, it must have a data import *session*. If the project does not have one, it must be added first. Then, an *experiment* needs to be created in the *session*. Since an experiment is always associated with a sample, and the sample list is empty for a new project, a sample needs to be added to the project's sample list before creating an new experiment. The new data import session is completely added once a new experiment is created for the session.

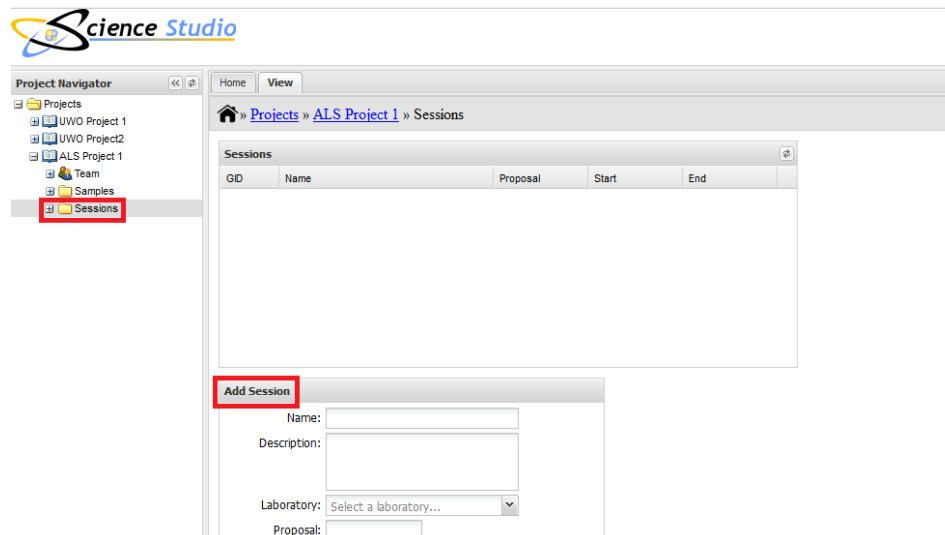
The following will give you instructions on how to completely add a data import session for a newly created project, including how to add a session, how to add a sample, and how to add an experiment.

1.5 Select or Create a Data Import Session in a Selected Project (Administrators)

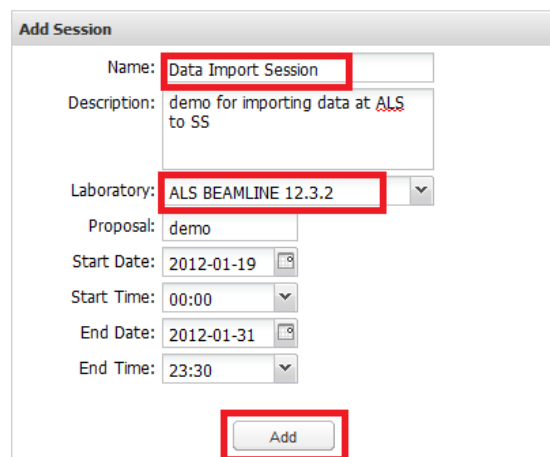
To import a data set into a project, you must first select the data import session inside the project. For a newly created project, three empty folders are generated: "Team", "Samples", and "Sessions". To create a Data Import session, you need to add a session, add a sample, then add an experiment inside the session.

1.5.1 Add a Session

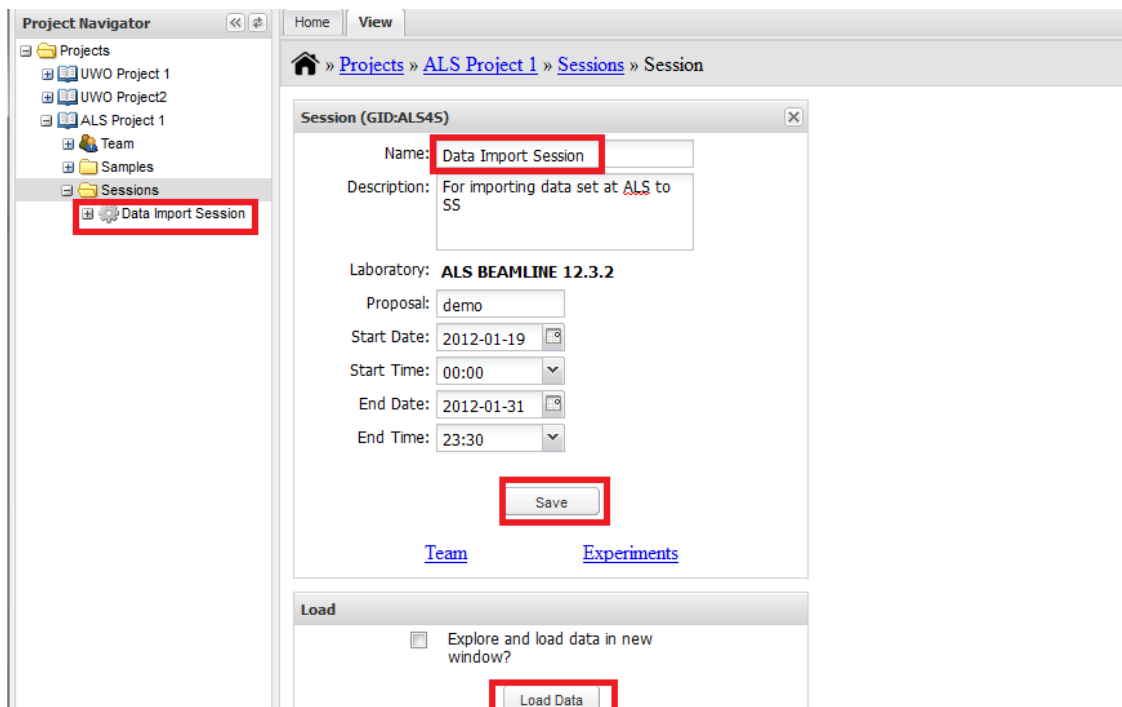
Click on the “Sessions” folder inside the selected project in the “Project Navigator” panel. It will bring you to the Sessions view panel.



