Lab 0: Preparing your laptop for the course – OS X

Five pieces of software are needed to complete this course:

1. VMD – Views and analyses molecular models.
2. NAMD – Performs molecular dynamics simulations.
3. Textmate 2.0
4. Gnuplot – Plots data
5. A modern web browser – Internet Explorer 10 or newer, recent versions of Chrome or Firefox.

Several assumptions in this document:

1. You have admin access (i.e. permission to install new packages to you system)
2. You know what a terminal is.
3. You understand the difference between a text editor and word processor.
4. You will have a web browser already installed, if you need a more modern version then one is only a web search and standard installation away.

We will also add NAMD and Gnuplot to your PATH for ease of use.

VMD

Download

Click on this link http://www.ks.uiuc.edu/Research/vmd/ or use your web browser to navigate to the web page.

- Locate the 'Downloads' section that is highlighted (below the 'Overview' section) on the left side of the page
- Click on the 'Download (all versions)' link

Then you need to select the 'MacOS X OpenGL' link appropriate for your version of OS X for the most recent version of VMD (Version 1.9.2 at the time of writing).

- 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'
- Confirm that you are you and agree to the license
- The download should begin automatically

Installation

- Once the file has downloaded double click on it to run it
- Drag the icon that resembles a water molecule into your Applications folder

To open VMD from a terminal window (optional)

- Add the following to your ~/.bashrc file:
    - alias vmd='Applications/VMD\ 1.9.2.app/Contents/vmd/vmd_MACOSXX86'
    - VMDFILECHOOSER=FLTK
    - Export VMDFILECHOOSER

- Then type “source ~/.bashrc”

NAMD

Download

Click on this link http://www.ks.uiuc.edu/Research/namd/ or use your web browser to navigate to the web page.

- Follow the 'Download NAMD' link on the left side of the page
- Select the MacOSX-x86_64 link from the “Version 2.9 (2012-04-30) Platforms” section
    - We use version 2.9 to ensure that all input and output formats are compatible with other software used in the tutorial
- Enter the username and password you created before when installing VMD.
- Agree to the license and the download should start automatically

Installation

- In the terminal navigate to the directory where the file was downloaded and run the command:

```
sudo tar xvf NAMD_2.9_MacOSX-x86_64-multicore.tar -C /usr/local/bin
```

- You will need to enter your password to gain admin rights
- Now we need to make the program easily accessible from the command prompt, this involves setting an Environment Variable:

    1. Open the file ~/.bashrc in your text editor
    2. Add the following line:

```
export PATH=$PATH:/usr/local/bin/NAMD_2.9_MacOSX-x86_64-multicore
```

    3. Save the file
    4. Type `source ~/.bashrc`
    5. Open the file ~/.bash_profile in your text editor
    6. Add the following line:

```
if [-f ~/.bashrc];then . ~/.bashrc;fi
```

Textmate (optional – the TextEdit app that comes with OS X can be used)

Download

Navigate to http://macromates.com/

- Click on the download icon

Installation

- Once the file has downloaded double click on it to run it
- Drag the icon that resembles a water molecule into your Applications folder

Gnuplot

Download

There are a variety of ways of installing Gnuplot. All of which have different dependencies. Ask one of the course administrators which option is best for you.

Perhaps the nicest is via homebrew (http://brew.sh/)but even this requires a working installation of Xcode.

Testing NAMD and Gnuplot Installations

If the installation has worked then NAMD and Gnuplot should be available from the command line.

- To test NAMD type:

  ```
  namd2
  ```

  - If NAMD is installed and setup correctly then a message stating:

```
FATAL ERROR: No simulation config file specified on command line.
```

- To test Gnuplot type:

```
gnuplot
```

  - If Gnuplot is installed correctly a message giving the version of the code should appear and the terminal prompt should look like:

```
gunplot>
```

  - Try making a plot by typing:

```
plot sin(x)
```

  - Exit by typing:

```
exit
```

Getting the Course Files

All course content is available from:

https://sassie-web.chem.utk.edu/training/aps_2016/main.html

Download each days zip file onto your desktop as you progress.

Lab 0: Preparing your laptop for the course – Windows

Four pieces of software are needed to complete this course:

1. VMD – Views and analyses molecular models.
2. NAMD – Performs molecular dynamics simulations.
3. Gnuplot – Plots data
4. A modern web browser – Internet Explorer 10 or newer, recent versions of Chrome or Firefox.

Two more are required to make it a more pleasant experience:

1. Notepad++ - In fact any text editor rather than word processor will do.
2. CoreUtils – Provides some command line tools which make life a lot easier.

We make a couple of assumptions in this document:

1. You have admin access (i.e. permission to install new packages to you system)
2. You will have a web browser already installed, if you need a more modern version then one is only a web search and standard installation away.

NAMD and CoreUtils require some configuration of the operating system to use them conveniently, but the other software uses standard Windows installation methods.

VMD

Download

Click on this link http://www.ks.uiuc.edu/Research/vmd/ or use your web browser to navigate to the web page.

- Locate the 'Downloads' section
- Click on the 'Download (all versions)' link

In either case you need to select the 'Windows OpenGL' link for the most recent version of VMD (Version 1.9.2 at the time of writing).

- 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'
- Confirm that you are you and agree to the license
- The download should begin automatically

Installation

- Once the file has downloaded double click on it to run it
- Click 'Yes' when asked to give the program permission to install on your computer
- 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

Notepad++

Download

Click on this link https://notepad-plus-plus.org/ or use your web browser to navigate to the web page.

