ELSTRU
INSTALLATION AND TESTING

For Mac OS X 10.6.8

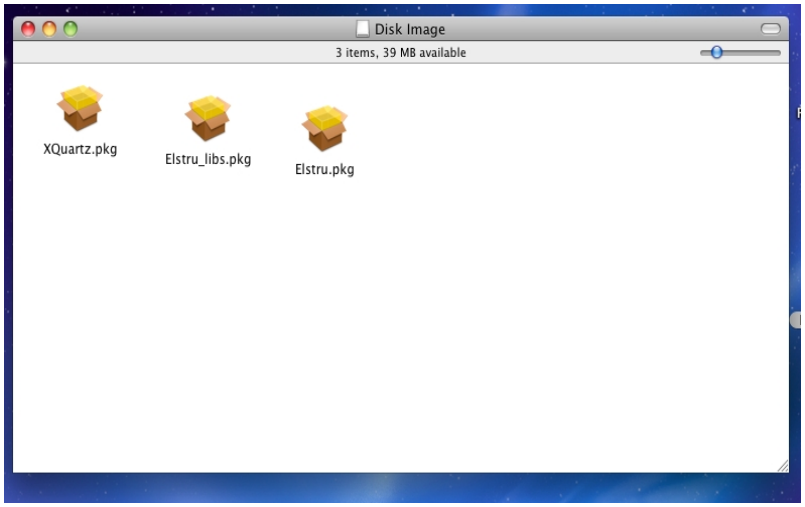
manual revision : 1.0

Software version 2.0

Contents

1.Installation

Currently the only version of ELSTRU for OS-X that is available is a 64 bit version compiled and testted on OS-X 10.6.8 (Snow-leopard).
The Installation package for Elstru can be downloaded as an DMG-file from our FTP-server :
ftp://nchrem.tnw.tudelft.nl/elstru/elstru.dmg
Copy this file to the machine where you want to install and than "*double click*" on it. A file called "Disk Image" will be created. Also "*double click*" on this file which will open a window containing the three installable packages in the file.



Xquartz.pkg contains version 2.6.3 of this X11-server. Installation of this package is not needed if you already have a working Xquartz 2.6.3 or a newer version.

Elstru_libs.pkg contains several installations obtained using MacPorts. It contains installations and its depencies for the following packages

- gtk2
- freetype
- freeglut
- fftw-3
- ImageMagick

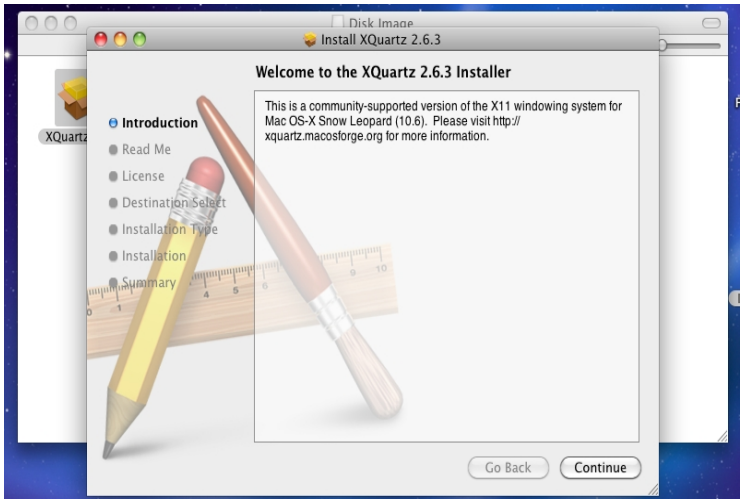
If you have recently installed these packages using MacPorts and if they are installed in /opt/local you do not have to install this package

Elstru.pkg contains the ELSTRU programs and data-files. Installation is always required.

Note that all installation should be performed using an account with administrator rights.

