SASSIE training course, Grenoble, France. 11 or 12 April 2019

Course description

SAXS and SANS are highly effective experimental techniques for investigating a broad range of soft matter science. The primary bottleneck in the interpretation of the experimental data is that it requires the use of as much a priori knowledge about the system as possible. The experimental X-ray and neutron data need to be interpreted using atomic-level models. This will replace the relatively crude shape models used up to now, which are based on rather simplistic overall shapes. It is only by doing this atomistic modelling that the real significance of the experimental data becomes clear. Work to develop such a package called SASSIE has been made possible by the CCP-SAS project (Collaborative Computational Project for Small Angle Scattering). This has been funded by the EPSRC in the UK and the NSF in the USA between 2013-2019 (**www.ccpsas.org**). Our open source software was released into the public domain in 2016, and easily accessible through a web interface. This package is being distributed to other centres outside the USA and UK.

SASSIE is a high-throughput, and user-friendly suite of software for the advanced atomistic and coarse-grained molecular modelling of SAXS and SANS data starting from physically accurate molecular structures. "SASSIE-Web" provides an online workflow framework into which modules are plugged to prepare structures, carry out simulations, calculate theoretical SAXS and SANS data and compare the outcome to experimental data. This provides a major step forward towards interpreting the experimental data down to atomistic level.

We are offering a 3.5 hour training course in Grenoble on both 11th and 12th April 2019 that is suitable for PhD students, academics and scientists who want to interpret their small angle x-ray and neutron scattering (SAXS and SANS) data of biological and soft matter polymer systems in order to obtain structural information down to the atomistic level.

In this training course, participants will get hands-on experience of using SASSIE-Web. They will perform molecular simulations of model biological and polymer systems, calculate theoretical scattering curves for them and infer the best-fit atomistic structures with respect to the experimental data. There will also be opportunity to discuss participants' own polymeric systems (biological molecules) in order to help them set up for SASSIE-Web analysis.

To secure a place on the course, applicants should make a booking during the poster session on Tuesday 9th April 2019. The CECAM meeting organiser is Dr Sylvain Prevost at the ILL (prevost@ill.fr). Participants will need to bring their own laptops to work on, they need to register themselves on the SASSIE web site as a new user (see https://sassie-web.chem.utk.edu/sassie2/), and they need to install some free software before the course begins.

Trainers: Prof Stephen J. Perkins (UCL) and Dr Jayesh S. Bhatt (UCL)

Schedule

Day 1 – 11th April

Time	Lead	Activity
16:30 – 17:00	JSB or SJP	SASSIE-web: Basic Usage. Micelles.
17:00 – 17:45	JSB or SJP	Lab 1: Introduction to VMD and NAMD. Running and visualising molecular dynamics simulation.
17:45 – 20:00	JSB or SJP	Lab 2: Use of SASSIE-web to analyse neutron scattering data of HIV-1 Gag protein. Involves Monte Carlo simulation.

Day 2 – 12th April

Time	Lead	Activity
08:45 – 09:15	SJP or JSB	SASSIE-web: Basic Usage. Micelles.
09:15 – 10:00	SJP or JSB	Lab 1: Introduction to VMD and NAMD. Running and visualising molecular dynamics simulation.
10:00 – 12:15	SJP or JSB	Lab 2: Use of SASSIE-web to analyse neutron scattering data of HIV-1 Gag protein. Involves Monte Carlo simulation.

JSB: Dr. Jayesh S. Bhatt (UCL)
SJP: Prof. Stephen J. Perkins (UCL)

A review of SASSIE and CCP-SAS is available to download from http://www.ccpsas.org/
Perkins, S. J., Wright, D. W., Zhang, H., Brookes, E. H., Chen, J., Irving, T. C., Krueger, S., Barlow, D. J., Edler, K. J., Scott, D. J., Terrill, N. J., King, S. M., Butler, P. D. & Curtis, J. E. (2016) Atomistic modelling of scattering data in the Collaborative Computational Project for Small Angle Scattering (CCP-SAS). *J. Appl. Crystall.* **49**, 1861-1875. DOI: 10.1107/S16005767160151X. Pubmed 27980506

SASSIE-web training course
Lab 0: Preparing your PC/laptop for the course – Windows

The following pieces of software are needed to complete this course. These must be installed on your PCs or laptops *before* the start of the course:
1. VMD – Views and analyses molecular models.
2. NAMD – Performs molecular dynamics simulations.
3. A modern web browser – recent versions of Chrome or Firefox. A lot of training will be done on a web portal. You will not be able to complete the training without one of these browsers.
   NOTE: Internet Explorer or the Edge browser are NOT suitable for SASSIE-web. Please do not use it for the course!
4. Notepad++ text editor. The standard Notepad that comes with Windows is *not* suitable, so please do not use that for the course.

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

VMD

Download

Use your web browser to navigate to the web page http://www.ks.uiuc.edu/Research/vmd/

- Locate the 'Download' 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 1.9.3 at the time of writing).

- Click the appropriate link

- You now need to register an account

   o Enter a username and password

   o Click "Continue with registration or download'

   o Fill in the form (including confirming your password)

   o 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

Use your web browser to navigate to the web page https://notepad-plus-plus.org/
- 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

Use your web browser to navigate to the web page http://www.ks.uiuc.edu/Research/namd/

- Follow the 'Download NAMD Binaries' link

- Select the Win32 link from the "Version 2.10 (2014-12-11) Platforms" section. Do NOT use a later version.