Fill in the contents of the “Add Session” form at the bottom of the sessions view panel. When you create a new session, you need to choose the proper laboratory. Some laboratories have a configured data source that supports importing, and some do not. Make sure to select “ALS BEAMLINE 12.3.2” as the “Laboratory” for importing data sets located at ALS, then click “Add”.



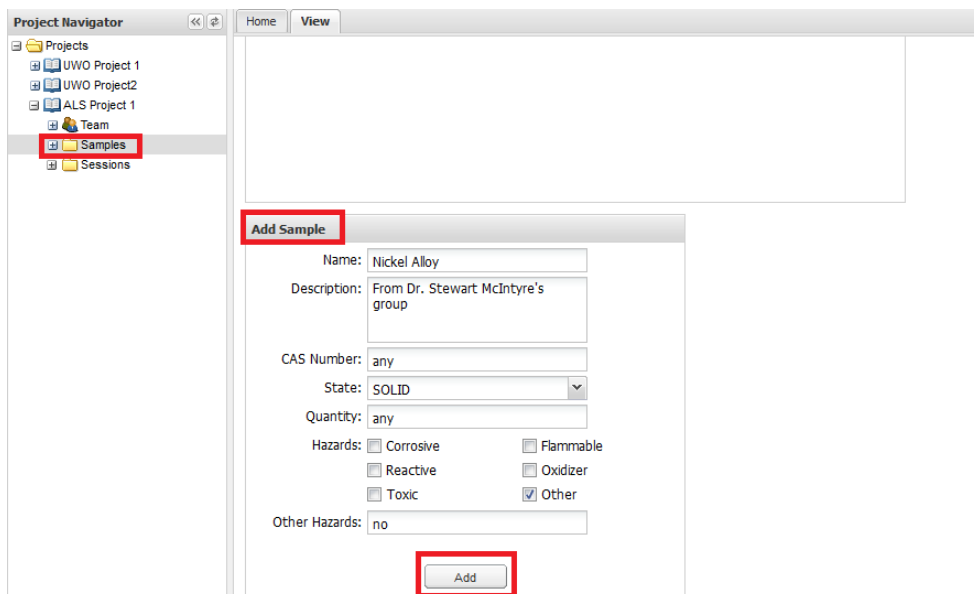
A new session called “Data Import Session” will then be added to the “Sessions” list in the “Project Navigator” panel.



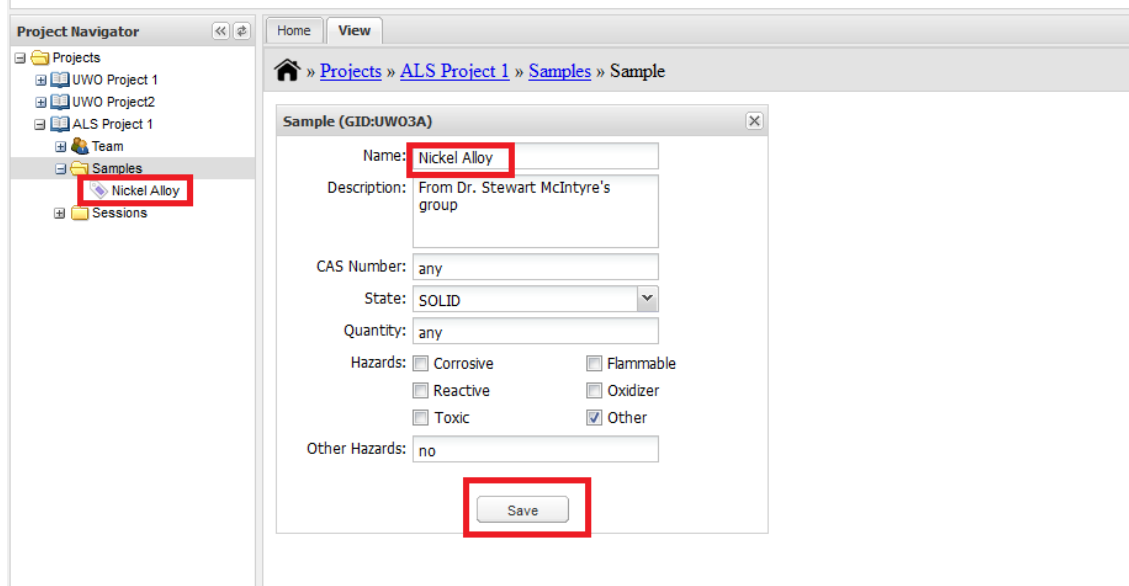
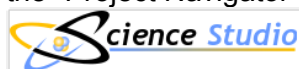
Click on “Save” to save this new session in Science Studio. Before you click “Load Data” in this session, you need to make sure that you have created an experiment in this session. If the Experiments list is empty when you expand the contents of this session (click on the “+” button for of “Data Import Session”), you need to add an experiment first. Since an experiment needs to be associated with a sample, if the Samples list in this project is empty, you need to add a sample first.

1.5.2 Add a Sample to the Project

Click on the “Samples” folder inside the selected project in the “Project Navigator” panel. It will bring you to the Samples view panel. Fill in the contents of the table “Add Sample”, then click “Add”.

