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Installation of XDS, XDSGUI, XDSSTAT, XDSCC12 and XDSViewer packages in Windows 10 Subsystem for Linux(WSL)

The programs of the XDS, XDSGUI, XDSSTAT, XDSCC12 and XDSViewer packages can be run on 64bit Windows 10 within the Windows Subsystem for Linux(WSL). For which the Linux bash shell has to be installed on windows. This allows installation of Ubuntu environment, which supports the apt package manager. Hence, allowing Ubuntu software's to be installed.

1. Installation of Linux bash shell on Windows 10

(https://www.howtogeek.com/249966/how-to-install-and-use-the-linux-bash-shell-on-windows-10/)

Steps to install Linux bash shell:

(i) Check the system type : should be 64-bit operating system

Control panel system and security system
system type : '64-bit operating system, x64-based processor

(ii) Enable the "Windows Subsystem for Linux" optional feature.

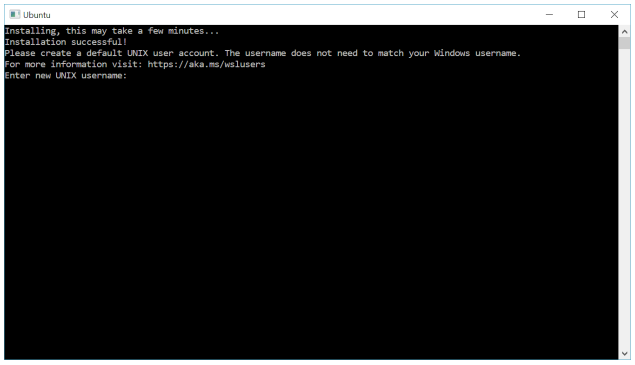
Control panel programs turn windows features on or off
New window 'windows features' pops up. In this window select, □ Windows Subsystem for Linux (and enable(√) it) and click ok.

2. Restart the computer.

3. Installation of Ubuntu in Linux bash shell on Windows 10.

Go to 'start menu'
Open 'Microsoft store
In search type ' Linux ' (and enter)
Gives results for : Linux
From this select the App 'Ubuntu 20.04 LTS'
To install a Linux distribution click Ubuntu, and then click the Get or install button. Ubuntu icon is saved on desktop or task bar.

First time when a newly installed Linux distribution is launched a console window will open followed by completion of installation. Finally we are asked to create a user account and password for the new Linux distribution.



2. Path assignment for executables of the XDS package accessible
(http://xds.mpimf-heidelberg.mpg.de/html_doc/downloading.html)

In Ubuntu bash window do following steps (red fonts to be typed): Type echo $SHELL to find out which shell you are using. For the bash shell type nano ~/.bashrc to open standard personal initialization file.

xyz@ZEPHYR: $ echo $SHELL
/bin/bash
xyz@ZEPHYR: $ nano ~/.bashrc

In the opened standard personal initialization file go to the end and append the following lines. The path /usr/local/bin is the location were the xds-programe file are located in Ubuntu.
export PATH=/usr/local/bin:$PATH

export KMP_STACKSIZE=8m

export DISPLAY=:0

The first line makes the executables of the XDS package accessible, while the second line defines the stack size limit of the Linux POSIX threads libraries used by OpenMP for xds_par. The third line makes the executables of the xdsgui and xdsviewer package accessible (for display of the images).

3) Downloading and Installation of XDS package

a) Go to the download site http://xds.mpimf-heidelberg.mpg.de/html_doc/downloading.html and download XDS-INTEL64_Linux_x86_64.tar.gz for operating system (Linux x86_64, 64 bit). Uncompress and untar the downloaded file. This will create a directory named XDS-INTEL64_Linux_x86_64. For installation the files in XDS-INTEL64_Linux_x86_64 folder should be included in the search path(/usr/local/bin) in Ubuntu.

Suppose the downloaded folder XDS-INTEL64_Linux_x86_64 is on the window desktop then the folders path is /mnt/c/Users/U/Desktop/ (check for the actual path of XDS-INTEL64_Linux_x86_64 folder). Log in as root - we need write permission for /usr/local/bin.