  ◦ We use version 2.10 to ensure that all input and output formats are compatible with other software used in the tutorial. **Later versions may have compatibility issues with SASSIE, so please do not use those.**

- Enter the username and password you created earlier when installing VMD.

- Agree to the license and the download should start automatically

Installation

- Open the downloaded NAMD_2.10_Win32-multicore.zip file in Explorer

- Copy the NAMD_2.10_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_2.10_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.
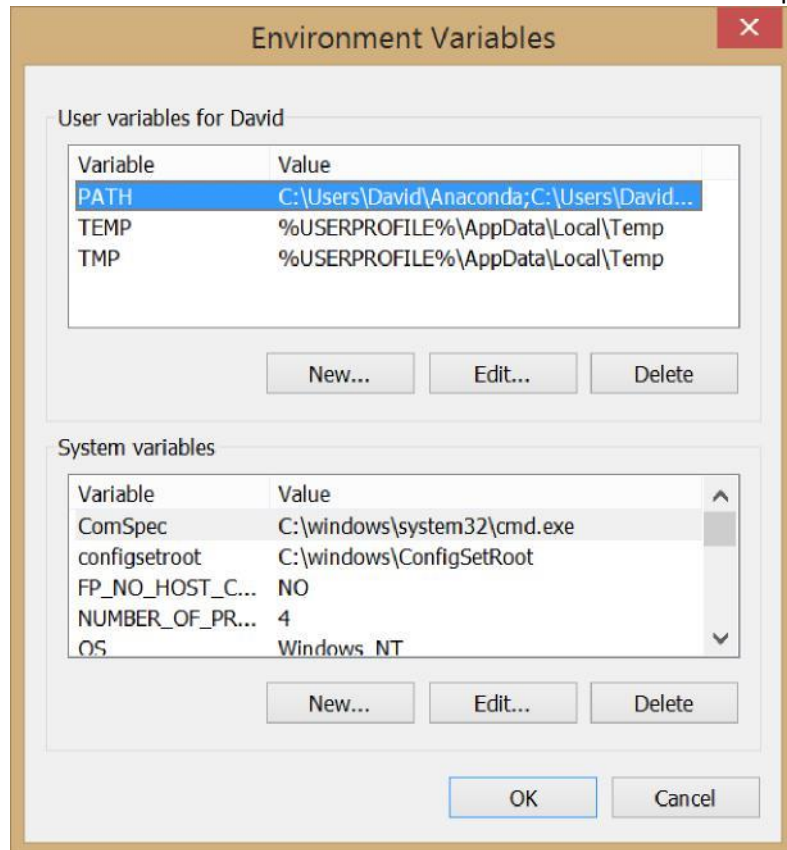
5. Ensure 'PATH' is selected in the 'User variables for xxxxx' listbox and then click the 'Edit' button beneath this section.

6. If there are no entries in 'Variable value' box simply paste in the location you copied earlier:
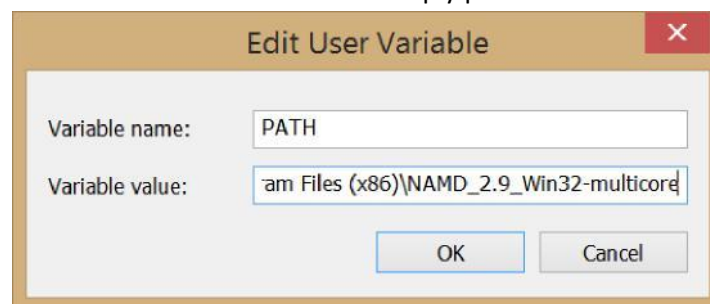
If entries already exist, place the cursor at the end of the text in the box. Enter a ; symbol and then paste in the folder location. So, if the entry read:

C:\Users\David\Anaconda

before, it should now say something like:

`C:\Users\David\Anaconda;C:\Program Files (x86)\NAMD_2.10_Win32-multicore`

7. Click 'OK'.

Testing NAMD installation

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):

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

- As for NAMD, 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_2.10_Win32-multicore; C:\Program Files (x86)\University of Illinois\VMD`

  ◦ Try opening VMD by typing:
     `vmd`

Lab 0: Preparing your PC/laptop for the course – Linux

Four pieces of software are needed to complete this course. These must be installed on your PCs or laptops *before* the start of the course:
1. VMD – Views and analyses molecular models.
2. NAMD – Performs molecular dynamics simulations.
3. A modern web browser - recent versions of Chrome or Firefox. A lot of training will be done on a web portal. You will not be able to complete the training without one of these browsers.

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 in the following instructions 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

Use your web browser to navigate to the web page http://www.ks.uiuc.edu/Research/vmd/

- 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 1.9.3 at the time of writing).

- Click the appropriate link

- You now need to register an account

    o Enter a username and password

    o Click "Continue with registration or download'

    o Fill in the form (including confirming your password)

    o 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-1.9.3.bin.LINUXAMD64.opengl.tar.gz
    ```

- Change into the vmd-1.9.3 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 2.10 (2014-12-11) Platforms" section

  ◦ We use version 2.10 to ensure that all input and output formats are compatible with other software used in the tutorial. **Later versions may have compatibility issues with SASSIE, so please do not use those.**

- 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_2.10_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_2.10_Linux-x86_64-
multicore
```

3. Save the file