- 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

Installation

- Once the file has downloaded double click on it to run it
- Click 'Yes' when asked to give the program permission to install on your computer
- 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

NAMD

Download

Click on this link http://www.ks.uiuc.edu/Research/namd/ or use your web browser to navigate to the web page.

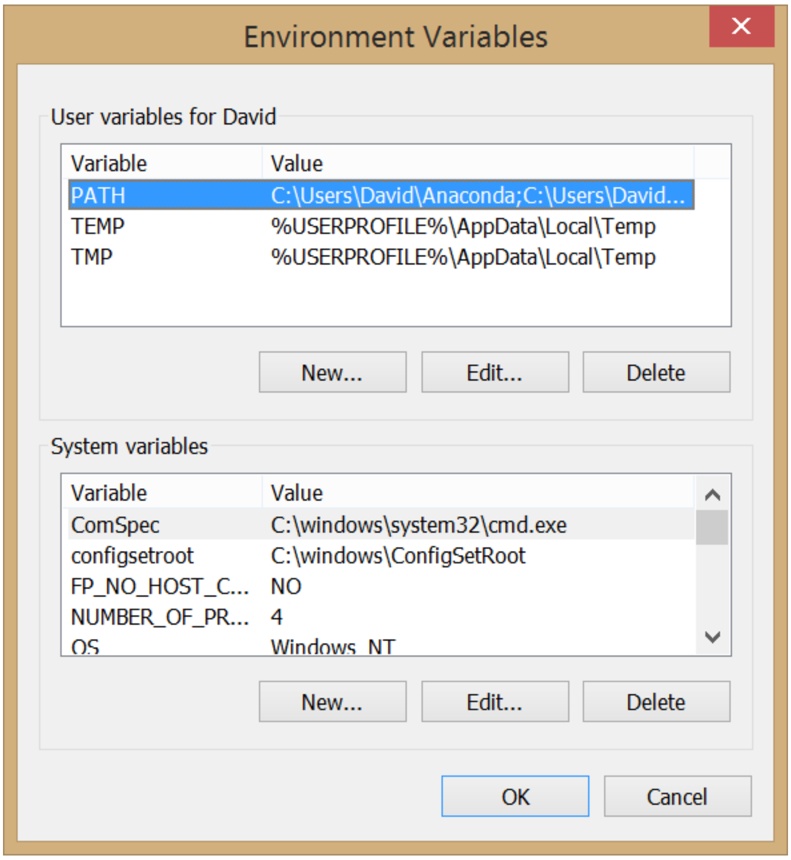
- Follow the 'Download NAMD Binaries' link
- Select the Win32 link from the “Version 2.9 (2012-04-30) Platforms” section
    - We use version 2.9 to ensure that all input and output formats are compatible with other software used in the tutorial
- Enter the username and password you created before when installing VMD.
- Agree to the license and the download should start automatically

Installation

- Open the downloaded NAMD_2.9_Win32-multicore.zip file in Explorer
- Copy the NAMD_2.9_Win32-multicore folder
- Paste the folder in a location of your choice (C:\Program Files (x86)\ is a good option)
- Now we need to make the program easily accessible from the command prompt, this involves setting an Environment Variable:
    1. Navigate in Explorer into the NAMD_2.9_Win32-multicore folder
    2. Left click in the address bar and copy the contents
    3. Open Advanced System Settings (Windows 7, 8, 10):
        - From the Start Menu:
            - Click on Control Panel, then System Security, then System, then Advanced System settings

       OR

        - Open File Explorer:
            - Type Control Panel\System and Security\System, then click Advanced System Settings
    4. Click the 'Environment variables' button. A window like that below should appear.



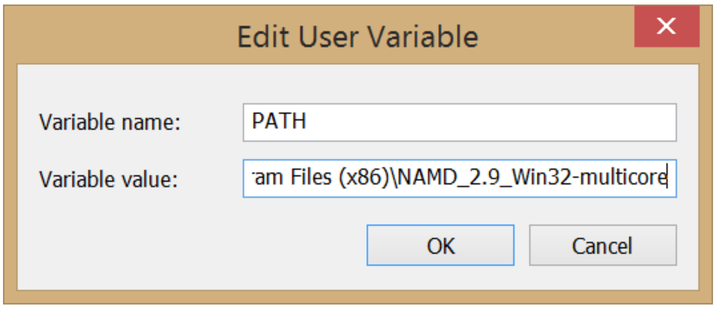
User variables for David

Variable	Value
PATH	C:\Users\David\Anaconda;C:\Users\David...
TEMP	%USERPROFILE%\AppData\Local\Temp
TMP	%USERPROFILE%\AppData\Local\Temp

System variables

Variable	Value
ComSpec	C:\windows\system32\cmd.exe
configsetroot	C:\windows\ConfigSetRoot
FP_NO_HOST_C...	NO
NUMBER_OF_PR...	4
OS	Windows_NT

5. Ensure 'PATH' is selected in the 'User variables for xxxxx' listbox and then click the 'Edit' button beneath this section.
6. If there are no entries in 'Variable value' box simply paste in the location you copied earlier:



Variable name: PATH

Variable value: am Files (x86)\NAMD_2.9_Win32-multicore

If entries already exist, place the cursor at the end of the text in the box. Enter a ; symbol and then paste in the folder location. So, if the entry read:

C:\Users\David\Anaconda

before it should now say something like:

C:\Users\David\Anaconda;C:\Program Files (x86)\NAMD_2.9_Win32-multicore

7. Click 'OK'.

CoreUtils

Download

Click on this link http://gnuwin32.sourceforge.net/packages/coreutils.htm or use your web browser to navigate to the web page. (If typing that in does not appeal to you, search the web for 'CoreUtils Windows'.)