In the bash terminal perform the following steps to place the programs of the XDS package (red fonts to be typed).
xyz@ZEPHYR:~$
xyz@ZEPHYR:~$ cd /mnt/c/Users/U/Desktop/

xyz@ZEPHYR:/mnt/c/Users/U/Desktop$ sudo cp -r XDS-INTEL64_Linux_x86_64 /usr/local/bin/
[sudo] password for xyz:

xyz@ZEPHYR:/mnt/c/Users/U/Desktop$ cd
xyz@ZEPHYR:~$ cd /usr/local/bin/
xyz@ZEPHYR:/usr/local/bin$ ls
XDS-INTEL64_Linux_x86_64 (Confirms that the XDS-INTEL64_Linux_x86_64 folder is copied)

xyz@ZEPHYR:/usr/local/bin$ sudo ln –sf XDS-INTEL64_Linux_x86_64/*. (copies files from XDS-INTEL64_Linux_x86_64 folder to /usr/local/bin)
xyz@ZEPHYR:/usr/local/bin$ ls (check the files copied from XDS-INTEL64_Linux_x86_64 folder)

This completes installation of the XDS package. As a check you can open a new terminal window and issue the command *which xds* or *which 2cbf* or *which forkxds*.
xyz@ZEPHYR:/usr/local/bin$ which xds
/usr/local/bin/xds
xyz@ZEPHYR:/usr/local/bin$ which 2cbf
/usr/local/bin/2cbf
xyz@ZEPHYR:/usr/local/bin$ which forkxds
/usr/local/bin/forkxds

(b) Alternative way to install XDS package (: https://strucbio.biologie.uni-konstanz.de/xdswiki/index.php/Installation)

Download and unzip & untar XDS package directly from the programme site using these commands.
i) xyz@ZEPHYR:~$ cd /usr/local/bin
xyz@ZEPHYR:/usr/local/bin$
In the above path add sudo wget -O- ftp://ftp.mpimf-heidelberg.mpg.de/pub/kabsch/XDS-INTEL64_Linux_x86_64.tar.gz | sudo tar xzvf –

xyz@ZEPHYR:/usr/local/bin$ sudo wget -O- ftp://ftp.mpimf-heidelberg.mpg.de/pub/kabsch/XDS-INTEL64_Linux_x86_64.tar.gz | sudo tar xzvf -
[sudo] password for xyz: [sudo] password for xyz:

xyz@ZEPHYR:/usr/local/bin$ ls
XDS-INTEL64_Linux_x86_64
By this command the XDS-INTEL64_Linux_x86_64 folder is extracted in the path from the internet site.

ii) xyz@ZEPHYR:/usr/local/bin$ sudo ln -sf XDS-INTEL64_Linux_x86_64/* .
xyz@ZEPHYR:/usr/local/bin$ ls

By this command the files from XDS-INTEL64_Linux_x86_64 folder get copied in the path /usr/local/bin

4. Installation of XDS-Viewer, XDSSTAT, XDSCC12, XDSGUI, XSCALE_ISOCLUSTER
(https://strucbio.biologie.uni-konstanz.de/xdswiki/index.php/Installation)

Make a new directory say ‘ test’ in /usr/local/bin and do the following steps.

sudo wget https://strucbio.biologie.uni-konstanz.de/pub/linux_bin/get_folder.sh
sudo chmod +x get_folder.sh
sudo ./get_folder.sh

i) Make directory 'test' in the path /usr/local/bin
xyz@ZEPHYR:/usr/local/bin$ sudo mkdir test
[sudo] password for xyz:
xyz@ZEPHYR:/usr/local/bin$ ls
test
xyz@ZEPHYR:/usr/local/bin$ cd test
xyz@ZEPHYR:/usr/local/bin/test$

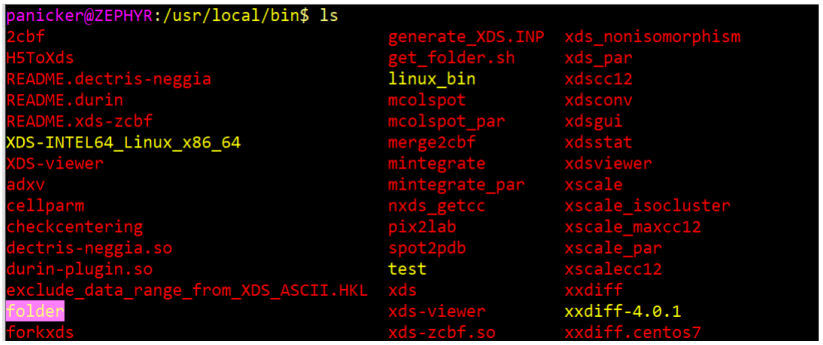
ii) Download programme from the internet site
xyz@ZEPHYR:/usr/local/bin/test$ sudo wget https://strucbio.biologie.uni-konstanz.de/pub/linux_bin/get_folder.sh
xyz@ZEPHYR:/usr/local/bin/test$ ls
get_folder.sh

xyz@ZEPHYR:/usr/local/bin/test$ sudo chmod +x get_folder.sh
xyz@ZEPHYR:/usr/local/bin/test$ ls
get_folder.sh

iii) by doing this step the files from downloaded folder gets placed in /usr/local/bin/
xyz@ZEPHYR:/usr/local/bin/test$ sudo ./get_folder.sh

xyz@ZEPHYR:/usr/local/bin/test$
xyz@ZEPHYR:/usr/local/bin/test$ ls
get_folder.sh

xds@ZEPHYR:/usr/local/bin/test$ cd ..
xds@ZEPHYR:/usr/local/bin$ ls
Will show all files extracted.



