

# Lab 0: Preparing your laptop for the course

Three pieces of software are needed to complete this course:

1. VMD – Views and analyses molecular models.
2. A modern HTML5 compatible web browser with Javascript enabled – Internet Explorer 10 or newer, recent versions of Chrome or Firefox.
3. A good text editor that handles different line endings (i.e. not Windows Notepad)

The majority of the exercises will use SASSIE-web; available on the internet, nothing to install.

## VMD

### Download

Navigate to the VMD site and download the package by following these instructions:

- Open <http://www.ks.uiuc.edu/Research/vmd> in your web browser
- Locate the 'Downloads' section
- Click on the 'Downloads (all versions)' link

Once at the downloads page, search under the heading for the current version (1.9.2 at the time of writing) to find the link for your operating system:

**Windows:** Windows OpenGL

**OS X:** MacOS X OpenGL (32-bit Intel x86)

**Linux:** LINUX\_64 OpenGL, CUDA

- Click the appropriate link
- You now need to register an account
  - Enter a username and password
  - Click "Continue with registration or download"
  - Fill in the form (including confirming your password)
  - Click Register"

### Installation

**Windows:** Run (double click) the downloaded file. It is a self-extracting executable, and will start the VMD Windows installer program. A standard Windows installer will appear, accept all defaults as they are offered to you and then click 'Install' when the option is presented to you. Note: You will need administrator privileges in order to install VMD correctly.

**OS X:** Open the downloaded file (disk image) and drag the VMD application into an appropriate directory (such as Applications). Once placed appropriately VMD should be ready for immediate use, no other installation steps are required.

**Linux:** Installation is slightly more complicated than for the other operating systems, full instructions are given below. Note: If the version you have downloaded is not 1.9.2 then update the paths given accordingly.

- In the terminal, migrate to the download directory
- Run the command:  
`tar xvfz vmd-1.9.2.bin.LINUXAMD64.opengl.tar.gz`
- Change into the *vmd-1.9.2* directory
- Open the *configure* file in a text editor; change the values for `$install_library_dir` and `$install_bin_dir` to the directories in which VMD data files and executables should be installed.
  - Note: `$install_bin_dir` values should be in your PATH
  - If you have admin access good choices might be:  
`$install_bin_dir="/usr/local/bin"`  
and  
`$install_library_dir="/usr/local/lib/$install_name"`
- Run the command:  
`./configure`
- Change into the *src* directory
- Run the command:  
`make install`

With a correctly set PATH variable you should now be able to simply run the command *vmd* from the terminal.

## Text Editor

If you are running OS X or Linux the chances are you have one or more suitable text editors installed (such as vim, emacs, gedit, kate, .....). If you are running Windows then a good option is to install one of the following options;

### Atom:

- Navigate to <https://atom.io/> in your web browser
- Click on the red button labelled 'Download Windows Installer'
- Click on the downloaded file to run it
- Accept all defaults as offered to you and click 'Install' when the option appears

### Notepad++:

- Navigate to <https://notepad-plus-plus.org/> in your web browser
- Click on the 'download' link on the left hand side of the page
- Click on the big download icon, the correct version should download automatically
- Once the file has downloaded double click on it to run it
- Accept all defaults as offered to you and click 'Install' when the option appears

# SASSIE-web: Basic Usage

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## [Access](#)

- **SASSIE-web:** One can access the full version of SASSIE on our server machine at <https://sassie-web.chem.utk.edu/sassie2>. By creating an account on our server, each user will have a persistent account and can re-login any time in the future and maintain access to your user filesystem. This software on this version is updated frequently and is most likely up to date.
- **NOTE:** A modern HTML5 compatible web browser with Javascript enabled such as Chrome, Firefox, Opera or Safari is required to run the application. You can check the compatibility of your browser to HTML 5 at <https://html5test.com>.

When you access the page you will see the following layout on the web page.

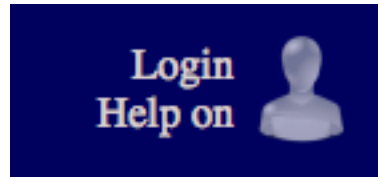


By default, roll-over help is "on" and therefore when your mouse passes over most icons and input fields a small amount of descriptive text will appear. At any time you can toggle help to be on or off.

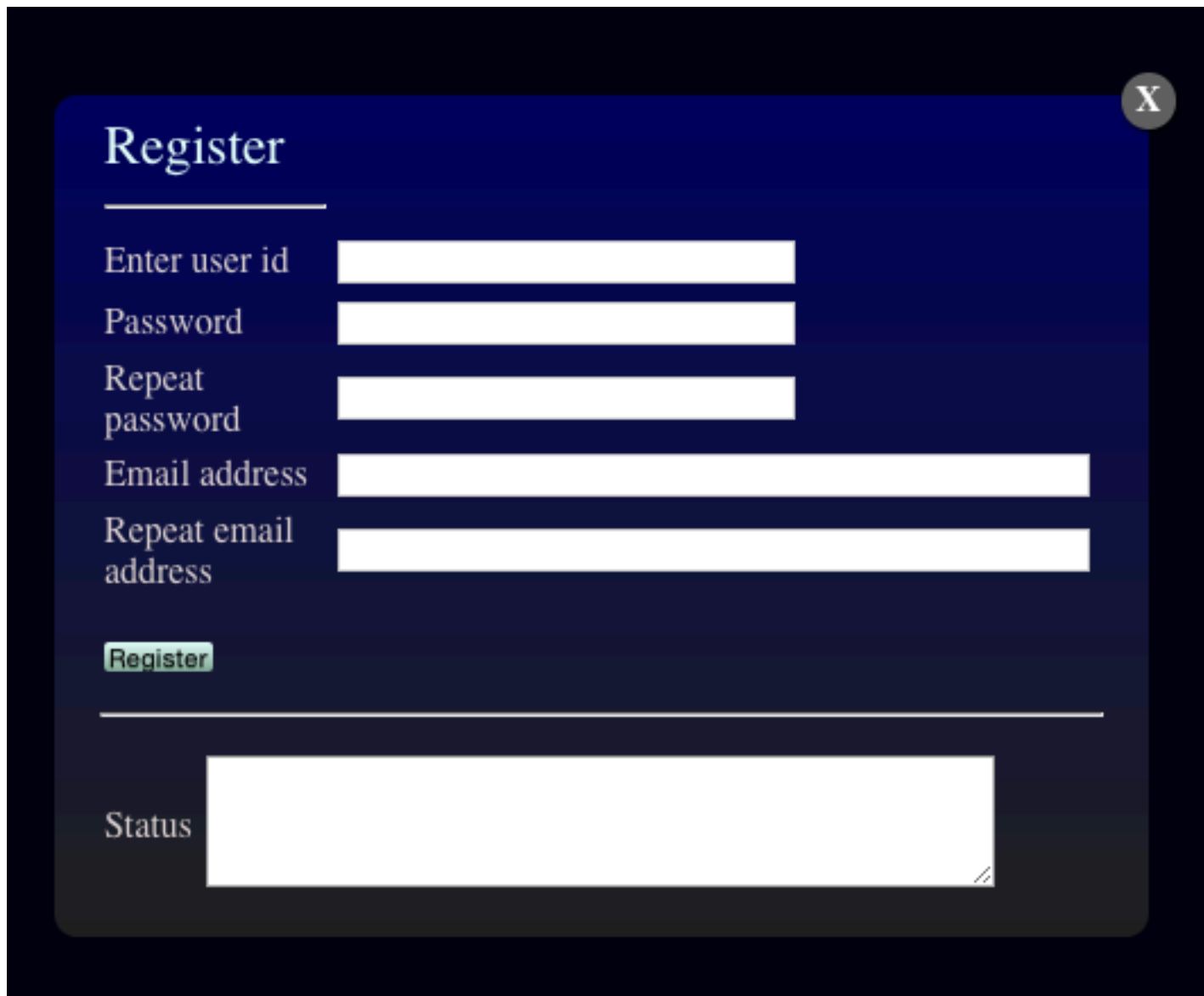
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## Register