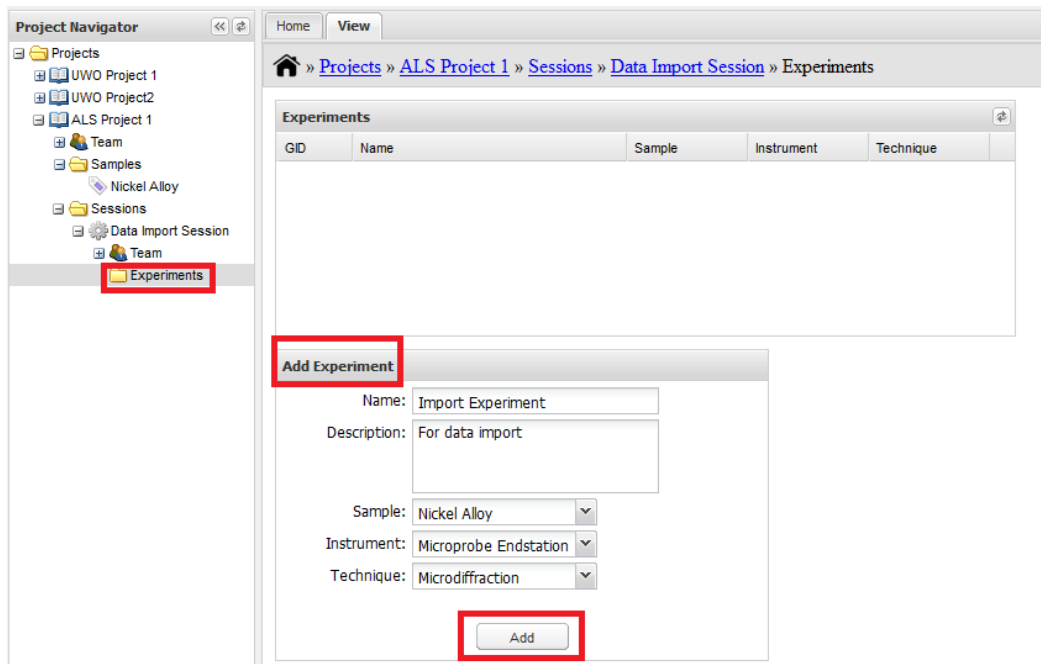


You will see that the new sample named “Nickel Alloy” is added to the “Samples” list in the “Project Navigator” panel. Click “Save” to save it in Science Studio.

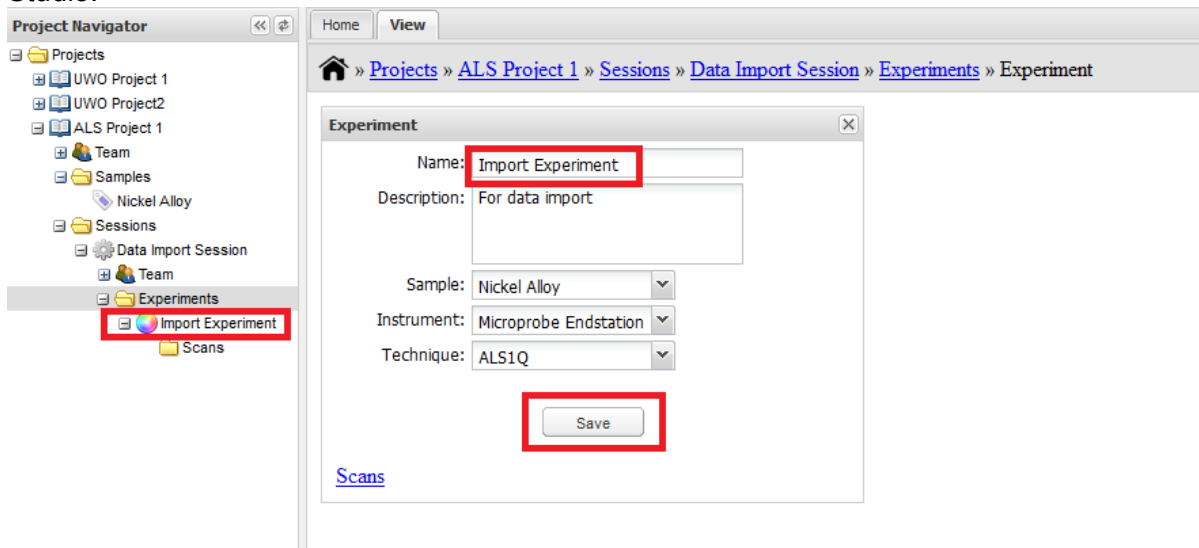


1.5.3 Add an Experiment in the Data Import Session

Click on the “Experiments” folder inside the data import session that is added in 1.5.1 from the “Project Navigator” panel. It will bring you to the Experiments view panel. Fill in the contents of the table “Add Experiment”, then click “Add”.



