ST-analyzer Quick Tutorial

Ver. 0.1.0

Committee

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Objective

ST-analyzer tutorial is written for users who want to learn ST-analyzer from a quick example analysis. As following this tutorial, users will experience overall usage of ST-analyzer from installation to submitting jobs. For more information about ST-analyzer, please refer ST-analyzer manual.

Installation

ST-analyzer can be installed by running install script (i.e., #HOME/install.sh) as following:

```
#HOME/install.sh
```

Or setup tools (i.e., easy_install and pip)

```
sudo easy_install install Django
sudo easy_install Pyhull
sudo easy_install -U GridDataFormats
sudo pip install MDAnalysis
```

Python

Python v2.7 or above is required.
Python is available through http://www.python.org/download/

Django

ST-analyzer is optimized Django v1.4.1.
Django is available through https://www.djangoproject.com/download/

MDAnalysis

ST-analyzer is optimized MDAnalysis v0.7.6 and above.
MDAnalysis requires other modules to complete its installation. To make the installation simple, we encourage installing all-in-one package. Please visit the following individual packages websites and check the system requirements prior to the installation.

All-in-one package

- Anaconda (http://continuum.io/downloads.html) for Linux, Windows and Mac.
- Enthought Canopy (https://www.enthought.com/products/canopy/) for Linux, Windows and Mac.

Install MDAnalysis

- First install one of the all-in-one packages listed above.
- Download and install MDAnalysis through https://code.google.com/p/mdanalysis/
- Details of installing MDAnalysis can be found in https://code.google.com/p/mdanalysis/wiki/Install
- We have received reports about problems during the installation. Most of them are caused by outdated version of Python and GNU C compiler (http://gcc.gnu.org/). If you have problems with the installation process, please check the version of your GNU C compiler and Python, and discuss with your system administrator.
- For more questions about installation procedures, please use the discussion board at https://code.google.com/p/mdanalysis/wiki/Install

Pyhull

Details of instruction for installing Pyhull can be found at http://pythonhosted.org/pyhull/

GNUplot

Details of instruction for installing GNUplot can be found at http://www.gnuplot.info/