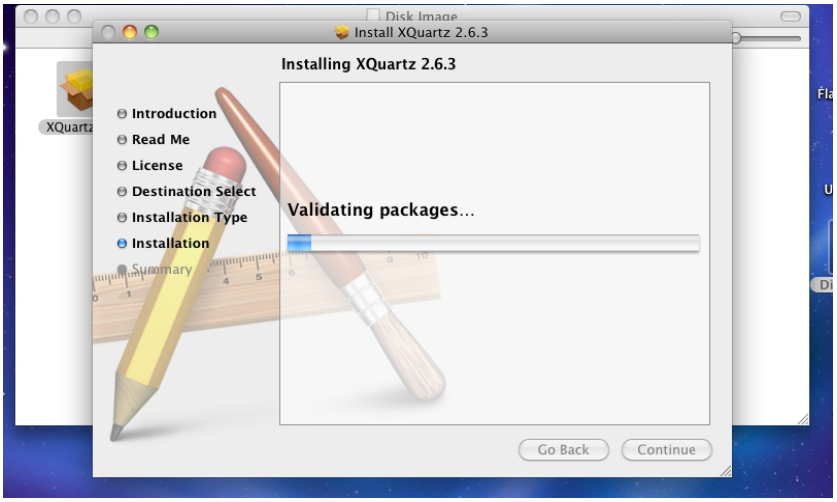
1.1 Installation of Xquartz

Install the Xquartz utility if you do not have already installed version 2.6.3 or later by *"double click"* on the Xquartz.pkg file. You will get the following window.

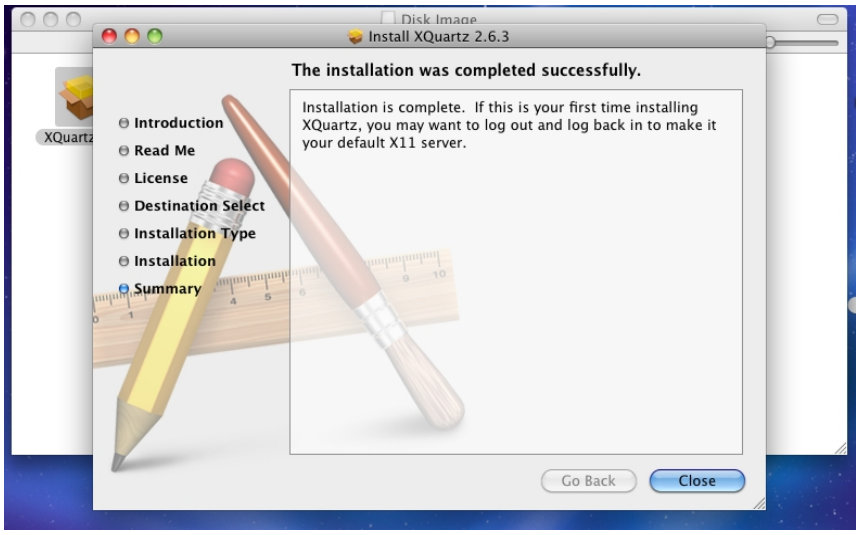


Click successively in the windows that are shown on *"continue"*, *"continue"*, *"continue" and "agree"*.

Click now on the blue area labeled "Install for all user of this computer" and in the windows that show successively on *"continue"* and *"install"*. A request for a password will pop-up. Information for an account with administrator-rights should be used here.
Wait now for several minutes watching the following screen, while the application is installed.



Finally you will get:



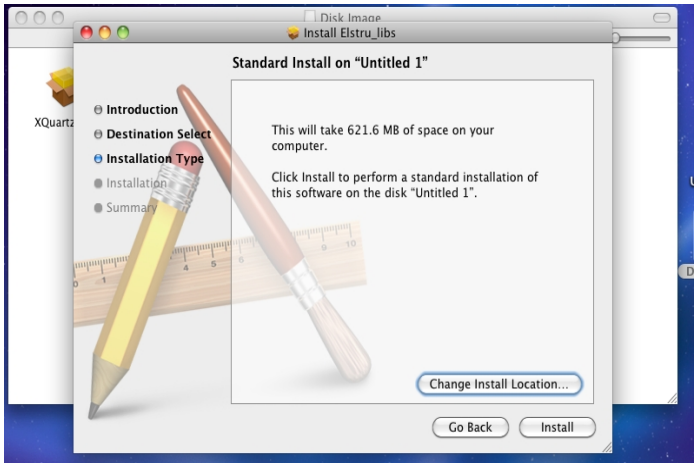
Select *"close"* to finish the installation.
To make Xquartz available you have to restart your computer. When you logon in the first time after the restart, start-up Xquartz manually. It is in the folder : Applications->Utilities. When this is done Xquartz will startup automatically whenever it is needed (also after restart of the machine)