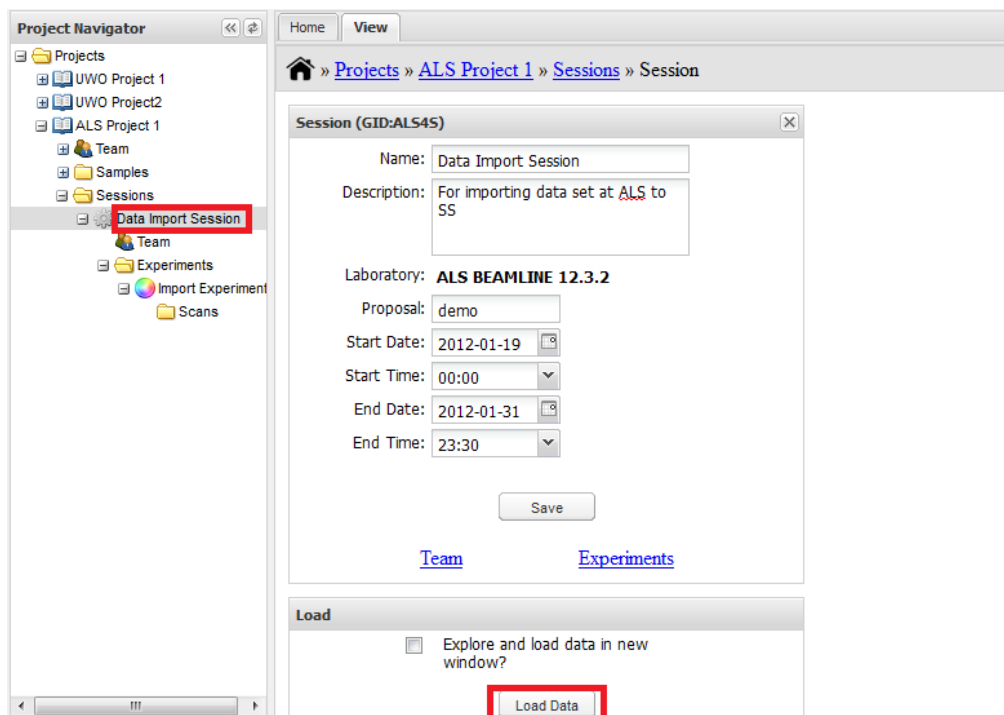
As for this example, you will see that the new experiment named “Import Experiment” is added to the “Experiments” list in the “Project Navigator” panel. Click “Save” to save it in Science Studio.



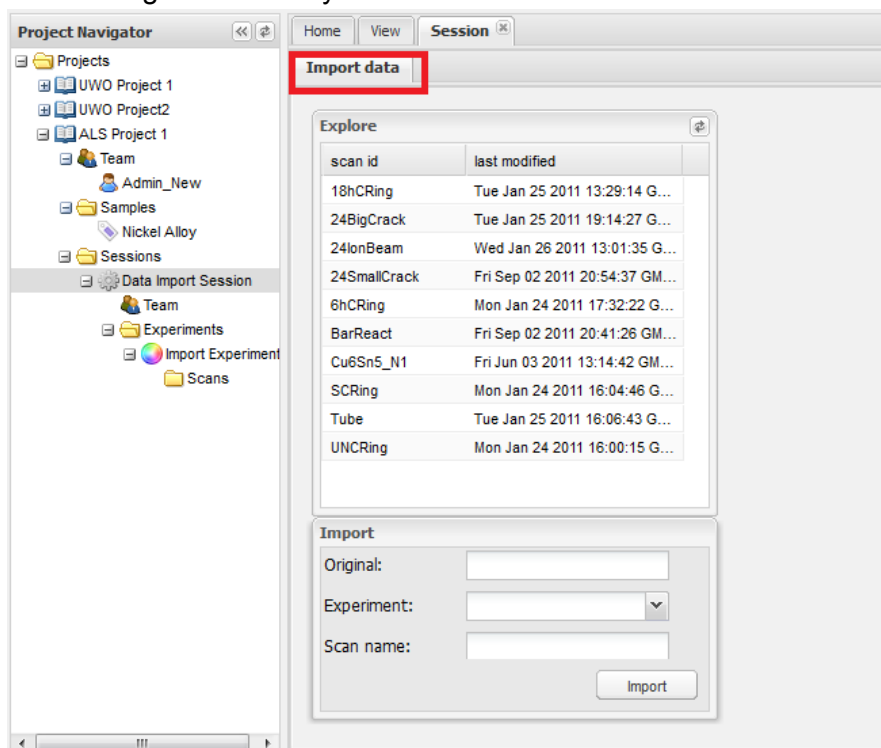
For the new experiment that was just created, an empty folder “Scans” is created for the experiment. The next section will instruct you on how to import scan data that is located at the ALS to this Scans folder.

1.6 Import a scan into Science Studio (Administrators)

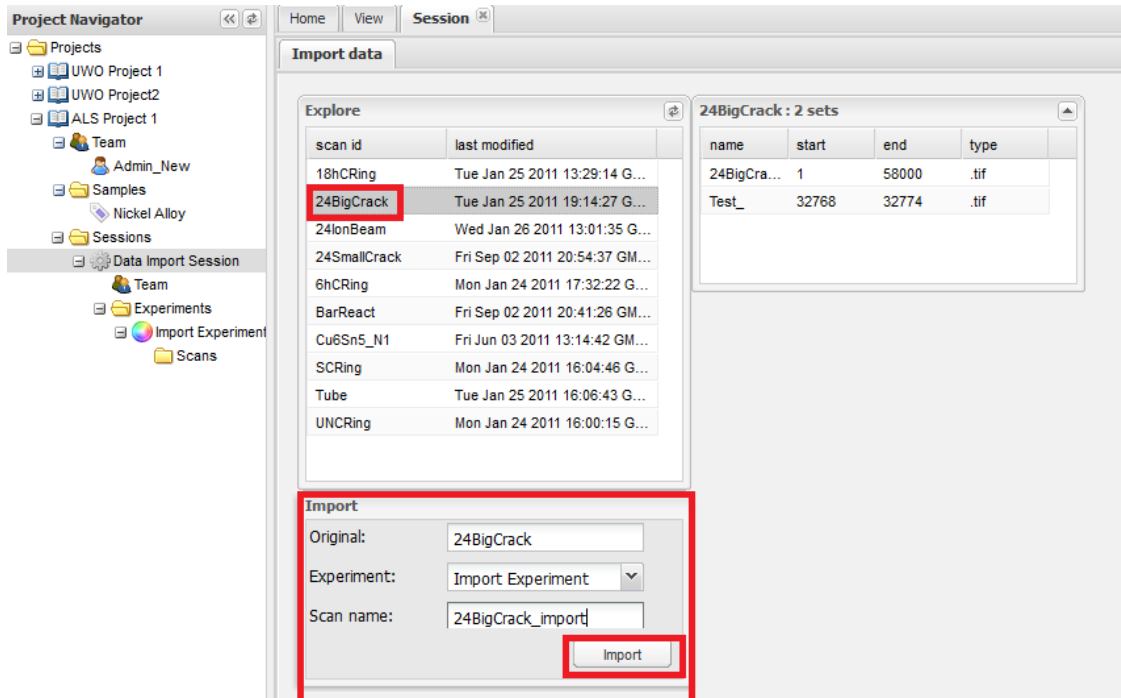
Once you have a Data Import session in your project, click to select it. It will bring you to the Session view panel. Click the *Load Data* button to start importing.