ST-analyzer

Download ST-analyzer from Git-hub: choose one of methods shown below

- Manual download: https://github.com/stanalyzer/ST-analyzer

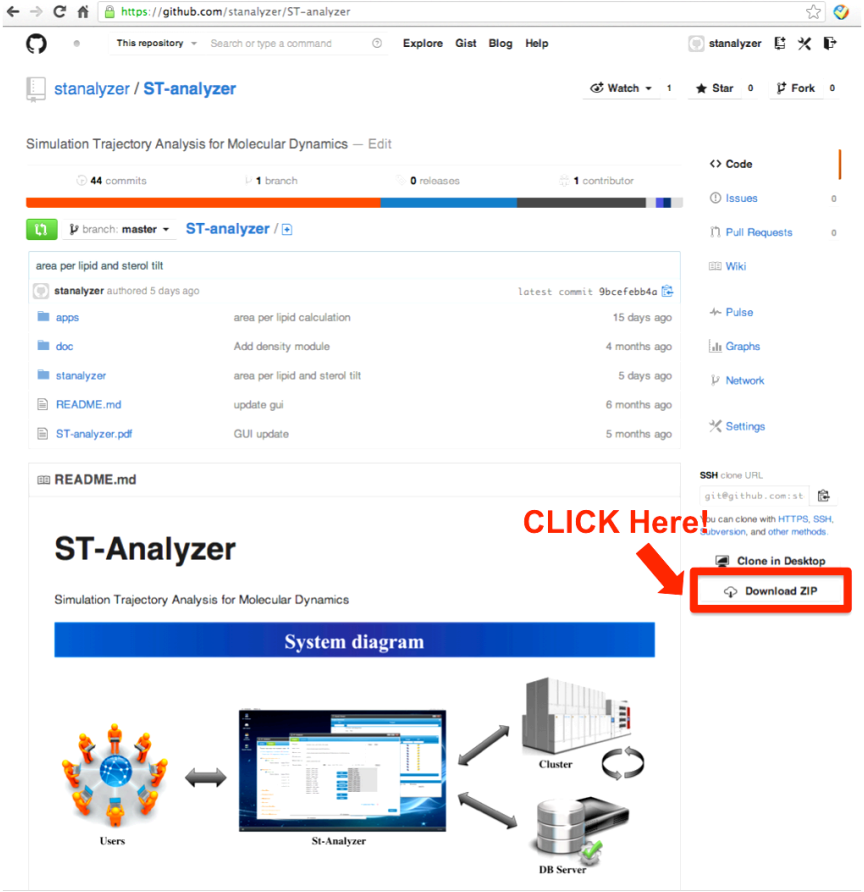


Figure 1 Manual download through Github

  - Unzip the zip file: *unzip ST-analyzer-master.zip*

- Git clone (using commandline): *git clone git@github.com:stanalyzer/ST-analyzer.git*

```
[jcjeong@stanalyzer]$ git clone git@github.com:stanalyzer/ST-
analyzer.git
Initialized empty Git repository in /Users/jcjeong/ST-analyzer/.git/
remote: Counting objects: 9326, done.
remote: Compressing objects: 100% (4882/4882), done.
remote: Total 9326 (delta 4290), reused 8764 (delta 3732)
Receiving objects: 100% (9326/9326), 129.10 MiB | 8493 KiB/s, done.
Resolving deltas: 100% (4290/4290), done.
Checking out files: 100% (2845/2845), done.
```

Figure 2. Using *git clone* to install ST-analyzer

Running ST-analyzer

1. Cnfiguration

Assume ST-analyzer is stored in *$LOC=/home/your_account/ST-analyzer/stanalyzer*

2. Checking DB consistency

This only requires for first run, right after the installation.
At your system command line prompt, use followings:

- user@stanalyzer> *cd $LOC*
- user@stanalyzer> *python manage.py syncdb*

3. Launch Django & ST-analyzer

- user@stanalyzer> *cd $LOC*
- user@stanalyzer> *python manage.py runserver 8000*
  the number '8000' are used as a port number communicating with ST-analyzer.
  Thus the port number can be changed

4. Forwarding port

Open terminal and type:
ssh -L 8000:localhost:8000 userid@your.hostname.edu

5. Connecting to ST-analyzer through your web-browser

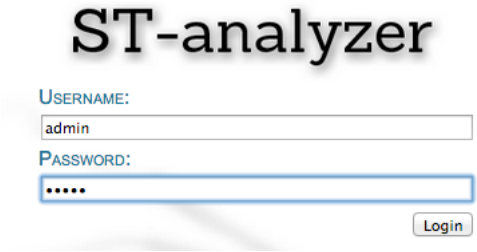
- Connect ST-analyzer through *http://127.0.0.1:8000/*
- You will see the ST-analyzer login.
- Initial account and password are ***'admin'*** and ***'12345'***

Examples for using ST-analyzer

Login

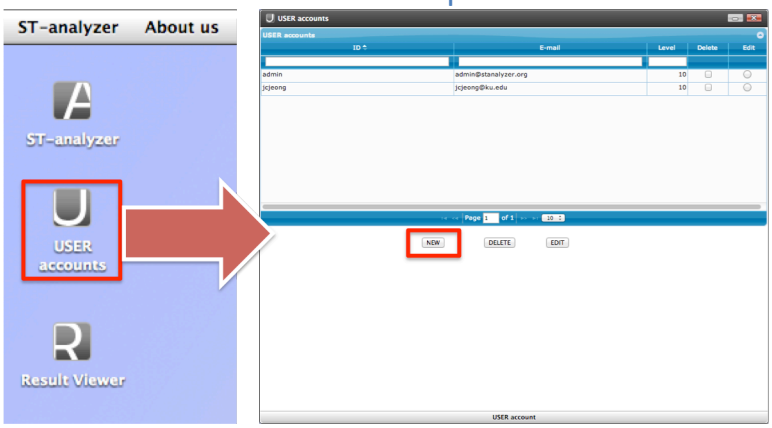
Username & Password

The initial user name and password is '***admin***' and '***12345***' respectively.