5. Additional programme to be installed for smooth performance of XDS, XDS-Viewer, XDSSTAT, XDSCC12, XDSGUI
(https://strucbio.biologie.uni-konstanz.de/xdswiki/index.php/Installation)

(i) Graphical Linux programs (xdsgui and xdsviewer) require installation of X server like Xming (https://sourceforge.net/projects/xming/support) or VcXsvr on the Windows host. **Before using xdsgui and xdsviewer programme, open Xming programme.** If Xming programme is not opened it gives a "error message xdsgui: cannot connect to X server :0 .

To use the X server, one has to say in the shell window. export DISPLAY=:0

(ii) Since XDSGUI depends on graphics packages which need to be installed. Check the XDSGUI binary with this command ldd `which xdsgui` and this will show the libraries it found and that it didn't find.

xyz@ZEPHYR:~$ cd ..
xyz@ZEPHYR:/home$ cd ..
xyz@ZEPHYR:/$ ldd `which xdsgui`
xyz@ZEPHYR:/$

(iii) In Ubuntu 18.04: if libQtOpenGL.so.4 is missing, use sudo apt install libqt4-opengl

(iv) xds-viewer needs libpng12.so.0 to work. But libpng12-0 is missing in Ubuntu 18.04, 19.10 or 20.04. To fix this issue install libpng by using a PPA created with an updated libpng12-0 package (www.linuxuprising.com › 2018/05 › fix-libpng12-0-mi...). Use these commands to add the PPA and install libpng12-0:

(a) sudo add-apt-repository ppa:linuxuprising/libpng12
(b) sudo apt update
(c) sudo apt install libpng12-0

xyz@ZEPHYR:/$ sudo add-apt-repository ppa:linuxuprising/libpng12
xyz@ZEPHYR:/$
xyz@ZEPHYR:/$ sudo apt update
xyz@ZEPHYR:/$
xyz@ZEPHYR:/$ sudo apt install libpng12-0

Or download the libpng12-0 DEB package from the PPA and install it manually (only need the libpng12-0 DEB package, e.g. libpng12-0_1.2.54-1ubuntu1.1+1~ppa0~eoan_amd64.deb).

(v) The xxdiff binary is provided by the get_folder.sh script i.e it is there in the Ubuntu path. In case the xds programs does not work than google to get xxdiff for Ubuntu and place in Ubuntu path (https://sourceforge.net/projects/xxdiff/files/latest/download). xxdiff is a graphical browser for viewing the differences between two or three files, or between two directories, and can be used to produce a merged version.

(vi) Running XDSGUI under WSL's Ubuntu may require installation of a packages with command:
sudo apt-get install libgompl libqtgui4

(vii) to generate_XDS.INP requires a number of packages which is detector specific. One e.g
sudo apt-get install coreutils binutils gawk sed bc grep

6) How to access external USB drive connected to the Window PC in Windows Subsystem for Linux.

Create the mount point using this command.
sudo mkdir/mnt/g (add g matching letter to the windows drive or whatever word or letter you want).

Mount the drive to the directory using this command.
sudo mount -t drvfs G: /mnt/g

The data from the pen drive can now be used from Ubuntu bash window.

Once all programmes are installed open the bash terminal and run the xds programs. (How to use these programmes see on internet.)

xyzr@ZEPHYR:~$ xdsgui (xdsgui window opens)

xyz@ZEPHYR:~$ xdsviewer (xdsviewer window opens)

xyz@ZEPHYR:~$ xds (to run xds programme, XDS.INP file is required, can be downloaded from internet)

xyz@ZEPHYR:~$ merge2cbf (to run merge2cbf programme, MERGE2CBF.INP file is required, can be downloaded from internet)

It was observed that in Ubuntu bash window only .cbf image files were displayed in xdsgui and xdsviewer programmes. Other image file like .img etc were not displayed. Even though the images were not displayed the data processing did take place and all results seen in both bash and xdsgui windows.

By using merge2cbf programme you can try to convert non cbf images to .cbf images (keep the no of frame one in this line: NUMBER_OF_DATA_FRAMES_COVERED_BY_EACH_OUTPUT_FRAME= 1). To convert the MERGE2CBF.INP file is to be placed in the folder were image files are located. Make the required changes in MERGE2CBF.INP file and run on the terminal (xyz@ZEPHYR:/mnt/c/Users/U/Desktop/data$ merge2cbf). The path given is where the images are located. The converted file is placed in the same folder.

Using merge2cbf, .img files do get converted to .cbf, which is displayed in xdsgui window, but all image details like distance from detector, etc is lost.
Hence, these values to be feed in XDS.INP file before processing in xdsgui.