1.2 Installation of Elstru libraries

Skip the installation of the libraries in this paragraph if you recently used MacPorts to install the following packages in /opt/local:

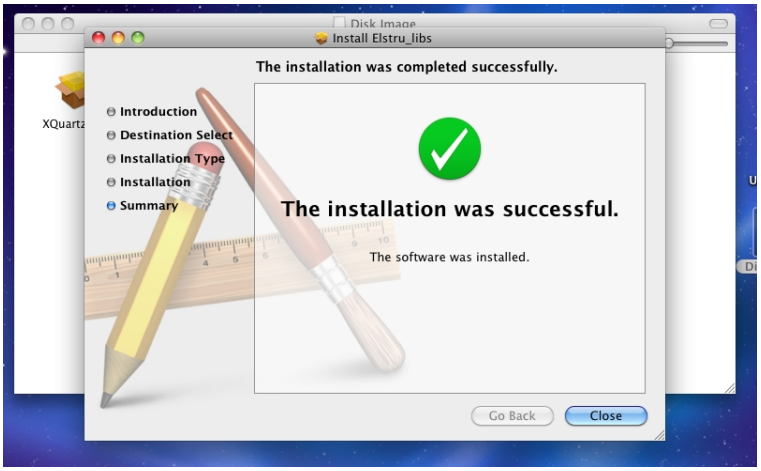
- gtk2
- freetype
- freeglut
- fftw-3
- ImageMagick

To install the libraries *"double click"* on Elstru_libs.pkg and select *"continue"* on the window that pops-up.



Select *"install"* and give username/Password information of am account with administrator-rights in the window that pops-up. Wait for several minutes to let the procedure copy all the files to the destination.

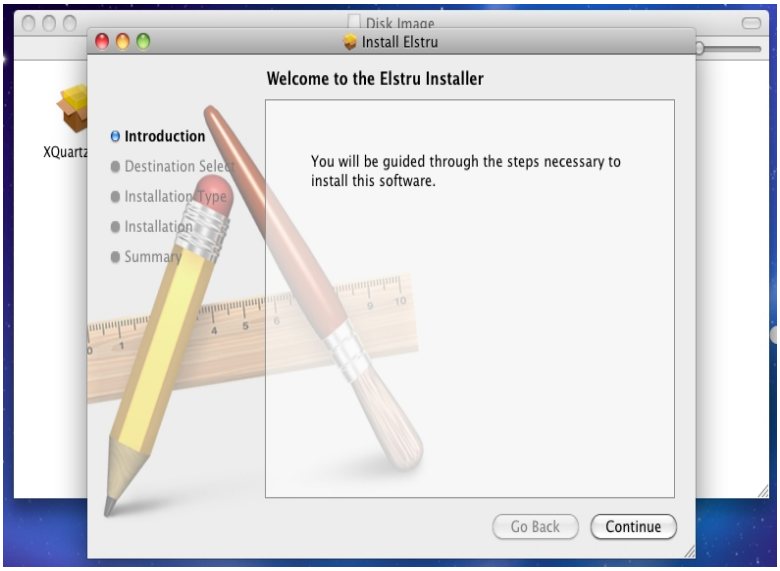
When it is finished it shows the following window.



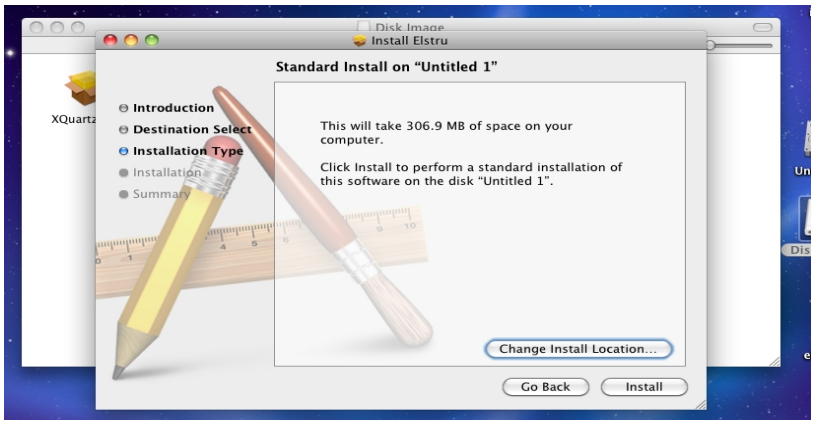
Select *"close"* to finish the installation.