Users must register to use software on SASSIE-web. To register you should click the Settings Manager icon, which is the white silhouette at the top-most right of the web-page.



This will open the following pop-up window to enable your initial registration.



**Register**

Enter user id

Password

Repeat password

Email address

Repeat email address

**Register**

Status

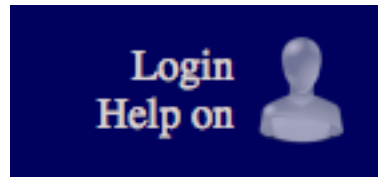
Choose a user id (name), a password which is at least twelve (12) characters in length and a verifiable e-mail address, then click the "Register" button.

Registering with SASSIE-web will also enroll you in the [CCP-SAS: SASSIE-web](#) Google group. This will allow you to provide feedback from within the web application.

This completes the registration process. **You must login to access the software using your new credentials.**

## [Login](#)

Registered users can login by pressing the "Login" button near the top right of the web page.



This will open the following pop-up window to enable you to login

A dark blue pop-up window with a white border and a close button (X) in the top right corner. The window contains the following elements:

- The word "Login" in a large white serif font, underlined with a white horizontal line.
- The text "Enter user id" followed by a white rectangular input field.
- The text "Password" followed by a white rectangular input field.
- The text "Forgot password" followed by a small white square checkbox.
- A green "Login" button.
- A white horizontal line separating the login fields from the status field.
- The text "Status" followed by a large white rectangular area for displaying the status.

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### **Forgotten your password?**

If you do not remember your password then enter your user id and check the "Forgot password" box and then click the "Login" button. This system will send you a temporary password at the e-mail address you entered during the registration process. You must login with the temporary password within one hour or you will have to begin the process again. Once you login you can change your password using [Settings Manager](#)

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After you are logged in, the top-panel will change to indicate the currently logged in user id (name) and two new icons are available.

The icon that looks like a filing cabinet is the [File Manager](#) that is used to inspect and download files and folders created while using SASSIE-web.

The icon that looks like two gears is the [Job Manager](#) that is used to inspect jobs (calculations carried out by SASSIE-web modules), check locked jobs, or re-attach to either running or completed jobs.

**Multiple logins** You can login to as many browser windows on as many computers & devices as you wish. Note that by default, you can only submit and run one job at a time in a given project. See [Job Manager](#)

## Logoff

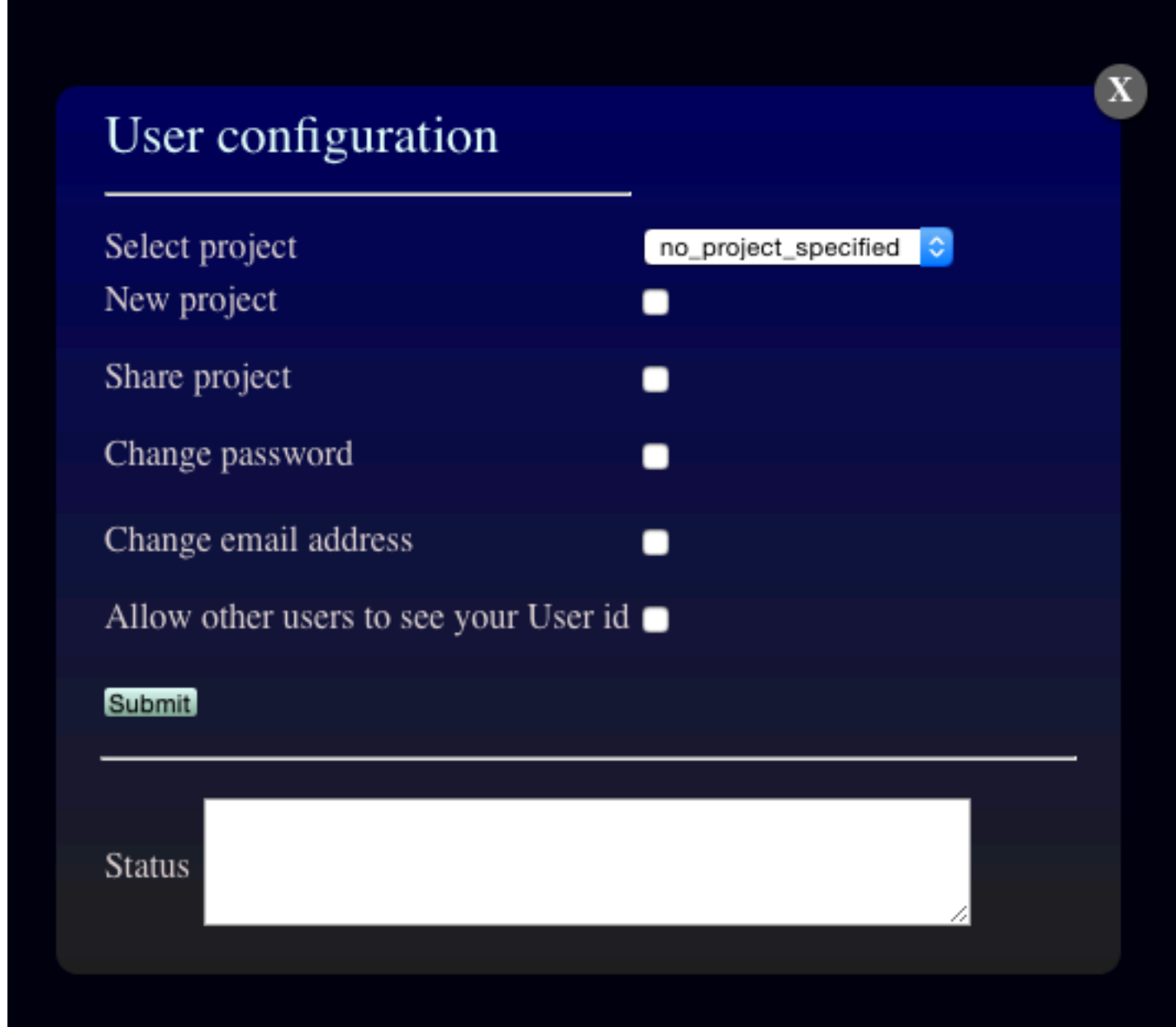
At any time, to logoff from SASSIE-web you can press the "Logoff" button. Alternatively, merely closing the browser tab/window also logs off the current user from that tab/window.