Go to the 'Download' section of the page and click on the 'Setup program' link, the download should start automatically.

Installation

- Once the file has downloaded double click on it to run it
- Click 'Yes' when asked to give the program permission to install on your computer
- 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
- As for NAMD you now need to set an Environment Variable. Follow the same procedure as before (if you did not change the destination CoreUtils will have been installed in C:\Program Files (x86)\GnuWin32\bin).
    - If you had no Environment Variables set at the start of this process the PATH variable value should now be:

```
C:\Program Files (x86)\NAMD_2.9_Win32-multicore;C:\Program Files
(x86)\GnuWin32\bin
```

Gnuplot

Download

Click on this link http://sourceforge.net/projects/gnuplot/files/gnuplot/5.0.0/ or use your web browser to navigate to the web page.

- Click on the gp500-win64-mingw.exe link
- The download should start automatically (a short delay is normal)

Installation

- Once the file has downloaded double click on it to run it
- Click 'Yes' when asked to give the program permission to install on your computer
- A standard Windows installer will appear, accept all defaults as they are offered to you, accept the license agreement and then click 'Install' when the option is presented to you
- As for NAMD and CoreUtils you now need to set an Environment Variable. Follow the same procedure as before (if you did not change the destination the program will have been installed in C:\Program Files\gnuplot\bin).
    - If you had no Environment Variables set at the start of this process the PATH variable value should now be:

```
C:\Program Files (x86)\NAMD_2.9_Win32-multicore;C:\Program Files
(x86)\GnuWin32\bin;C:\Program Files\gnuplot\bin
```

Testing NAMD, CoreUtils and Gnuplot Installations

If the installation has worked then NAMD and all the programs in Coreutils should be available directly from the Command Prompt.

- Open Command Prompt (Windows 7, 8, 10):
    - Using the Search feature:
        - Search for “cmd”
- To test CoreUtils type:

```
basename --version
```

    - If CoreUtils is installed and setup correctly message giving the version number and other program details should appear.

- To test NAMD type:

```
namd2
```

  - A window bearing an alarmist message may appear, if so click 'Cancel'
  - If NAMD is installed and setup correctly then a message stating:

```
FATAL ERROR: No simulation config file specified on command line.
```

- To test Gnuplot type:

```
gnuplot
```

  - If Gnuplot is installed correctly a message giving the version of the code should appear and the terminal prompt should look like:

```
gunplot>
```

  - Try making a plot by typing:

```
plot sin(x)
```

  - Exit by typing:

```
Exit
```

To make VMD run from the Command Prompt (optional):

- As for NAMD, CoreUtils and Gnuplot, you need to set an Environment Variable to make VMD available from the Command Prompt. Follow the same procedure as before (if you did not change the destination the program will have been installed in C:\Program Files (x86)\University of Illinois\VMD).
  - If you had no Environment Variables set at the start of this process the PATH variable value should now be:

```
C:\Program Files (x86)\NAMD_2.9_Win32-multicore;C:\Program Files
(x86)\GnuWin32\bin;C:\Program Files\gnuplot\bin;C:\Program Files
(x86)\University of Illinois\VMD
```

  - Try opening VMD by typing:

```
vmd
```

Introducing the Command Prompt

Have a quick look at the tutorial in the following link:

http://tutorial.djangogirls.org/en/intro_to_command_line/README.html

Getting the Course Files

All course content is available from:

https://sassie-web.chem.utk.edu/training/aps_2016/main.html

Download each days zip file onto your desktop as you progress.

Lab 0: Preparing your laptop for the course – Linux

Four pieces of software are needed to complete this course:

1. VMD – Views and analyses molecular models.
2. NAMD – Performs molecular dynamics simulations.
3. Gnuplot – Plots data
4. A modern web browser – Internet Explorer 10 or newer, recent versions of Chrome or Firefox.

Several assumptions in this document:

1. You have admin access (i.e. permission to install new packages to you system)
2. You know what a terminal is.
3. You are using 64 bit Linux (if not then select the 32 bit versions of VMD and NAMD and correct all paths accordingly)
4. You understand the difference between a text editor and word processor.
5. You will have a web browser already installed, if you need a more modern version then one is only a web search and standard installation away.

We will also add NAMD to your PATH for ease of use.

VMD

Download

Click on this link http://www.ks.uiuc.edu/Research/vmd/ or use your web browser to navigate to the web page.

- Locate the 'Downloads' section that is highlighted (below the 'Overview' section) on the left side of the page
- Click on the 'Download (all versions)' link

In either case you need to select the 'LINUX_64 OpenGL, CUDA' link for the most recent version of VMD (Version 1.9.2 at the time of writing).