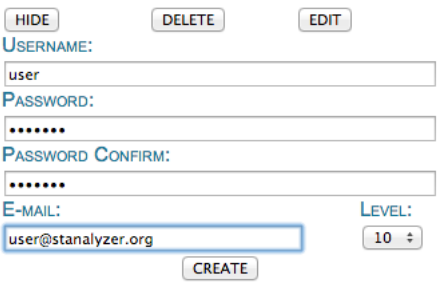
Creating personal account

1. Double click USER accounts icon at desktop

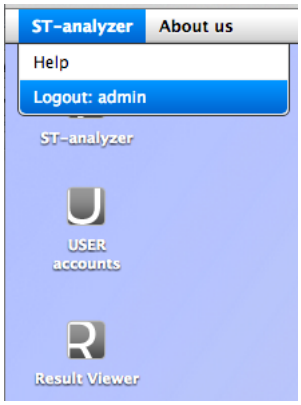


2. Click "NEW" and fill out the information & Click "CREATE"

Example:
Username: user
Password: userpwd

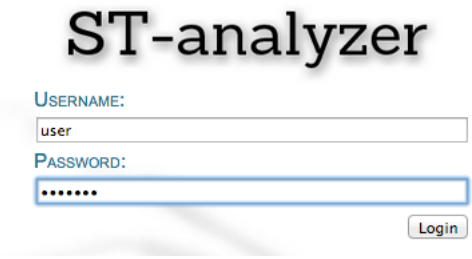


3. Log out



4. Log in with new ID

Username: user
Password: userpwd



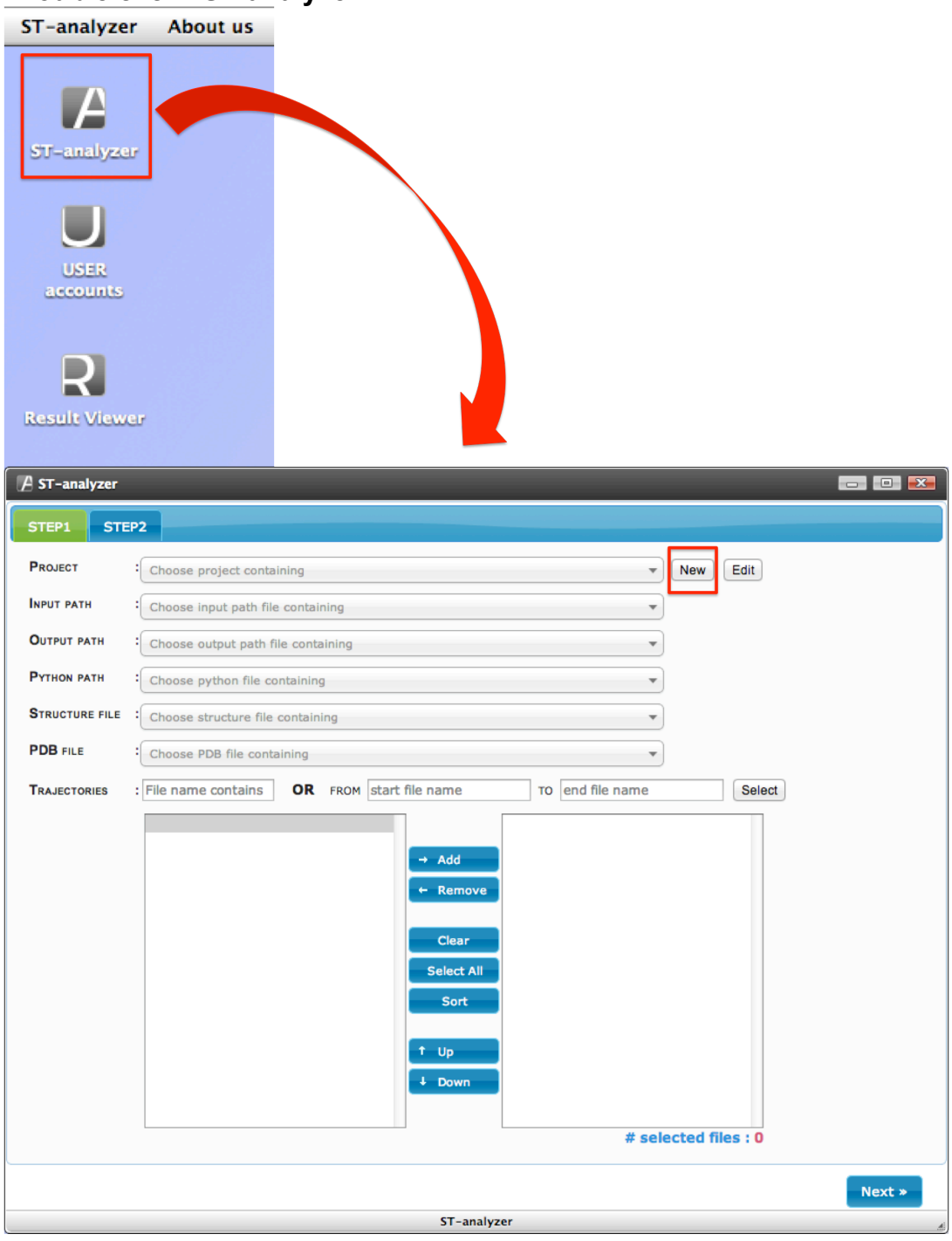
Submitting jobs

The example trajectory files can be found in *$LOC/trajectory*

Creating project

"*Project*" is the storage of the system environment, so users can store information about trajectories and retrieve it to prepare new jobs for further analysis.

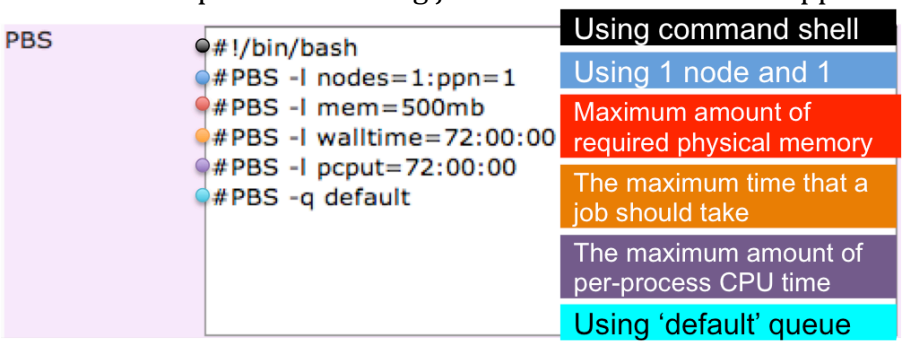
- **Double click "ST-analyzer"**



- **Click "New"**
  - Users will see "project" window as shown below
  - Next step will show the way to add information into this window