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## [Settings Manager](#)

The same icon that you used to register becomes the Settings Manager after you login.



There are utilities to change your password and/or your e-mail address.

The "Share project" and "Allow other users to see your User id" check boxes are for future applications and are not currently functional.

## Projects:

When logging in users are automatically placed into a workspace folder named **no\_project\_specified**. One can complete all work in this directory, or alternatively, one can create new project directories checking the "New project" box and entering a project name. Thus, in the future the new project will be available as a selection in the "Select project" list box.

If you create a new project then when you return to the main web page the current project name will be listed. For example, if you create a project named "demonstration" your current project would be indicated as shown below.



Therefore, by default, if you do not see the word "Project" followed by a project name that you have created and/or selected, then your current project is always **no\_project\_specified**.

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## Main Menu

On the left hand side of the web page there is a series of vertically organized icons. Clicking on one of the six possibilities will open the appropriate sub-set of modules corresponding to that section. An overview of these sections and the modules that they contain can be found in the [SASSIE modules at a glance](#) page.



One can minimize or expand the main menu at any time by clicking the three bar icon at the top of the image above. This icon can be found in the top left corner of every SASSIE-web page.

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## Documentation

On the right hand side of the web page there is a tab labeled **DOCS**. Clicking on this tab opens a new window to the main page for SASSIE-web documentation.

If you click this tab after you have selected a specific section (i.e Tools, Build, Interact, etc.) then the specific documentation page for that section will open in a new tab.

If you click this tab after you have selected a specific module (i.e. Align, Data Interpolation, etc.) then the specific documentation page for that module will open in a new tab.

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## Basic Module Usage

SASSIE-web modules are designed to share similar interfaces and methods of user interaction despite their diverse functions. The purpose of this section is to introduce some of these usage abilities without worrying about the goal of any specific module.

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### run name

Each module requires a user to define a "run name" which serves as the name of a folder within the current project directory that will contain the results of a given calculation.



Within each "run name" directory, the files and folders that are generated by the specific module are placed into a folder with the same name as the module in question. For example, when running the "data\_interpolation" module where the "run name" entered is **run\_0** the results will be written to a folder called

```
run_0/data_interpolation/
```

inside the current project directory.

The selected "run name" must be compatible with allowed path names on computer systems. The following characters are not allowed

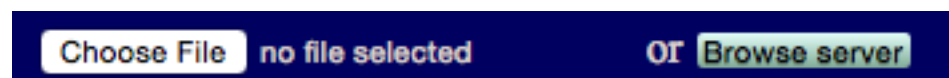
```
< > | \ \ : ( ) & ; # ? * or blank space
```

or an error message will be presented. The first character can not be a period, ".". Any files or folders with the same name that pre-exist the run will be overwritten. The characters mentioned above are also not allowed for any file name that exists on the server.

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### file input

Two options are given for each file input.



The "Choose File" option on the left corresponds to a file you wish to upload from your local computer/device.

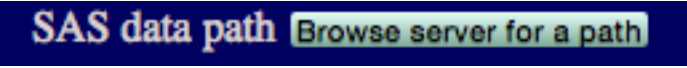
The "Browse server" option on the right corresponds to a file you wish to upload from the server that hosts SASSIE-web.

Selecting either option will open a pop-up window for you to select the desired file from the chosen system.

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## path input

A few modules process all files that are located in a single directory. In these cases, there is no option to upload a directory of files to the SASSIE-web server. In these cases an option is provided to select a path on the server




SAS data path

Clicking the "Browse server for a path" will open a pop-up window to select the path from the server that hosts SASSIE-web.

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## input / output structure file types

In many modules the input trajectory files (files that contain structure(s) to be analyzed or used in some way) can either be in text file format (PDB) or binary file format (DCD). For a typical input such as



trajectory file name [1]  no file selected

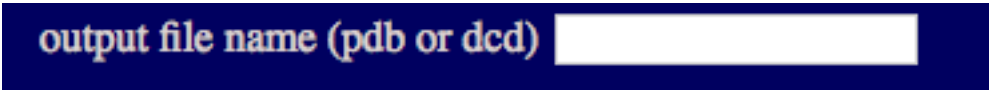
the user will select either a PDB or DCD file. The module will determine the file type from the last four characters

```
*.pdb --> PDB file input
```

```
*.dcd --> DCD file input
```

where the preceding "\*" is at least one allowed character (see above for allowed characters).

Likewise, for modules that request the name of an output trajectory file such as the input such as



output file name (pdb or dcd)

the software will determine the required output type by the last four characters as described above.

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## dynamic text area and progress bar

When a job is submitted in a module a message will be displayed under the progress bar. It will state