1.3 Installation of Elstru application

To install the applications *"double click"* on Elstru.pkg

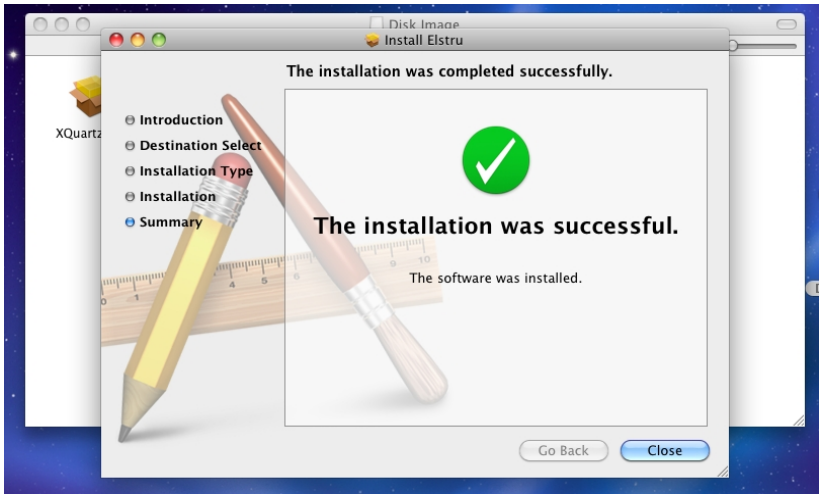


Select *"Continue"*



Select *"install"* and give username/Password information of am account with administrator-rights in the window that pops-up. Wait for several minutes to let the procedure copy all the files to the destination.

When it is finished it shows the following window.

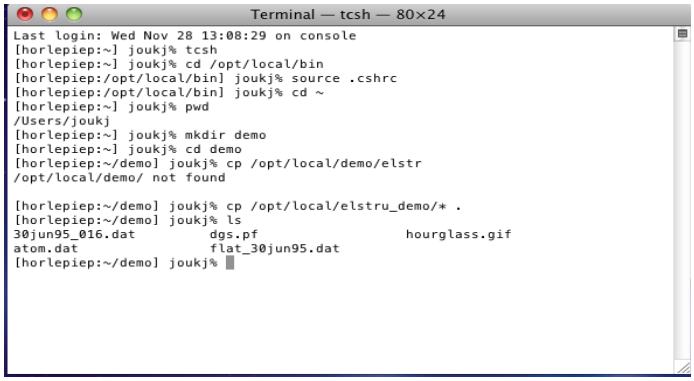


Select *"close"* to finish the installation.

2. Testing the installation

Open a Terminal (it is an application in Applications->Utilities). The following set of commands will set-up the Elstru software and copy the *"demonstration-files"* to a folder demo in the users home-folder:

```
tcsh
cd /opt/local/bin
source .cshrc
cd ~
mkdir demo
cd demo
cp /opt/local/elstru_demo/* ./
ls
```



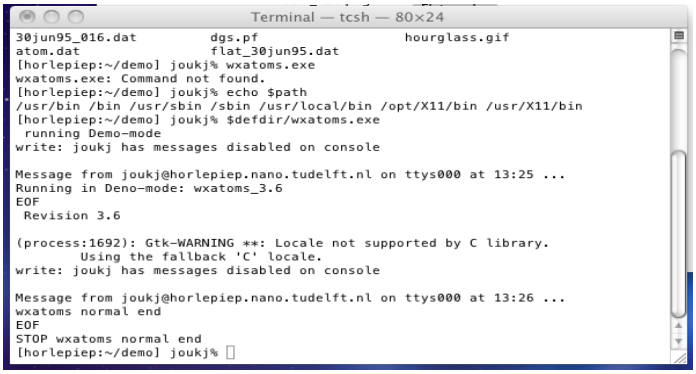
The current default folder (demo) contains five files:

30jun95_016.dat	: a diffraction pattern of the [001] zone of $Ce_5Cu_{19}P_{12}$
dgs..pf	: general parameter file for Elstru
hourglass.tiff	: artwork for Elstru
atom.dat	: File containing the atomic parameters of $Ce_5Cu_{19}P_{12}$
flat_30jun95.dat	: Flatfield for the CCD which was used to record 30jun95_016.dat

To run the first program type the following command in the terminal window

```
$defdir/wxatoms.exe
```

Ignore messages like



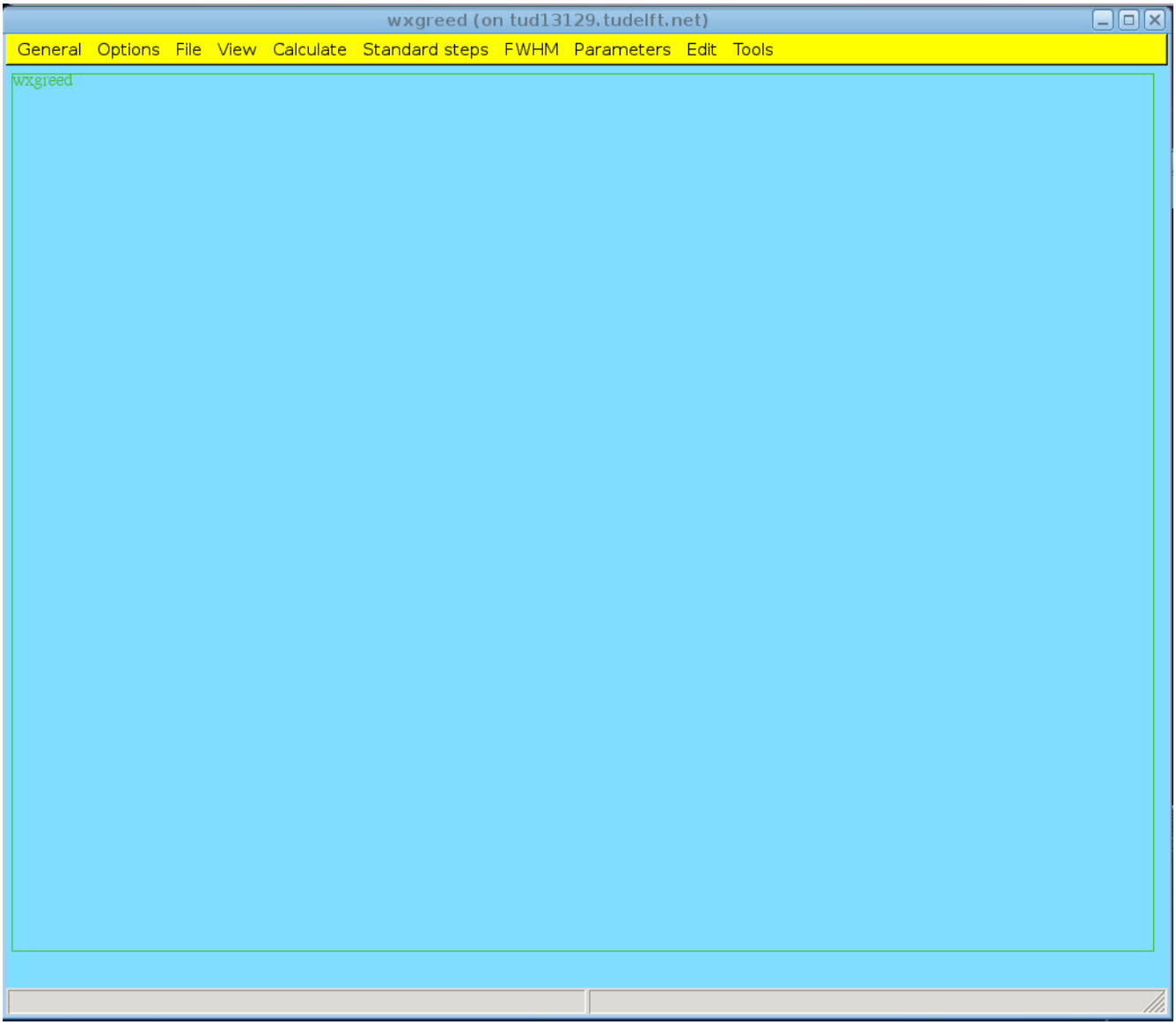
The following window should appear.