- 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'
- Confirm that you are you and agree to the license
- The download should begin automatically

Installation

- 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: the $install_bin_dir value should be in your PATH

  - With 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
```

This will generate a Makefile based on these configuration variables

- Change into the src directory,
- Type:

```
sudo make install
```

NAMD

Download

Click on this link http://www.ks.uiuc.edu/Research/namd/ or use your web browser to navigate to the web page.

- Follow the 'Download NAMD Binaries' link
- Select the Linux-x86_64-multicore link from the "Version 2.9 (2012-04-30) Platforms" section
  - We use version 2.9 to ensure that all input and output formats are compatible with other software used in the tutorial
- Enter the username and password you created before when installing VMD.
- Agree to the license and the download should start automatically

Installation

- In the terminal run the command

```
sudo tar xvfz NAMD_2.9_Linux-x86_64-multicore.tar.gz -C /usr/local/bin
```

- You will need to enter your password to gain admin rights
- Now we need to make the program easily accessible from the command prompt, this involves setting an Environment Variable:
  1. Open the file ~/.bashrc in your text editor
  2. Add the following line:

```
export PATH=$PATH:/usr/local/bin/NAMD_2.9_Linux-x86_64-multicore
```

  3. Save the file

Gnuplot

Download & Installation

You should be able to obtain Gnuplot via your standard package manager, for example:

Ubuntu/Debian:

```
sudo apt-get install gnuplot
```

CentOS:

```
sudo yum install gnuplot
```

Testing NAMD and Gnuplot Installations

To ensue that the various packages are available in your path you will need to start a new terminal. This will ensure that the .bashrc file is read. You can manually do this in an existing terminal using the command:

```
source ~/.bashrc
```

If the installation has worked then NAMD and Gnuplot should be available from the command line.

- To test NAMD type:

  ```
  namd2
  ```

  - If NAMD is installed and setup correctly then a message stating:

```
FATAL ERROR: No simulation config file specified on command line.
```

- To test Gnuplot type:

```
gnuplot
```

  - If Gnuplot is installed correctly a message giving the version of the code should appear and the terminal prompt should look like:

```
gunplot>
```

  - Try making a plot by typing:

```
plot sin(x)
```

  - Exit by typing:

