

How to install QSpace library

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QSpace comes as a collection of precompiled C++ core routines (MEX function binaries with `.mex64` or `.mexmaci64` extensions) and a MATLAB environment wrapped around them. By being precompiled, users can simply copy the files to their own directory, to run the library. However, it puts constraints on the operating systems (OS). The binaries have been precompiled (1) for the environment of the workstations and HPC cluster at ASC (Linux), and (2) for Macbooks (macOS).

Below we explain how to install QSpace for different OS. To have the complete package necessary for tutorials, you should be able to access the ASC workstations; see `SSH_X_instruction.pdf` for details.

I. Installation on Linux

I.A. Installation at your home directory on ASC workstations

QSpace is optimized for being used with the workstations and cluster machines in the Arnold Sommerfeld Center (ASC). Thus it is the recommended way of installing and using QSpace.

Since your home directory (`/home/...`) is mounted on the network drive, it is enough to copy only once, to use the library for all the ASC workstations. The following instruction assumes that you install at `~/Documents/MATLAB/QSpace`.

For installation, first log into the ASC workstations. Then create the directory to place the package under your home directory.

```
mkdir -p ~/Documents/MATLAB/QSpace
```

Copy the files from the repository to the created directory.

```
rsync -avuh /home/s/S.Lee/X/QSpace_TNcourse/ ~/Documents/MATLAB/QSpace/
```

It is advisable also to copy some system setting files that defines useful environment settings and shortcut functions. The next command overwrites `.bashrc`, `.bash_profile`, or `.inputrc` to your home directory. If you haven't set these file before or don't know what they mean, you may run:

```
rsync -avuh /home/s/S.Lee/X/QSpace_TNcourse/system/ ~/
```

If you have set `.bashrc` or the others, then don't run the command not to overwrite your own. Instead, add a line at the end of your `.bashrc`:

```
source ~/Documents/MATLAB/QSpace/system/.bashrc
```

Restart SSH session or type `source ~/.bashrc` in the command line, so that shortcuts and environment setting are recognized. Then go to the QSpace directory which you installed the package, by typing:

```
go qs
```

Start the MATLAB **from** the QSpace directory. (Otherwise, `startup.m` needs to be run manually, which is a bit inconvenient.) With the `.bashrc` copied from the repository, you can start MATLAB by simply typing:

```
ml
```

The full MATLAB desktop with graphic user interface will start. But this might be slow and unstable when you work from home. To suppress the graphic interface, give `-nn` option (which means `-nosplash` -

nodesktop option in starting MATLAB):

```
ml -nn
```

In this case, MATLAB desktop does not show up; instead just command-line interface appears. It is the text interface version of the `Command Window`, the main panel of MATLAB installed at your laptop. When you configured X11 properly, you can plot figures.

I.B. Installation at your Linux machines

You may try the binaries for LMU workstations whether they work as they are. However, this will likely depend on the particular hardware of and libraries installed on your computer. Thus there is no guarantee whether it works. Please let us know whether you manage to get this to work or not.

II. Installation on macOS

This way is advantageous in that you can directly use the library within the local MATLAB installation at your Macbook.

The library for macOS can be downloaded from: <https://bitbucket.org/aweichselbaum/qspace-3.2-os-x10-catalina/downloads/> Click “Download repository”. Unzip the downloaded .zip file under `~/Documents/MATLAB/QSpace` of your laptop. Then copy the rest of files needed for tutorial:

```
rsync -avuh /home/s/S.Lee/X/QSpace_TNcourse/ ~/Documents/MATLAB/QSpace/
```

Don't worry about overwriting, as the binaries have different extensions for macOS from Linux.

When you try to use the QSpace, some versions of macOS (including Catalina) might complain that the developer of the MEX function binaries is not verified, so it cannot run them. (Of course, the library does not contain malware!) To solve this issue, try out an approach mentioned in:

http://www.fieldtriptoolbox.org/faq/mexmaci64_cannot_be_opened_because_the_developer_cannot_be_verified/

Please let us know if you experience any trouble in using QSpace in your macOS machine.

III. Installation on Windows

As of now, there are no MEX function binaries available for Windows. One may try out Cygwin or Windows Subsystem for Linux (WSL). Please let us know whether you manage to get this to work or not.

IV. Workflow guideline

This section applies only to the users of the library installed for the ASC workstations.

You may directly write your codes in your home directory mounted on the network drive, by using terminal-based editors such as `vi`. Using the graphic interface (including `.mlx` scripts) via network can be extremely slow. It is especially the case when you are connecting from the outside of MWN (e.g., your home).

Another way is to work on the codes and data in your laptop, and synchronize your working directory with

the counterpart on the network drive. It is robust against network problem. Even when network fails, you can keep editing your code! The details of this approach are:

- Copy the QSpace library to your laptop, even though the library would not run on your laptop. Use `rsync` (for Mac and Linux laptop users) or FTP (for general users) to download the directory from workstations. Place the library to a different directory, **not** in the TN directory used for the other tutorials, to avoid possible path conflicts.
- The QSpace directory contains MATLAB functions that can be recognized by local MATLAB session on your laptop. For MEX functions under `bin` directory, there are `.m` files with the same name. For example, there is a pair of `contractQS.m` and `contractQS.mexa64`. Such `.m` files contain the documentation of the corresponding MEX functions. Even more, with the local copy of the QSpace library, your MATLAB session recognizes that there are functions of such names, enabling convenient features such as auto-completion and Code Analyzer.
- Save your code in your local `Work` directory in your laptop. And use `rsync` or FTP to upload your code to the QSpace directory under your ASC home directory. Similarly, you can also download the computation result in your ASC home directory, e.g., to plot figures.

There are a few general, important remarks.

- While you are using graphic interface, do not close the terminal window (PuTTY, Terminal, etc.) from which you have started MATLAB. The whole graphic interfaces (MATLAB desktop, editor, figures, etc.) are bound to that terminal window. So if you close the terminal window, you will lose all the other windows as well.
- The current version of QSpace is 3.2, and it is confirmed to be compatible with MATLAB R2018a. Please let us know if it does not work with your MATLAB version.
- After using a MATLAB session running on the ASC workstations, quit the MATLAB session properly by typing `exit` in the MATLAB command window or by clicking `x` button in case of graphic interface. There are limited number of licenses of MATLAB, shared for all the ASC members. So please only run interactive MATLAB sessions on one specific workstation at any given time. (Multiple concurrent matlab sessions on the same workstation are alright, as they only use one license.)

IV. Start tutorial

The exercises and solutions for T05 and T06 will be uploaded under the subdirectory `Tutorials` of the repository in the ASC network drive (`/home/s/S.Lee/X/QSpace_TNcourse/Tutorials`), **not** in the course webpage. So please download or copy files from the repository by using `rsync` or FTP, before you start working on tutorial materials.