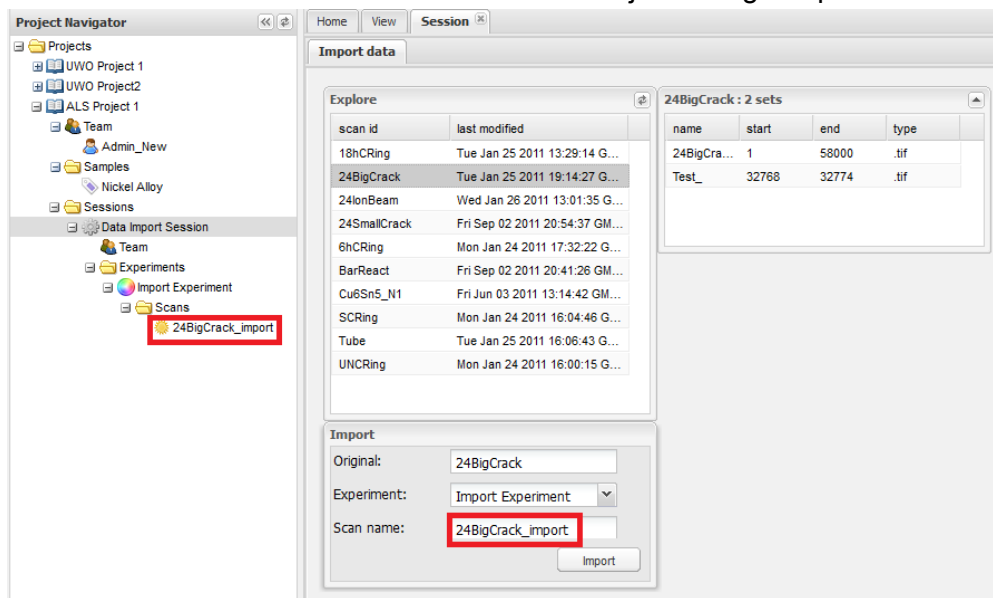
It will bring you to the “Import data” panel with a list of data sets that can be selected to import. If the “Import data” panel does not show up or an warning message appears, contact the administrator -- they may need to ensure that the service running on the laboratory server has been configured correctly.



Select a scan from the list; it will show some information about this data set on the panel on the right. Fill in the “Import” form at the bottom, and click the “Import” button.



Importing a data set can take several seconds. Once completed, you will see that the selected data set has been added to the Scans list in Project Navigator panel on the left.



If you see your new scan in the Scans list in the Project Navigator panel, you have successfully completed importing your data into Science Studio.

From now on, any user, who is added as a team member to this project, can perform data processing task by using FOXMAS.

1.7 Add a Person to a Project (Administrators)

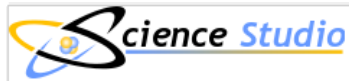
This section will instruct you on how to add a new regular user to a project and enable him/her

to process any scan data inside this project using FOXMAS.

Click on the “Team” entry inside the selected project, it will bring you to the Team view panel. Fill in the “Add Person” form for the new team member to be added.

The screenshot shows the Science Studio interface. On the left, the Project Navigator shows a tree view with 'ALS Project 1' selected, and its 'Team' sub-entry highlighted with a red box. The main panel displays the 'Team' view for 'ALS Project 1'. It contains a table with one entry: 'Admin New' with role 'RESEARCHER'. Below the table is the 'Add Person' form, which is highlighted with a red border. The form fields are: Name (Ge Baolai), Phone (empty), Mobile (empty), Email (bge@sharcnet.ca), and Role (COLLABORATOR). The 'Add' button at the bottom of the form is also highlighted with a red box.

Once you click “Add”, this new team member (with the name “LastName_FirstName” in the above example) will be added to the “Team” list in the Project Navigator panel on the left.



The screenshot shows the Science Studio interface after the 'Add' button was clicked. The Project Navigator on the left now shows 'ALS Project 1' selected, and its 'Team' sub-entry expanded to show 'Admin New' and 'Ge_Baolai', with 'Ge_Baolai' highlighted by a red box. The main panel displays the 'Person' view for 'ALS Project 1' > 'Team'. It contains a form for editing the person's details. The fields are: Name (Ge Baolai), Phone (empty), Mobile (empty), Email (bge@sharcnet.ca), and Role (COLLABORATOR). The 'Save' button at the bottom of the form is highlighted with a red box.

Click on “Save” to save this update in Science Studio.