```
exit
```

Getting the Course Files

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https://sassie-web.chem.utk.edu/training/aps_2016/main.html

Download each days zip file onto your desktop as you progress.

[Return to Main Documents Page]

SASSIE-web: Basic Usage

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 splash screen on the web page.

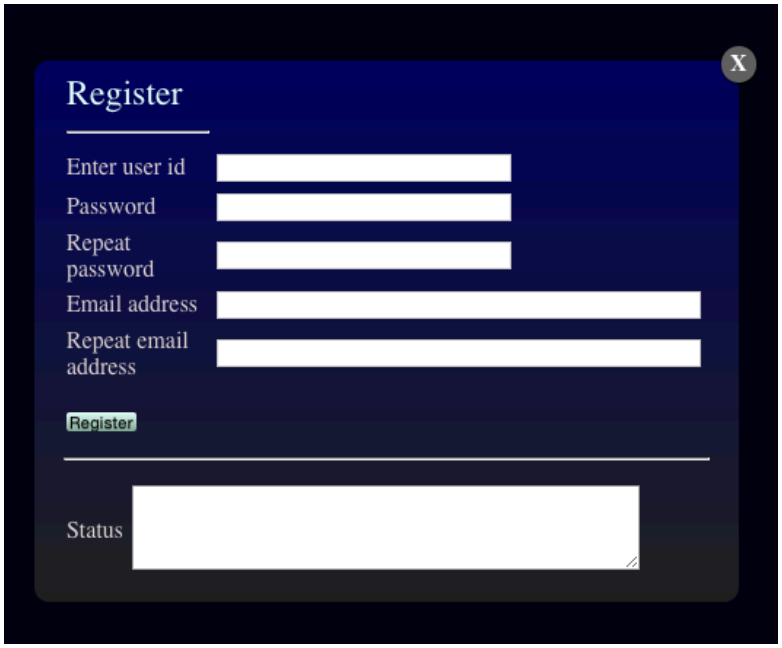
Generated on Wed Jun 29 16:47:46 UTC 2016
SASSIE-web Revision 937 on 2016-06-28 07:27:43 -0400 (Tue, 28 Jun 2016)
GenApp Revision 792 on 2016-05-28 14:26:19 -0400 (Sat, 28 May 2016)

Here one can either login or register if you are a new user. One can also access the documentation directly from here.

Register

Users must register to use software on SASSIE-web. To register you should click the Settings Manager icon, which is the white silhouette on the right side of the splash screen.

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



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 clicking "Login" on the left side of the splash screen.

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

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](#)

After you are logged in, the main SASSIE-web screen is visible. The currently logged in user id (name) is shown in the upper right and two new icons are available.

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.

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.

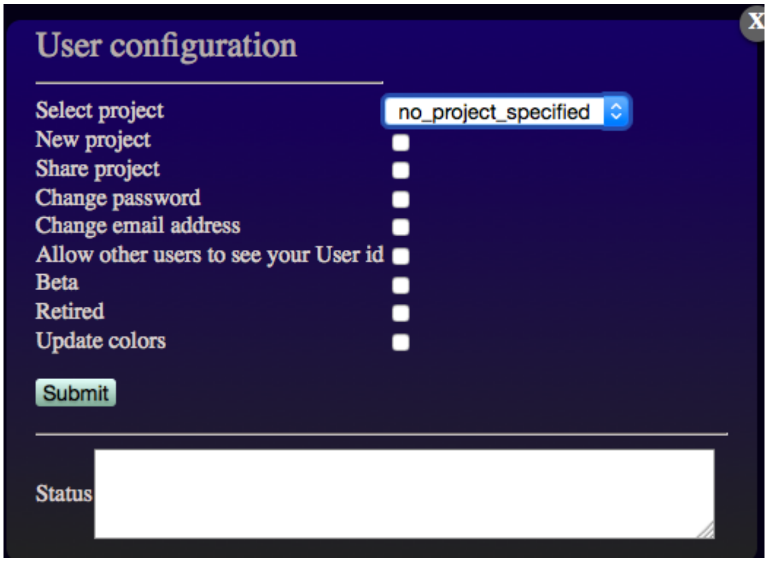
Multiple logins You can login to as many browser windows on as many computers & devices as you wish. Note that by default, you can only submit and run one job at a time in a given project. See Job Manager

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.

Settings Manager

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



User configuration

Select project: no_project_specified
New project ☐
Share project ☐
Change password ☐
Change email address ☐
Allow other users to see your User id ☐
Beta ☐
Retired ☐
Update colors ☐

Submit

Status

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.

Project demo
Logoff skrueger
Help on

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**.

Beta and Retired modules:

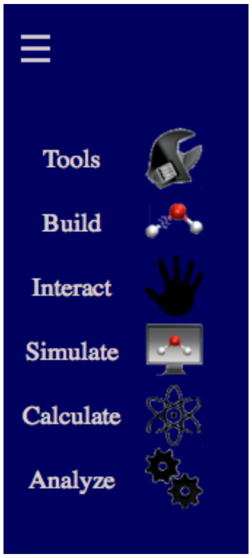
One can choose to display beta and retired SASSIE-web modules in the main menu by selecting the corresponding "Beta" and/or "Retired" checkbox in the Settings Manager. This will allow you to access beta and/or retired SASSIE-web modules as part of your work flow.

Update colors:

One can change the background and foreground colors of your SASSIE-web screen by choosing the "Update colors" checkbox in the Settings Manager. The new colors are saved and will take effect each time the user logs in.

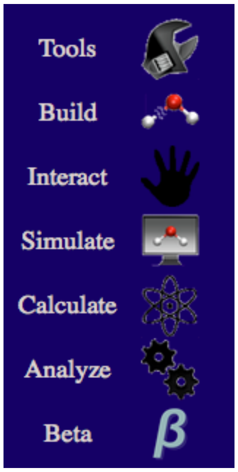
Main Menu

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.

If the Beta or Retired menu options have been activated in the Settings Manager, they will appear in the main menu. The image below shows an example of the main menu with the Beta icon.



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.

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.

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.

run name: run_0

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.

file input

Two options are given for each file input.

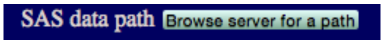
The "Choose File" option on the left corresponds to a file you wish to upload from your local computer/device.

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.

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



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

input / output structure file types

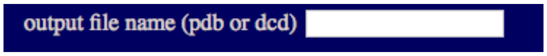
In many modules the input trajectory files (files that contain structure(s) to be analyzed or used in some way) can either be in text file format (PDB) or binary file format (DCD). For a typical input such as

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



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

---

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

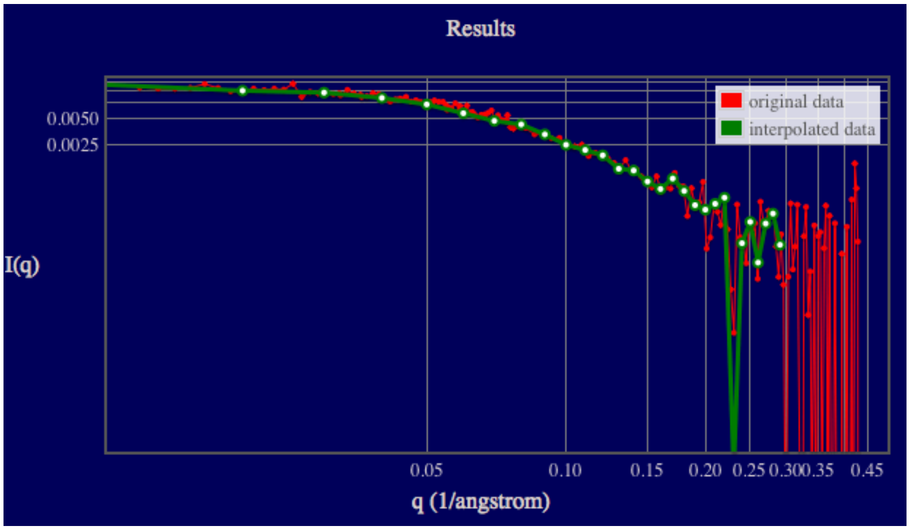
```
==============================================================
DATA FROM RUN: Wed Apr 29 16:27:16 2015