wxatoms is the atomic parameter editing program for Elstru. For the demonstration everything is filled in correctly. By selecting *"general->exit"* from the top-menu you can leave the program

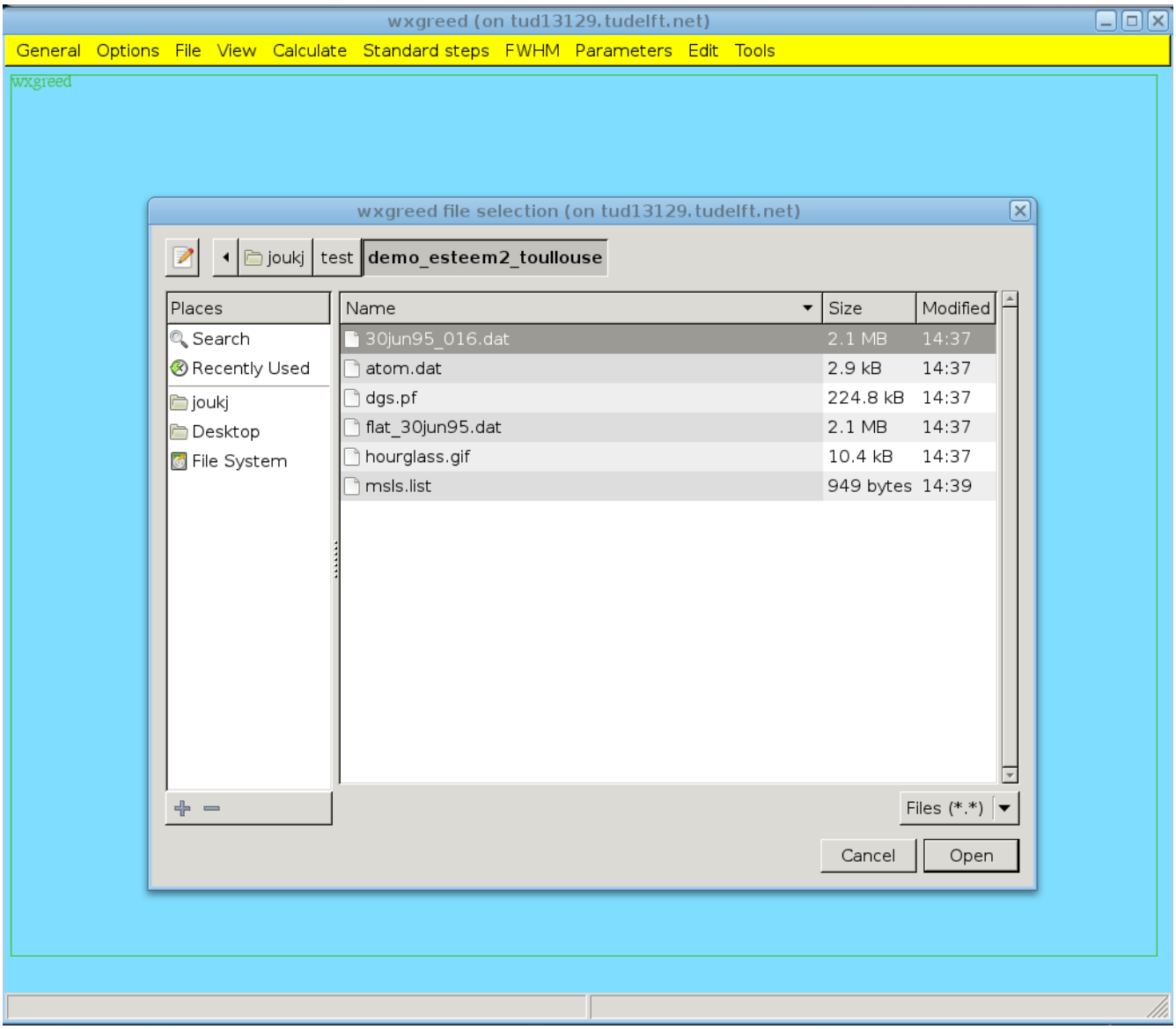
The next program to run is the data reduction program (greed=Graphical REduction of Electron Diffractiondata). Type the following command in the terminal window

$defdir/wxgreed.exe

The following window should appear.