starting job

Soon afterwards a white text box will appear and provide any module / run specific output, for example

```
=====
DATA FROM RUN: Wed Apr 29 16:27:16 2015

> merging trajectory files
reading 39 frames from /share/apps/genapp/sassie2test/results/users/joseph/merge_test/run_m1.dcd
reading 32 frames from /share/apps/genapp/sassie2test/results/users/joseph/merge_test/run_m2.dcd
wrote 71 frames to ./run_0/merge_utilities/merged_run_m1_m2.dcd

> merging sas files
wrote 71 sas files to ./run_0/merge_utilities/xtal2sas

=====

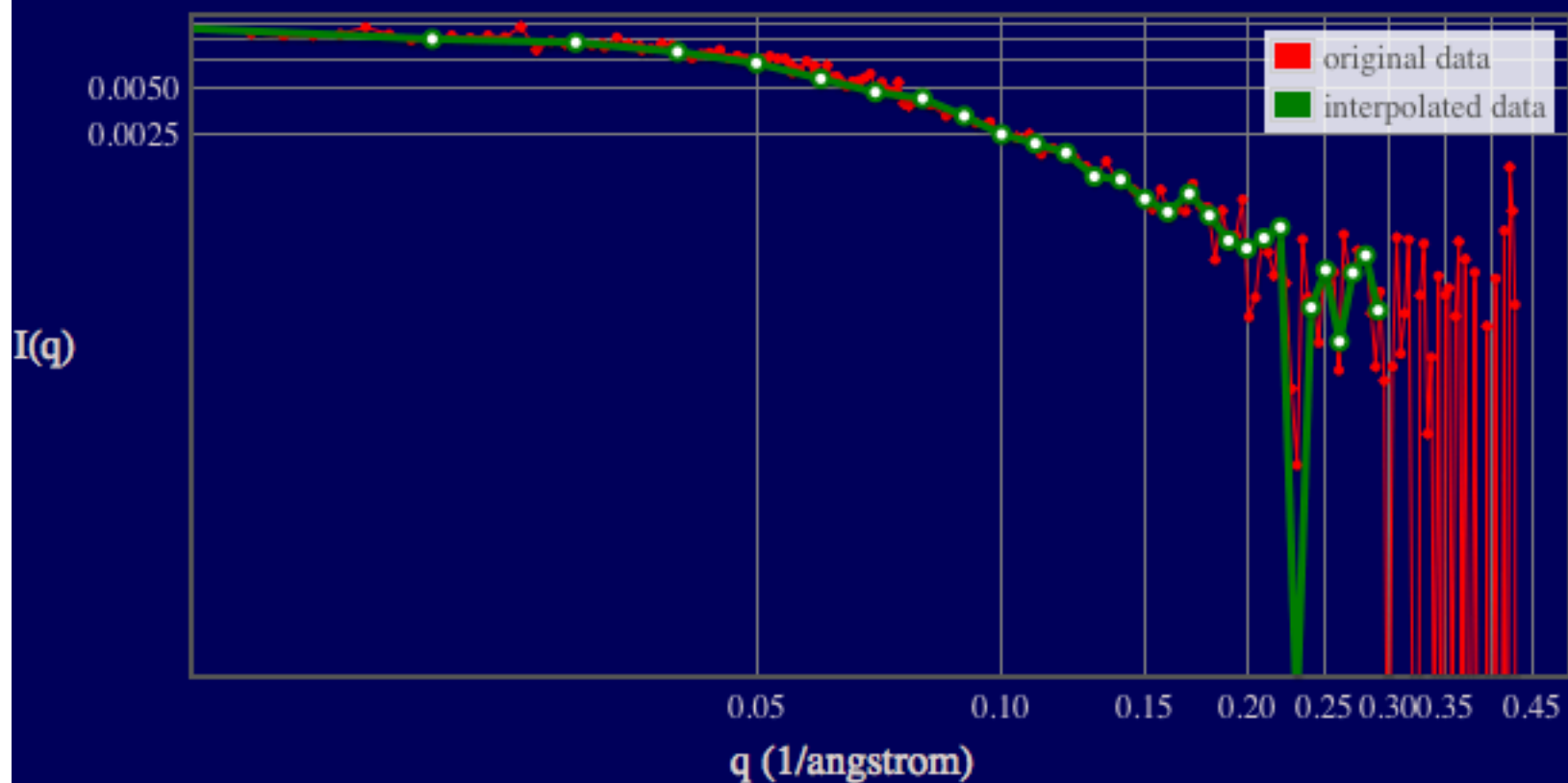
percent done: 100.0
```

If a submitted job does not start the progress bar and/or the text area is not displayed completely, then check the status of the job using [Job Manager](#). It could indicate that a run has failed due to an error in SASSIE-web software and/or the input files of the user and should be reported using [Feedback](#).

## plots

A few modules summarize the results of a run in graphical form. For example,

## Results

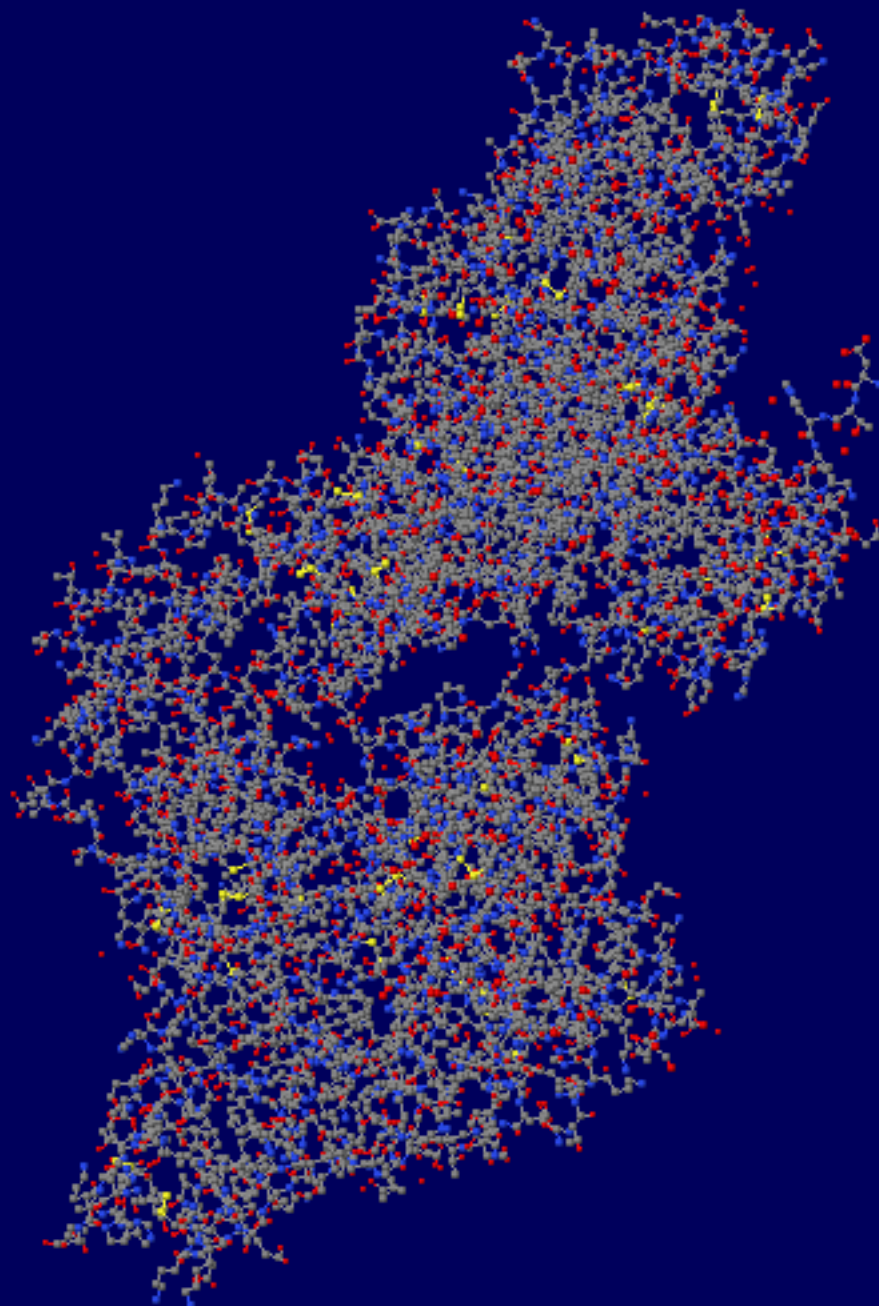


Users can zoom using your scroll-wheel on your input device, drag by clicking your mouse on the graph and moving while maintaining the click. Plots can be re-sized to their original view by clicking on the title or axis labels. One can also view values from the graph by placing the mouse pointer at any points on the plot.