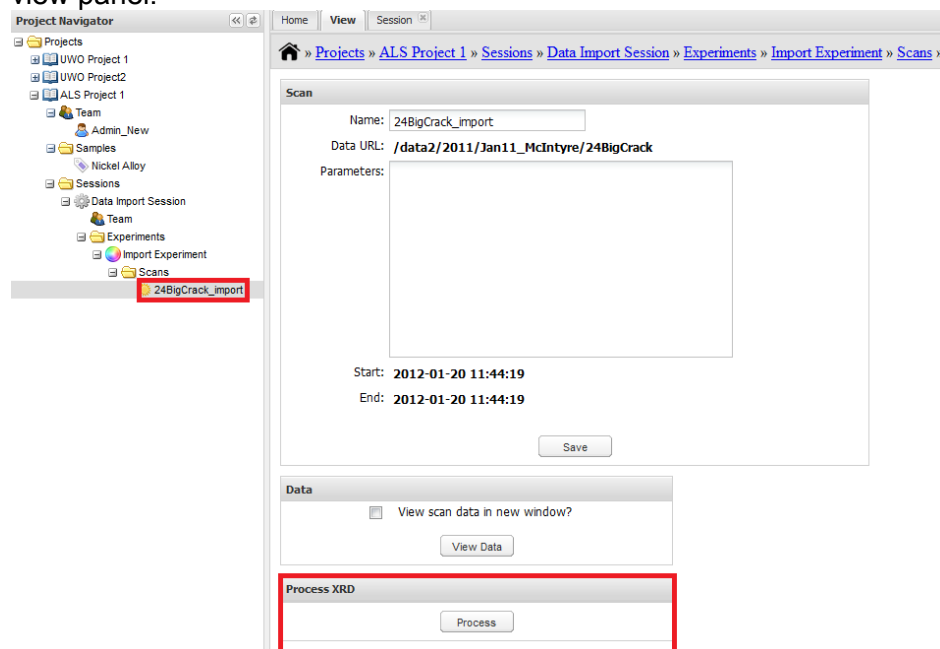
The next section will instruct you on how to process a data set using FOXMAS.

2. FOXMAS Processing (All Users)

Any user who has registered in Science Studio can use FOXMAS to process scans. New regular users must be added to the project containing the scan by an administrator. Adding users to projects is documented later in this guide. This section describes how to select a scan, process it with FOXMAS, and view the results online.

2.1 Select a Scan to be Submitted for Processing

In the Project Navigator window, select a scan from the Scans list under an experiment contained in a session. In the example shown below, the scan “24BigCrack_Import” from the Data Import Session is selected. Clicking on the scan to be processed will bring you to the scan view panel.



Click on the button “Process” inside the “Process XRD” panel at the bottom, it will bring you to the FOXMAS web interface.

2.2 Input Parameters Through the Web Interface

If the selected data set has been processed before, the last parameters you used will be loaded, otherwise default values will be loaded. Carefully check each of those parameters to ensure that they are correct. Many fields have tool tips which will appear if you hover your mouse over them.

Choose a name for the result of this processing by filling the field “Name of Result”. This will be the name used by Science Studio for the processing results.

FOXMAS
Fast Online X-ray Microdiffraction Analysis Software

Input Data

Name of Result: 24BigCrack fistTry Jan19 2012

Type of Image: PilatusTiff

High Priority:

Peak Search

Threshold (%): 1.2

Max Center To Fit Distance: 10

Type of Filter: Brukner

Type of Fit: Gaussian

Box Size: 10

Max R Factor: 0.9

Min Peak Width: 0.01

Max Peak Width: 20

Map Parameters

Scan Width: 580

Scan Height: 100

Micron Step Width: 1

Micron Step Height: 1

Material Structure

Crystal Structure: ni-i600.cri

Stiffness File: (ni-i600.cri): ni.stf

Buttons: New, View, Edit, Delete (under Crystal Structure); New, Edit (under Stiffness File)

Calibration, Laboratory, Analysis (expandable sections)

2.2.1 Select or Create Crystal Structure

If you can not find the appropriate crystal structure and stiffness files in the provided list, you can create new ones by click on the buttons “New”.

Expand the Calibration, Laboratory, and Analysis fields to enter parameters relating to different aspects of the required configuration information.

2.2.2 Input Calibration Parameters

Experiment calibration needs to be done by using XMAS, which can be downloaded at <https://sites.google.com/a/lbl.gov/bl12-3-2/user-resources> .You may request these values from a beamline scientist or you may do the calibration yourself by using XMAS. Once you have all the calibration parameters ready, expand the closed fields for Calibration parameters.

New Edit

Calibration

Center Channel (pixels)

X:

Y:

Detector

Sample Distance:

Tilt of Detector / Beam (degrees)

Roll:

Pitch:

Yaw:

▼ Laboratory

▼ Analysis

Reset Parameters Save Parameters Start

2.2.3 Input Laboratory Parameters

Expand those closed fields for “Laboratory parameters”. The default values in this section are for ALS beamline 12.3.2. Adjust any settings for which your experiment settings differ from the defaults.

▼ Calibration

Laboratory

CCD Camera (mm)

Width:

Height:

Polychromatic Beam Energy Bandpass (keV)

Min:

Max:

CCD Camera (pixels)

Width:

Height:

Detector Orientation

2θ (degrees):

Sample Tilt Matrix

1	0	0
0	-0.70711	-0.70711
0	0.70711	-0.70711

▼ Analysis

Reset Parameters Save Parameters Start

2.2.4 Input Analysis Parameters:

Expand those closed fields for “Analysis parameters”. These parameters influence how indexing and strain refinement are performed. Carefully select these parameters for your analysis.