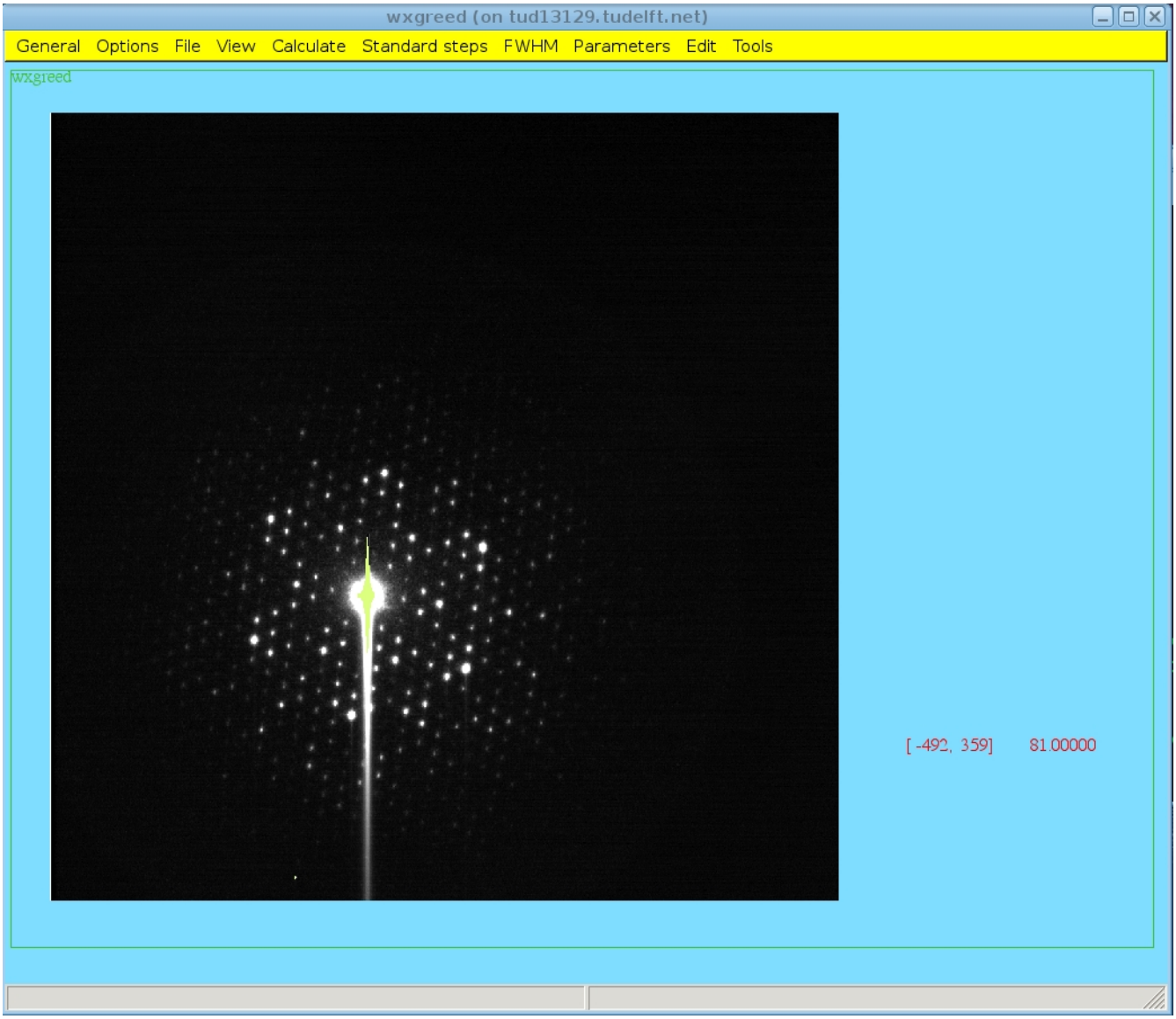


To open the data-file, select “File->Open file” from the menu bar. A file-selection window should pop-up.