> 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

==============================================================
```

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,

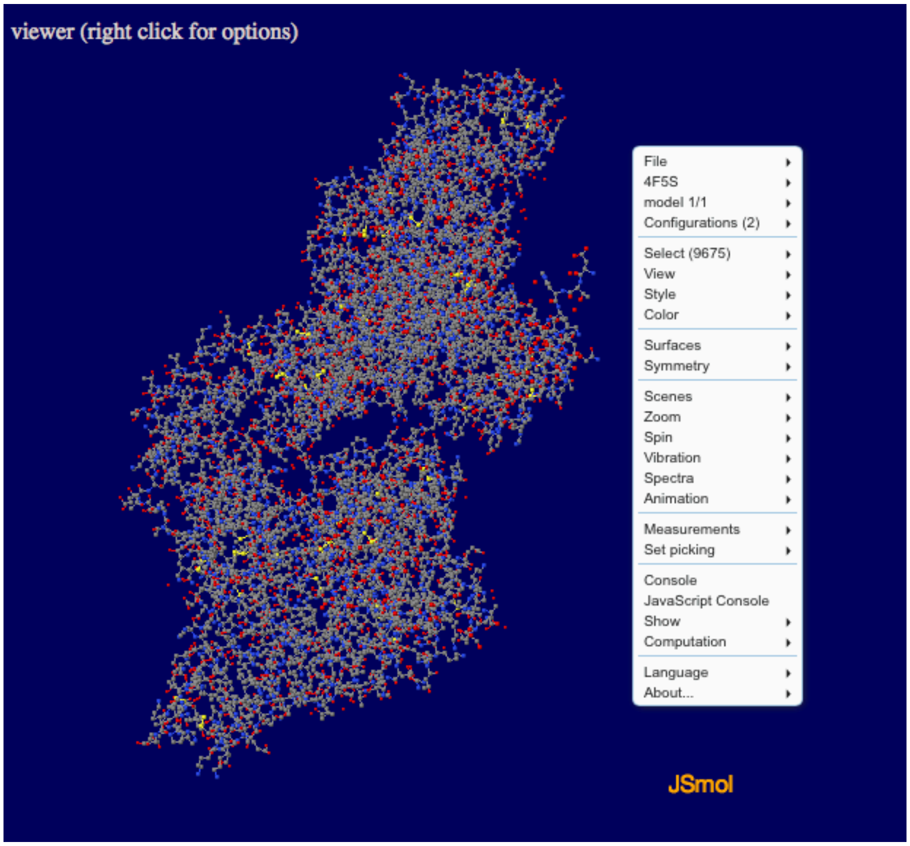


Users can zoom using your scroll-wheel on your input device, drag by clicking your mouse on the graph and moving while maintaining the click. Plots can be re-sized to their original view by clicking on the title or axis labels. One can also view values from the graph by placing the mouse pointer at any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



File Manager

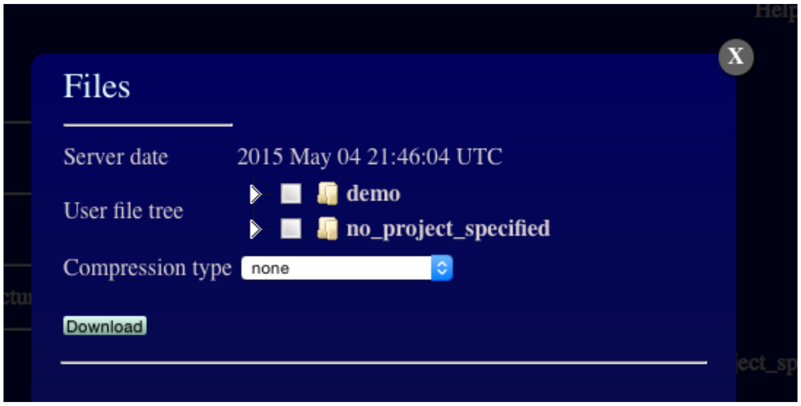
Each user has their own persistent file system. Your files will exist after you logout and they are backed up on a regular basis on our secure server.

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.

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



Files

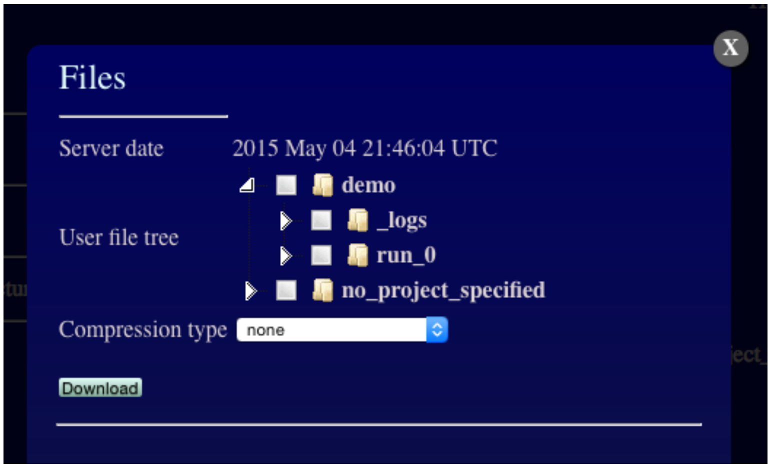
Server date 2015 May 04 21:46:04 UTC

User file tree
- ☐ demo
- ☐ no_project_specified

Compression type none

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.



Files

Server date 2015 May 04 21:46:04 UTC

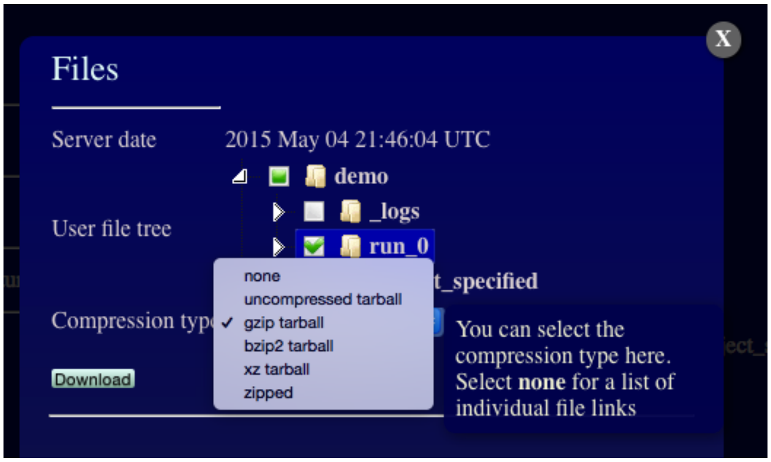