Calibration

Laboratory

Analysis

Indexing Parameters

Angular Tolerance:

Starting Set:

Min # Indexed:

Re-index

Refine Lattice Parameters

b/a

c/a

α

β

γ

$\alpha = \beta$

$\alpha = \beta = \gamma$

b = a

Refine Detector Parameters

pixel size ratio

distance

xcent

ycent

pitch

yaw

roll

Reset Parameters Save Parameters Start

2.3 Start Processing

Double check all the parameters that you input for analyzing the selected scan data set, click “Start” to start processing this data set with the current configuration. A message will tell you whether your job was submitted successfully or not.



FOXMAS

Fast Online X-ray Microdiffraction Analysis Software

Input Data

Name of Result:

Type of Image:

High Priority:

Peak Search

Threshold (%):

Max Center To Fit Distance:

Type of Filter:

Type of Fit:

Box Size:

Max R Factor:

Min Peak Width:

Max Peak Width:

Map Parameters

Scan Width:

Scan Height:

Micron Step Width:

Micron Step Height:

Material Structure

Crystal Structure:

Stiffness File: (ni-i600.cri):

Calibration

Laboratory

Analysis

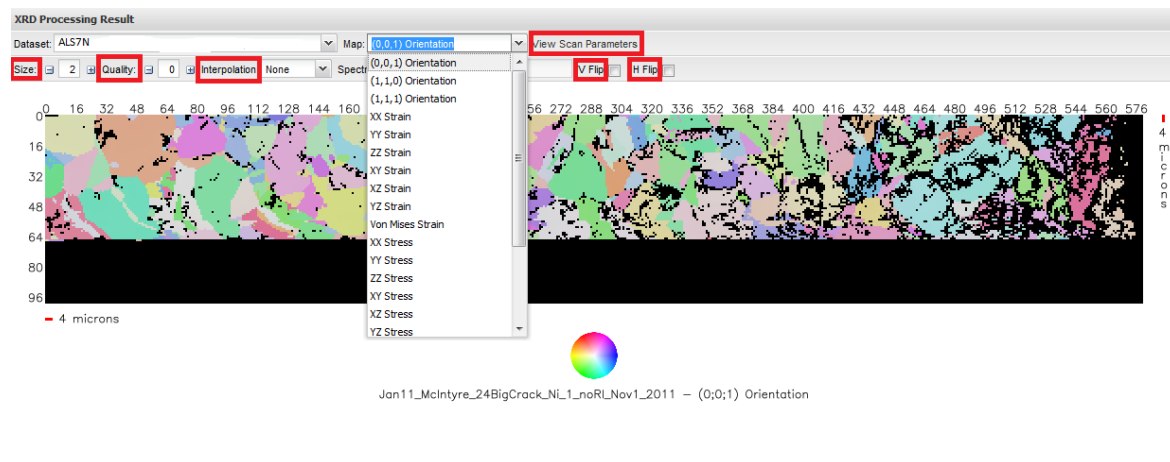
Job successfully submitted [Click to view the results.](#)

Once a job is submitted successfully, it will be processed according to priority. While many jobs can be run at once, preference is given to small scans, and scans for which data is still being collected. Users can submit multiple jobs at once, but should remember to change the result name when resubmitting. While giving multiple processed data sets the same name is technically allowed, it could become confusing. Some functions, such as such as viewing the status of a submitted job or cancelling or stopping a running job, are still under development and are not yet available.

2.4 View the Results

After the processing has been started, follow the link “Click to view the results” to the online “XRD Processing Result” map view page. The name in the “Dataset” field is just a system

generated unique ID for this scan data set. You can view different maps by choosing any of the maps that are provided in the list. If the processing is not yet completed, you can observe the progress as new data is loaded. Once the a map is completed, processing is finished.



The Results Viewer has the following features:

2.4.1 Change Map Size (Zoom)

The value in the “Size” field decides the size of the map. For example, if the value is 2, that means that each scan point in the map is represented by 2X2 pixels. Increase the value to get a larger size map, or decrease the value to get a smaller size map.

2.4.2 Filter Data by Minimum Indexing Quality

The indexing quality is decided here by a threshold value for the minimal number of indexed spots on an XRD image. Changing the value in the “Quality” field will give you maps with a different “quality”. For example, if the value in the “Quality” field is 10, the map will only show the scan points for which the associated XRD image had at least 10 spots indexed by FOXMAS. Any XRD images which cannot be indexed or have fewer than 10 indexed spots will become black spots in the map.

The default value in the “Quality” field for the map is shown as “0” at the beginning, but the actual map for the “lowest quality” is based on the value you input previously in the “Min # Indexed” field in the “Analysis parameters” on the job submit page.

2.4.3 Flip the Map

Check “V flip” to flip the map vertically, and/or check “H flip” to flip the map horizontally.

2.4.4 View Parameters

To view the parameter values that have been used in processing this result data set, click “View Scan Parameters”, it will open a window to show all the parameters.

2.4.5 Save a Map to Disk

To save any map to your local machine, right click on the map and select “Save Image As ..”