- **Fill information**
  - *Title*: name of project
  - *Input path*: the location of trajectory files (e.g *$LOC/trajectory/lipids*)
    - *Click "Add" button located next to the input box of "Input path"*
  - *Output path*: results storage directory
    - *Click 'Confirm' button located next to input box of 'Output path'*
  - *Python path*: the location of Python execution file
    - *The execution file could be "python" for most users unless users distinct installation of MDAnalysis in various versions of python*
    - *Click "Confirm" button located next to the input box of "Python path"*

- *PBS*: PSB script for submitting jobs to cluster machine if applicable



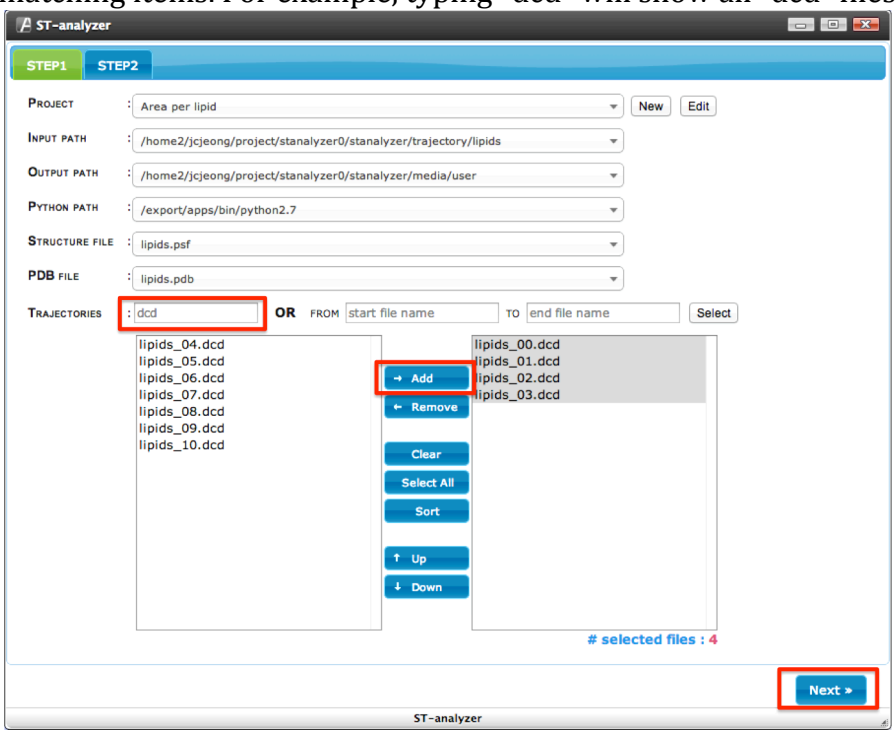
- **Click "Create" located at the bottom of "project" window (i.e. right below the input text box of PBS script)**
  - This will eventually create and store the project profile into database