User file tree
- ☐ demo
  - ☐ _logs
  - ☐ run_0
- ☐ no_project_specified

Compression type none

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.

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.



Files

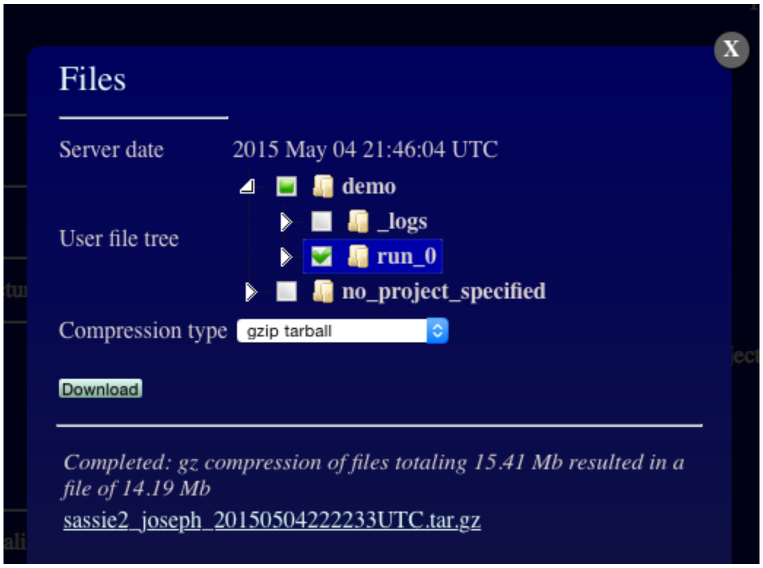
Server date 2015 May 04 21:46:04 UTC

User file tree

Compression type gzip tarball

You can select the compression type here. Select **none** for a list of individual file links

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.



Files

Server date 2015 May 04 21:46:04 UTC

User file tree

Compression type gzip tarball

Completed: gz compression of files totaling 15.41 Mb resulted in a file of 14.19 Mb

sassie2_joseph_20150504222233UTC.tar.gz

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.

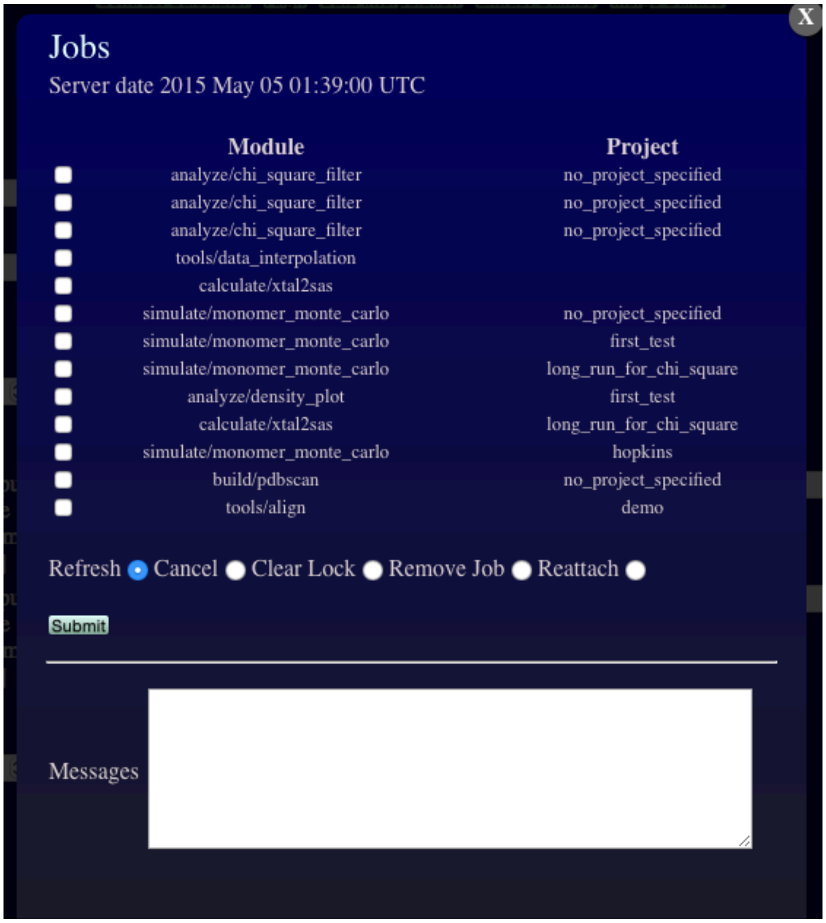
Notes

- 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.

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
☐	analyze/chi_square_filter	no_project_specified
☐	analyze/chi_square_filter	no_project_specified
☐	analyze/chi_square_filter	no_project_specified
☐	tools/data_interpolation	
☐	calculate/xtal2sas	
☐	simulate/monomer_monte_carlo	no_project_specified
☐	simulate/monomer_monte_carlo	first_test