### molecular viewing

A few modules allow the display of three-dimensional structures. Right clicking on the viewer menu will open a pop-up menu with viewing options. SASSIE-web uses [JSMol](#) to represent structures on the web application. See the [JSMol](#) documentation for further information regarding visualization options.

viewer (right click for options)



- File ▶
- 4F5S ▶
- model 1/1 ▶
- Configurations (2) ▶

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- Select (9675) ▶
- View ▶
- Style ▶
- Color ▶

---

- Surfaces ▶
- Symmetry ▶

---

- Scenes ▶
- Zoom ▶
- Spin ▶
- Vibration ▶
- Spectra ▶
- Animation ▶

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- Measurements ▶
- Set picking ▶

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- Console
- JavaScript Console
- Show ▶
- Computation ▶

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- Language ▶
- About... ▶

JSmol

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## File Manager

Each user has their own persistent file system. Your files will exist after you logout and they are backed up on a regular basis on our secure server.

Files are uploaded only within SASSIE-web modules from your local machine to the server. Files and directories are created by running modules and they are stored within the "project" directory that was current when the job was submitted.

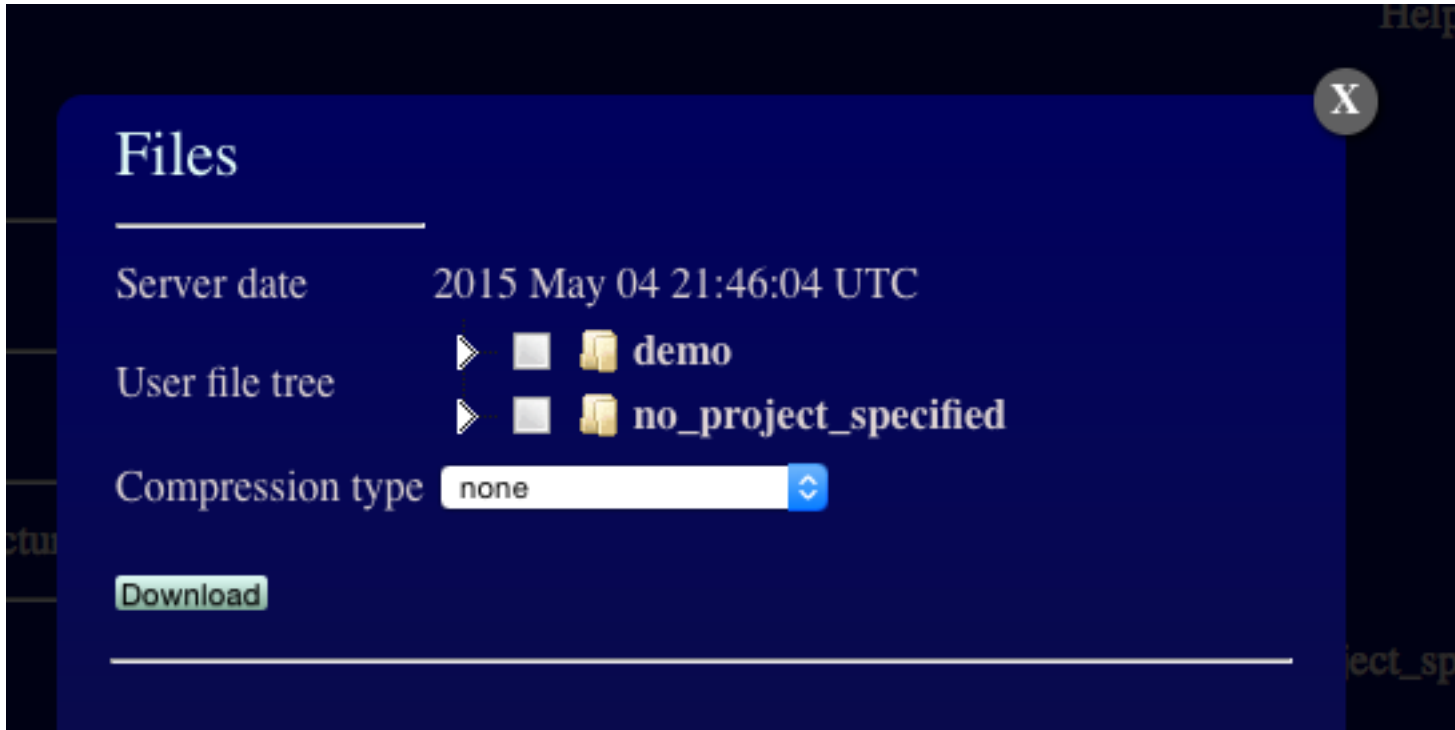
The role of the File Manager is to enable users to download files in their file system on the server to their local machine. In addition, one can remove files and folders from their file system.

One can access the File Manager by clicking the filing cabinet icon at the top right of the web page.