- **Click "Hide" located at the top of "project" window (i.e. next to the drop box of project)**

- **Specify Structure and PDB files from the drop down menus as shown in the next section**

Configure trajectory information

- **Select files of interest** stored in "*Project*," a list will be displayed in the selection window. Start typing part of the information to be selectd, a quick search engine will show matching items. For example, typing "dcd" will show all "dcd" files.

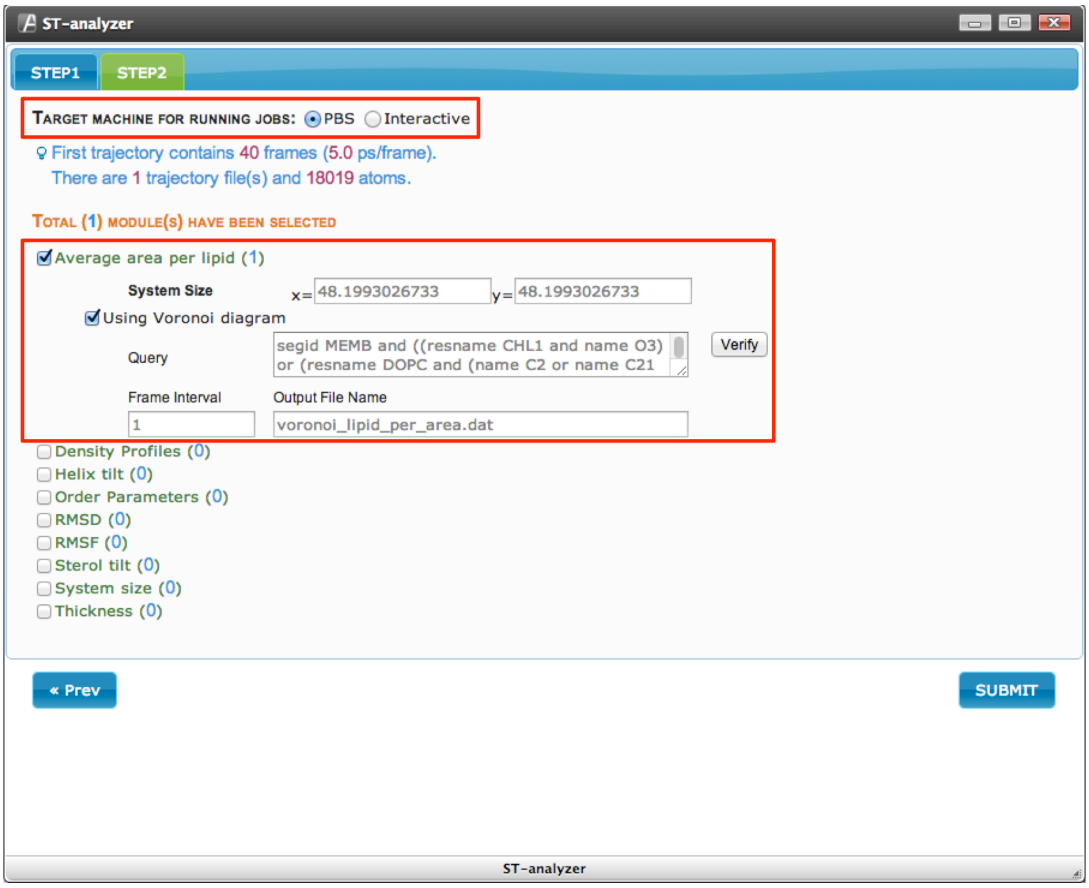


- **Click "Add" to move selected file to list of chosen files**

- **Click "Next" to specify analysis modules**

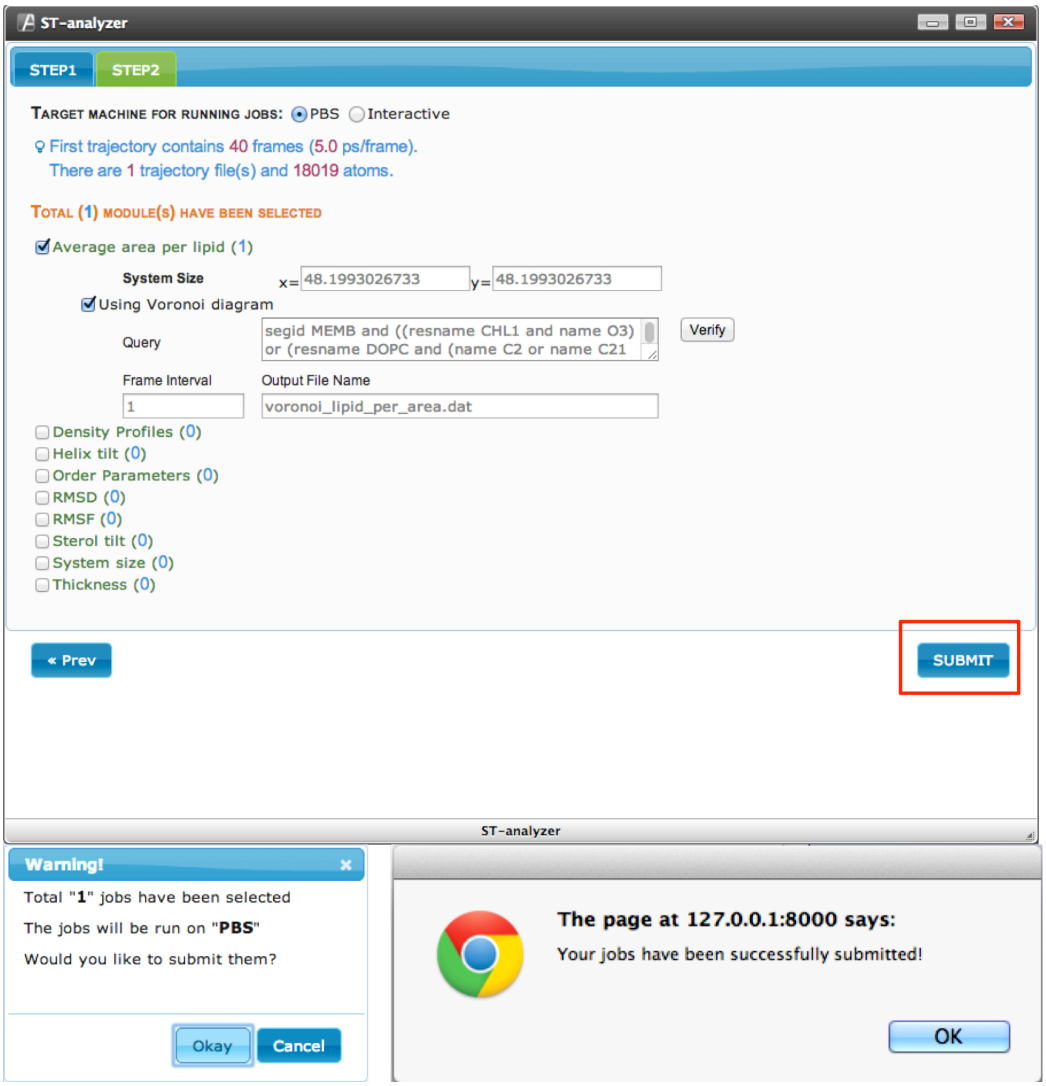
Setup analysis modules

- **Select machine to submit jobs:**
  - **PBS (**cluster machine) or **Interactive** (server where ST-analyzer is installed)