☐	simulate/monomer_monte_carlo	long_run_for_chi_square
☐	analyze/density_plot	first_test
☐	calculate/xtal2sas	long_run_for_chi_square
☐	simulate/monomer_monte_carlo	hopkins
☐	build/pdbscan	no_project_specified
☐	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.

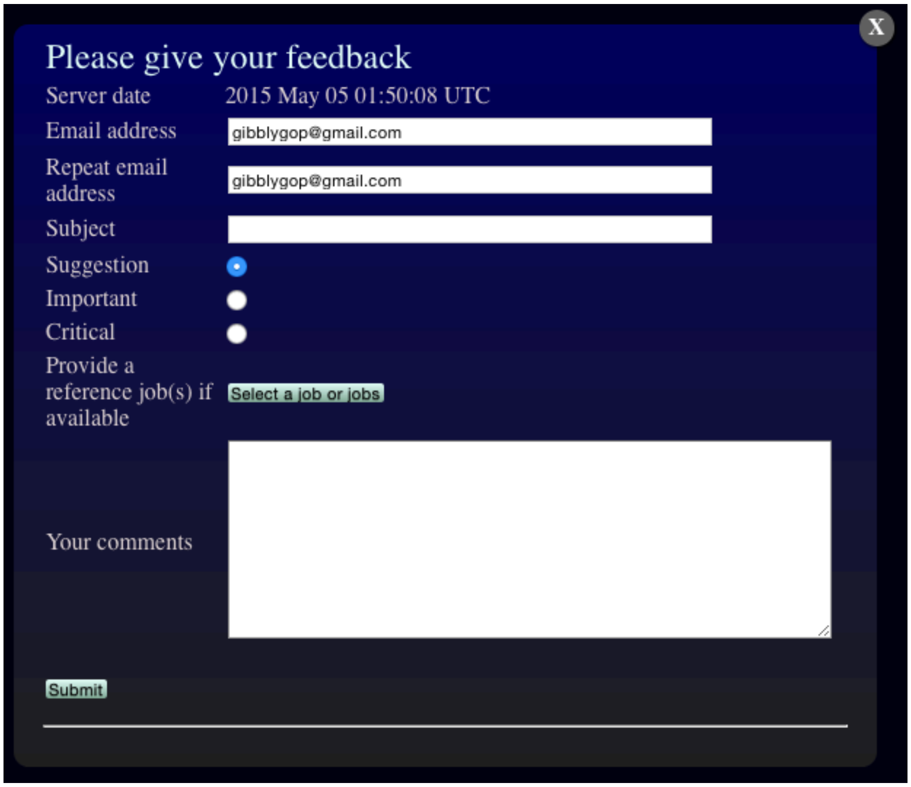
If a job is locked by a run in a different project directory it will be yellow

---

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



Please give your feedback

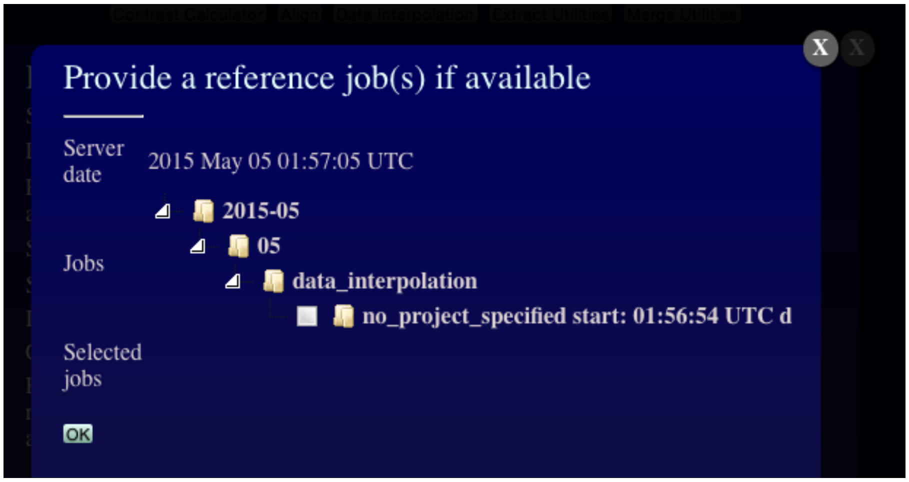
Server date 2015 May 05 01:50:08 UTC

Email address gibblygop@gmail.com

Repeat email address gibblygop@gmail.com

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



Provide a reference job(s) if available

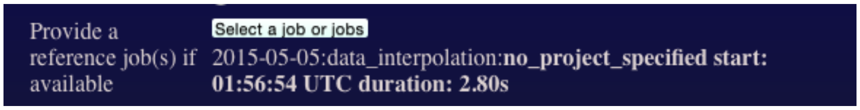
Server date 2015 May 05 01:57:05 UTC

◢ 2015-05
◢ 05
◢ data_interpolation
☐ no_project_specified start: 01:56:54 UTC d

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.



Provide a reference job(s) if available

2015-05-05:data_interpolation:**no_project_specified start: 01:56:54 UTC duration: 2.80s**

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

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