Project demo  
Logoff joseph  
Help off

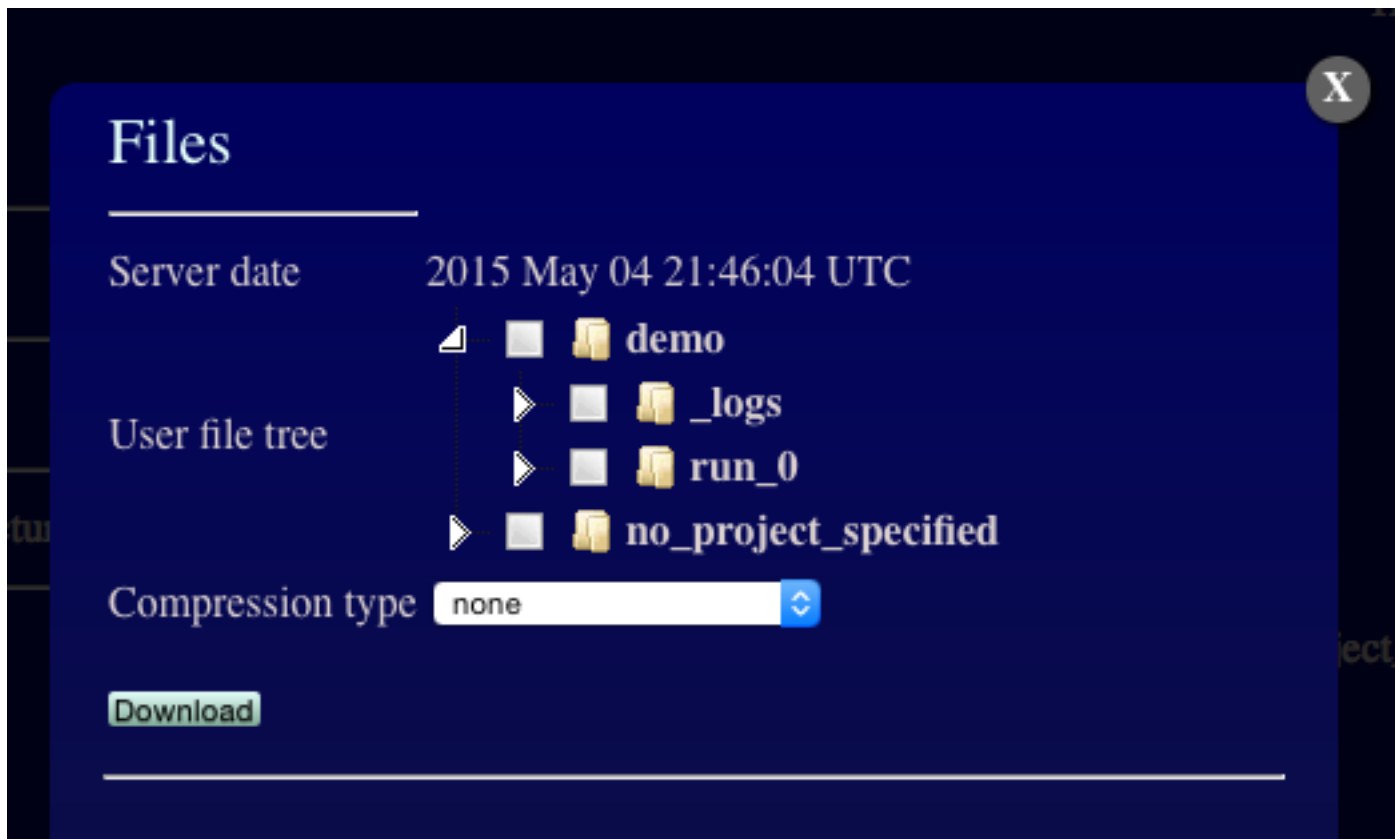


This will open the following pop-up window that lists the persistent file system for the logged in user.



The current time on the server is listed along with the "User file tree" containing the project directories. To open or close a given folder one can click on the arrow to the left of the empty box adjacent to the folder name.

For example, a test calculation was done using the Align module within Tools in the project "demo". Thus, clicking on the arrow next to the "demo" folder reveals the files and folders within.

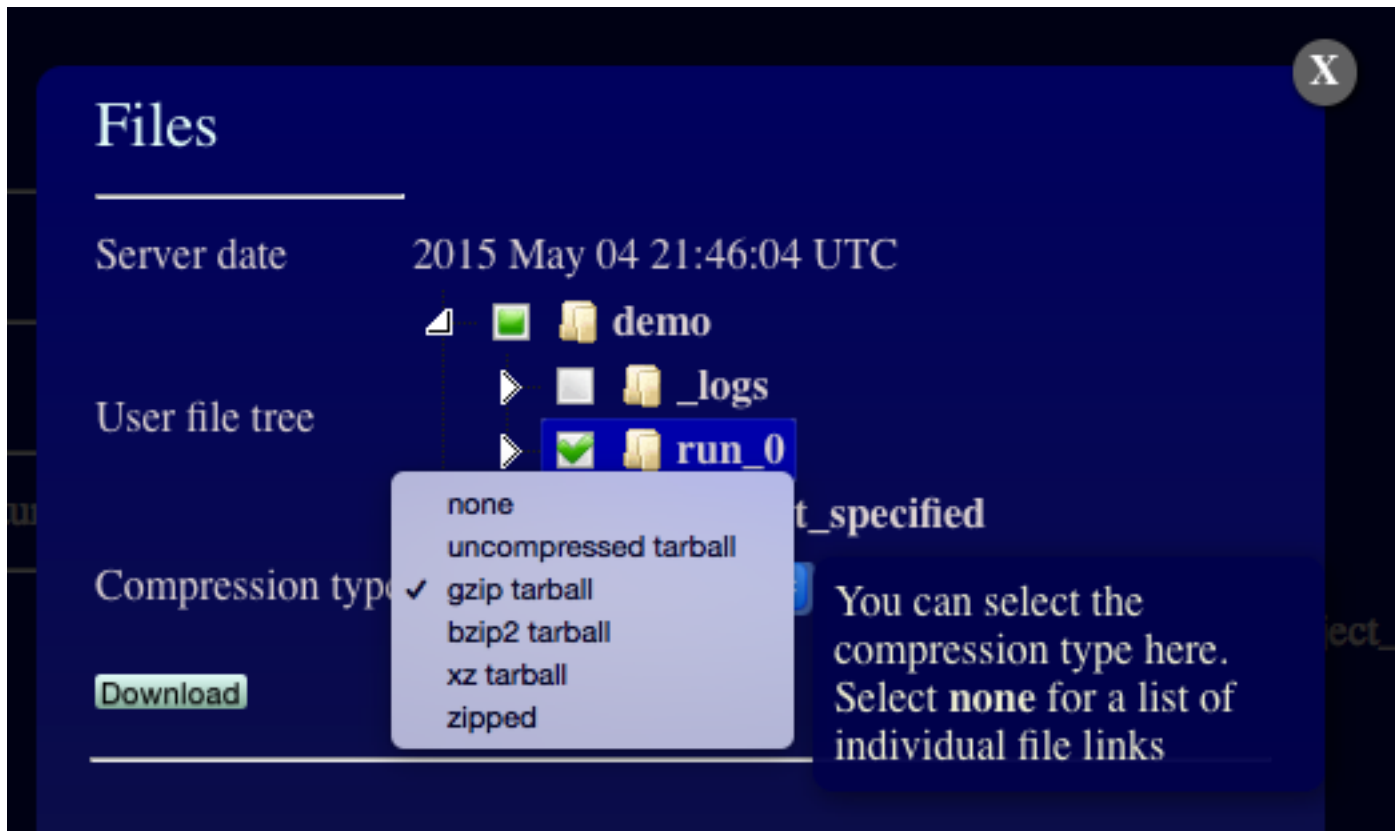


This reveals a folder called "\_logs" and a folder called "run\_0". Once a job has been run within a project directory the "\_logs" directory will exist. The files within this folder are mainly for debugging purposes as discussed in the [Feedback](#) below. The "run\_0" directory contains the pertinent output from our test calculation. More information regarding the internal file structure within a project can be found in [Basic Module Usage](#).