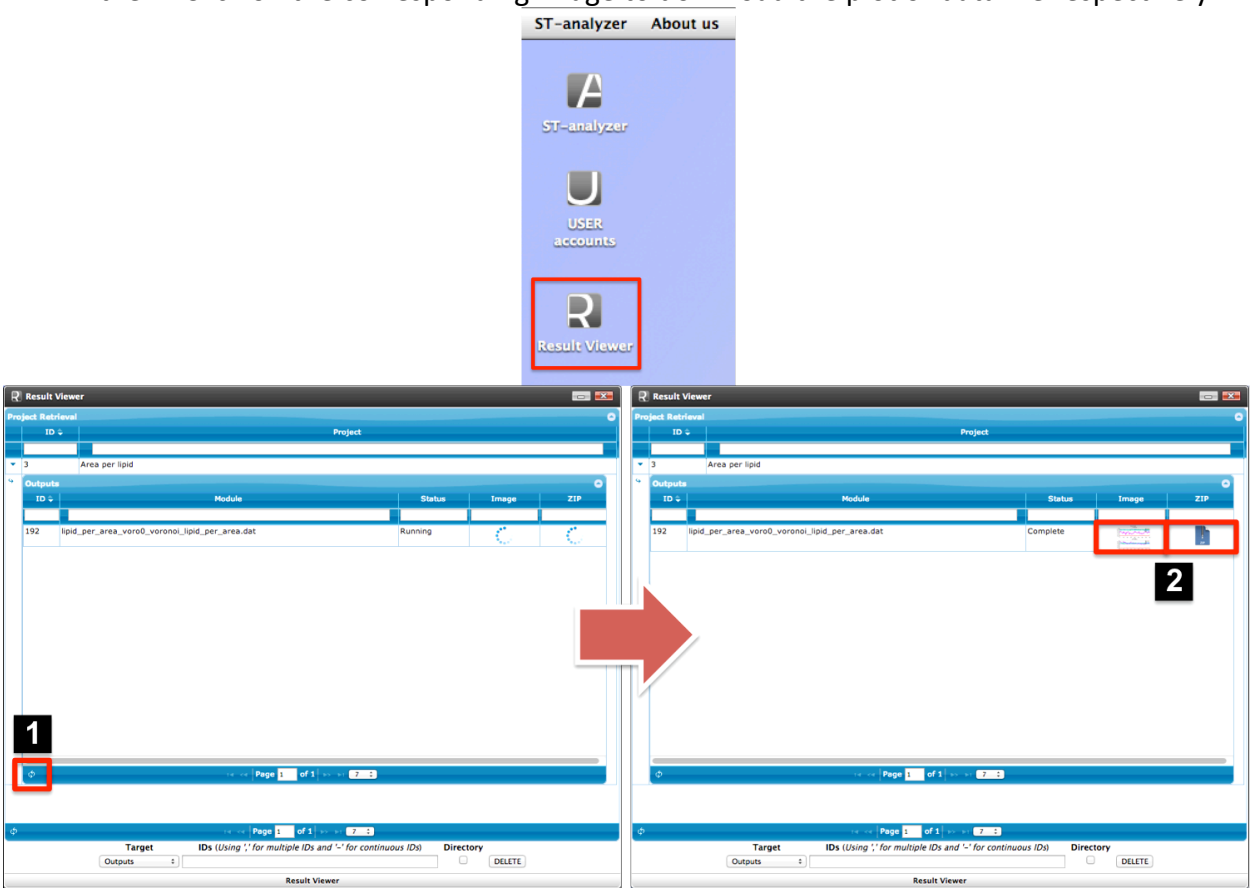
- **Select analysis modules and define parameters:** each module has sample values for user reference. Update the information to match the information of the system under study.
  - **Module name: "Average area per lipid"**
  - **System Size:** read information from first 'DCD' file
  - **Query:** e.g. **"***segid MEMB and ((resname CHL1 and name O3) or (resname DOPC and (name C2 or name C21 or name C31)) or (resname POPC and (name C2 or name C21 or name C31)) or (resname POPI and (name C2 or name C21 or name C31)) or (resname POPI13 and (name C2 or name C21 or name C31)))***"**
    The above string will select atoms having segment ID equal to 'MEMB', and atoms named O3 in residue name CHL1, as well as atoms named C2, C21, and C31 in residues DOPC, POPC, POPI, and POPI13.
  - **Verify:** click to verifying the query before submitting the job
  - **Frame Interval:** type "1" to read each frame in the trajectory files (DCD)
  - **Output File Name:** this name will be assign to output files stores in the selected output/results directory**.**

- **Click "SUBMIT":** ***Jobs will not be submitted until users click "OK" button***



Retrieve outputs

- **Double click "*Result Viewer*" in the main screen of ST-Analyzser interface**: A list of running jobs will be shown, click the "*refresh*" button at the bottom left to update job status. Completed jobs will have a small figure and a zipped file icon next to them. Click on the corresponding image to download the plot or data file respectively.



Log out

- **To prevent accidental data loss, users are encouraged to log out.**