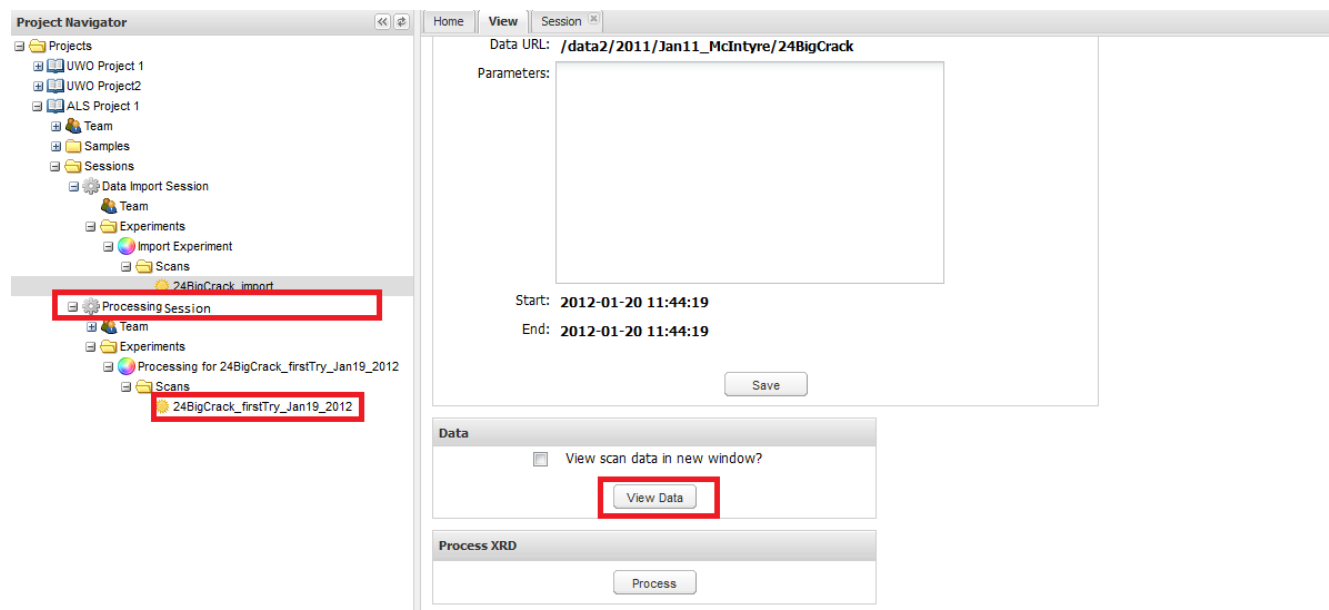
3. Download result files

This section describes how to download result files from a processing record in Science Studio.

3.1 Select a Processing Record

Find the main page of Science Studio in your previous window or tab. After you start processing a scan, if this is the first processing data in this project, Science Studio will create a new session called “Processing Session” in the project. The processing results will be added as a “scan” inside a new experiment in the Processing Session.

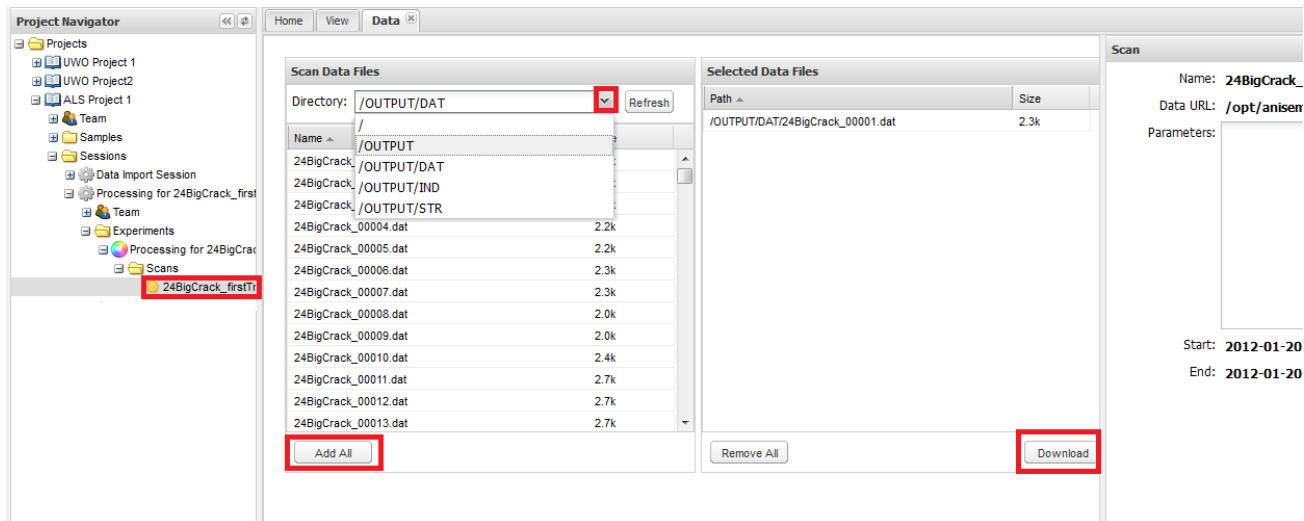
For example, we have processed data with the “Name of Result” field as “24BigCrack_firstTry_Jan19_2012”. You will see that a new experiment called “Processing for 24BigCrack_firstTry_Jan19_2012” is added to the Experiments list inside the “Processing Session” by Science Studio. The scan named as “24BigCrack_firstTry_Jan19_2012” is for the result files. Click on the scan name, it will bring you to the scan view panel.



Click on the “View Data” button in the scan view panel, it will open a data view panel.

3.2 Select Files for Download

The files contained in a FOXMAS processing result are organized into three sub folders of the “OUTPUT” folder. The three sub-folders are DAT, IND and STR. The DAT folder contains the peak searching result files for each of the images. The IND folder contains the indexing result files. The STR folder contains the strain calculation result files. Select one of the three sub-folders from the “Directry” list. The contents of the selected folder will then be displayed. Feel free to select any files by clicking on them to add them to the “Selected Data Files” panel on the right. You can also click on the “Add All” button at the bottom for selecting the entire folder.



Then click on the “Download” button. All your selected files will then be downloaded as a .zip file to your local machine.

4. After Downloading

After downloading all the result files, you may use some additional tools to further investigate those results. Please feel free to use some tools that were developed by Science Studio, and they are available for downloading at <http://sciencestudioproject.com/packages.php>.