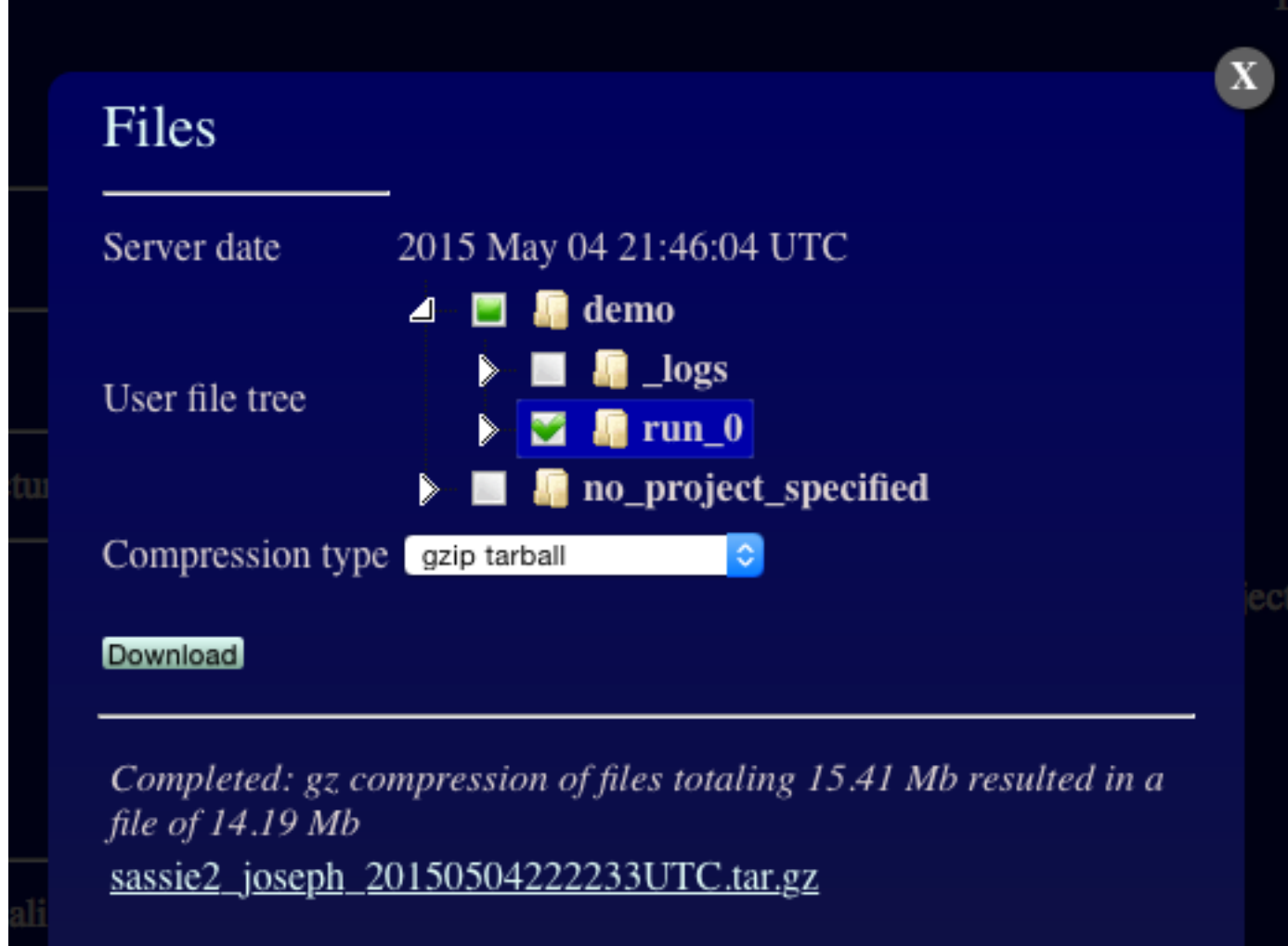
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## File / Folder Download

In this example we will download contents of the folder "run\_0" as a compressed tar file. In the image below the selection of the run\_0 folder is shown along with the list-box display of compression options.



Clicking the download button will create a link to a compressed file that, once pressed, will download the compressed file to your local machine. The status of the compression is noted and once completed a link to the compressed file is presented as shown below.



Clicking on the link will then enable you to download the file. The compressed file / folder will be saved in the same folder structure that existed in the user file tree. In other words, saving the folder "run\_0" and it's enclosed folders and files will show up as

```
demo/run_0/align/ac7.dcd
```

```
demo/run_0/align/ac7.dcd.minmax
```

Thus, for this example, "run\_0" contained a folder called "align" that contained two files "ac7.dcd" and "ac7.dcd.minmax".

### File / Folder Refresh and Remove

Selecting a file or folder and "right-clicking" on your input device (i.e. mouse) will pop up a small window with an option to either "Refresh" or "Remove" the selected file or folder.

Choosing "Refresh" is useful if you expect that contents in a folder have been updated, such as occurs in long running jobs.

Choosing "Remove" will spawn a message box to confirm if you wish to remove the folder and it's contents.

### Notes

- choosing "none" as the compression type for a folder containing many files will result in a list of files that must be downloaded individually.

- It is recommended that large binary trajectory files (DCD) are downloaded without compression.
  - There are currently no options to move files from one folder / project to another. One can access any folder or file within the user's file system directly from the modules as described in [Basic Module Usage](#).
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## [Job Manager](#)

When one performs a calculation by submitting a job in one of the SASSIE-web modules the calculation is sent to the server for execution. A list of all jobs that have been submitted by the current user can be observed in the Job Manager. One can access the Job Manager by clicking the two-gear icon at the top right of the web page.



This will open the following pop-up window that lists the jobs run by the user.

# Jobs

Server date 2015 May 05 01:39:00 UTC

	Module	Project
<input type="checkbox"/>	analyze/chi_square_filter	no_project_specified
<input type="checkbox"/>	analyze/chi_square_filter	no_project_specified
<input type="checkbox"/>	analyze/chi_square_filter	no_project_specified
<input type="checkbox"/>	tools/data_interpolation	
<input type="checkbox"/>	calculate/xtal2sas	
<input type="checkbox"/>	simulate/monomer_monte_carlo	no_project_specified
<input type="checkbox"/>	simulate/monomer_monte_carlo	first_test
<input type="checkbox"/>	simulate/monomer_monte_carlo	long_run_for_chi_square
<input type="checkbox"/>	analyze/density_plot	first_test
<input type="checkbox"/>	calculate/xtal2sas	long_run_for_chi_square
<input type="checkbox"/>	simulate/monomer_monte_carlo	hopkins
<input type="checkbox"/>	build/pdbscan	no_project_specified
<input type="checkbox"/>	tools/align	demo

Refresh  Cancel  Clear Lock  Remove Job  Reattach

Messages

One can scroll to the right and inspect the various fields and note the color of the job

**Module** section & module that the job was submitted

**Project** name of project used for job submission

**Start, End, Duration** time statistics for the job (Eastern Time US)

**Remote IP** internet address of the local machine from which the user submitted the job

**Resource** name of node on the cluster the job was run on.

If a job has finished (either normally or not) it will appear white.

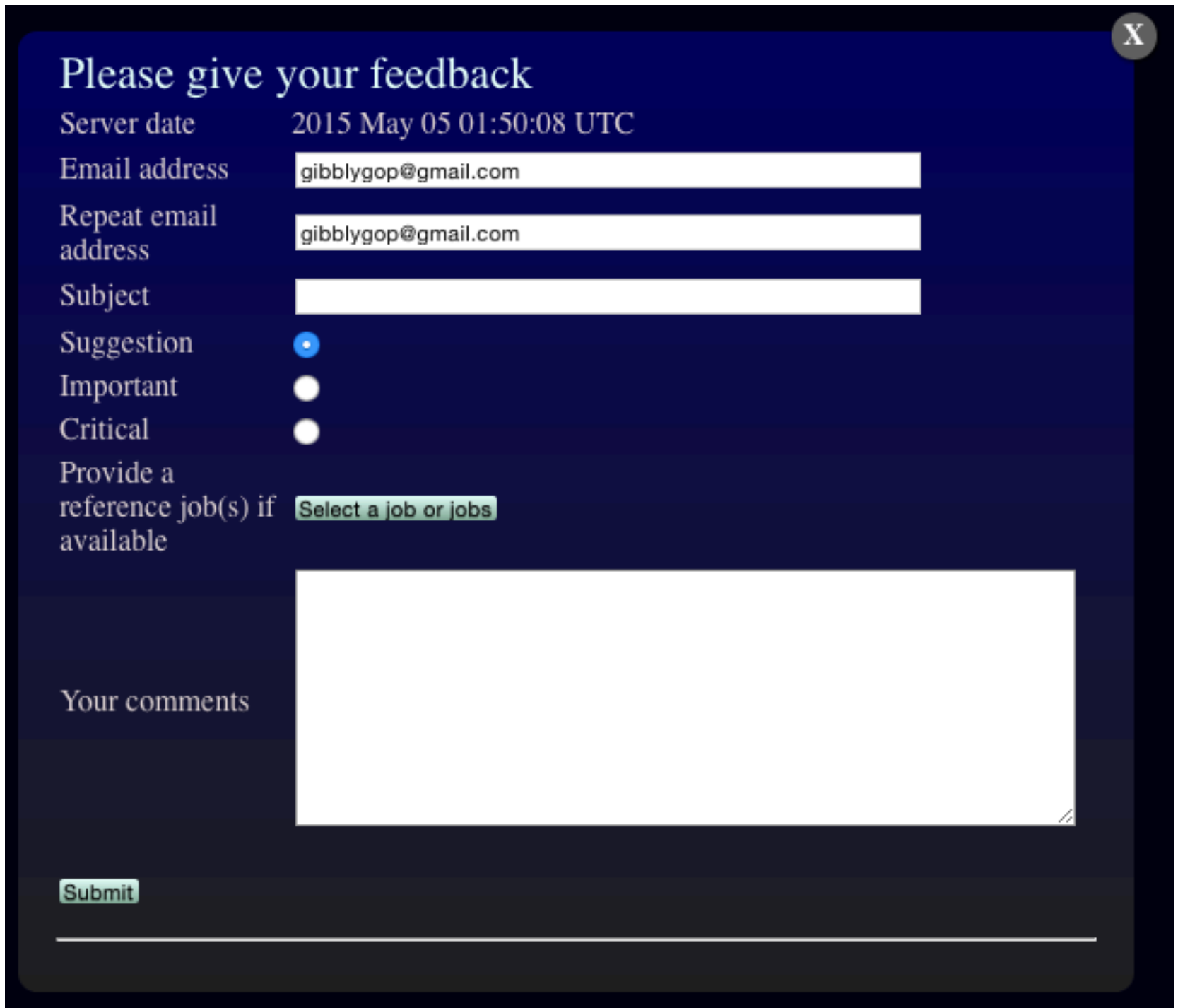
If a job is running and locks the project directory that it originated it will be red.

If a job is locked by a run in a different project directory it will be yellow

There are options to "Refresh" the list, "Clear Lock" to allow multiple jobs to run in the same project directory, "Remove Job" to clear the information from the list, and "Reattach" which allows users to connect to a job submitted previously whether it has finished or not.

## [Feedback](#)

On the right hand side of the web page there is a tab labeled **FEEDBACK**. Clicking on this tab opens a pop-up window



The screenshot shows a dark blue feedback form with a white 'X' close button in the top right corner. The form is titled "Please give your feedback" in white text. It contains the following fields and options:

- Server date:** 2015 May 05 01:50:08 UTC
- Email address:** gibblygop@gmail.com
- Repeat email address:** gibblygop@gmail.com
- Subject:** (empty text input field)
- Suggestion:**
- Important:**
- Critical:**
- Provide a reference job(s) if available:** Select a job or jobs (button)
- Your comments:** (large white text area)
- Submit:** (button)

SASSIE-web will supply the e-mail address associated with your account. Your feedback will automatically be posted to the [CCP-SAS: SASSIE-web](#) Google group page.

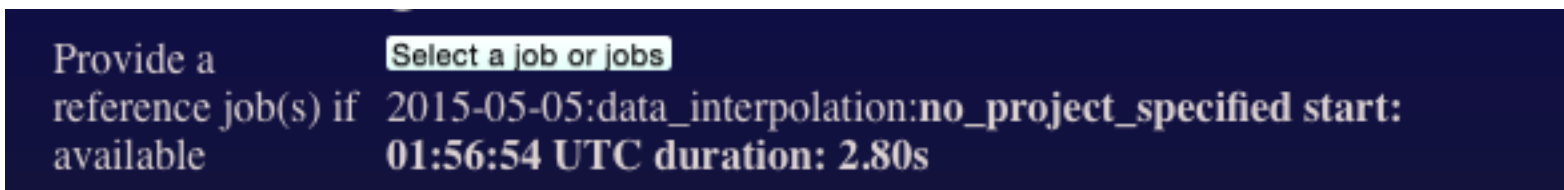
If you are reporting feedback regarding specific job(s), then you can click the "Select a job or jobs" button which will open a pop-up window such as



where for illustrative purposes we show the expanded tree structure. The folders are shown in chronological order "year - month", which has "day" as an interior folder. In the example, only one job has been run by this test user:

**data interpolation module was run in the no\_project\_specified project on May 5, 2015**

Clicking this job and pressing OK then attaches the \_logs for this particular run and attaches them to the feedback e-mail as shown below.



The \_logs are useful in order to debug error reports. Their inclusion is not necessary for general feedback.

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