Select the file “30jun95_016.dat” and click on “Open”

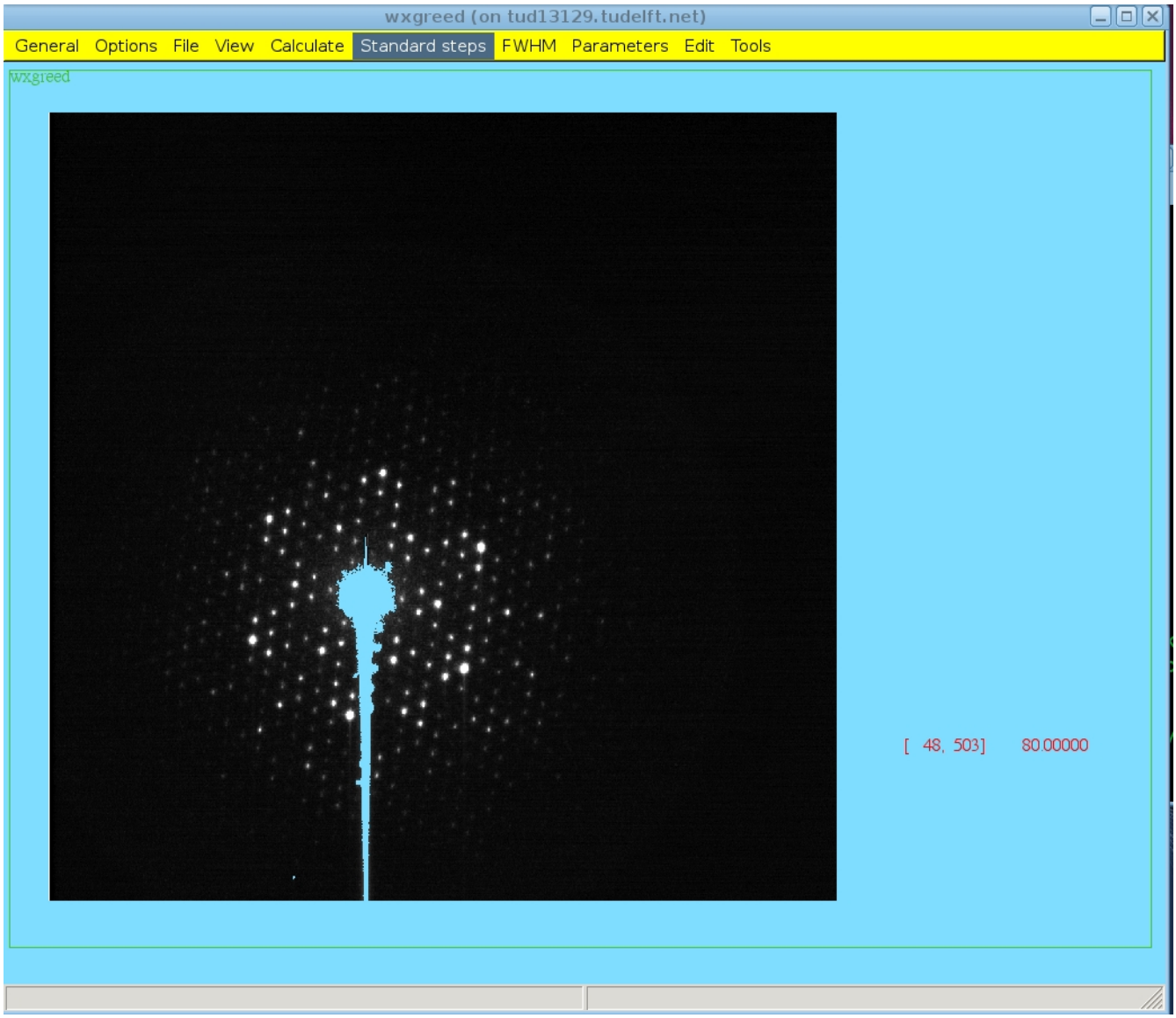
The diffraction patterns should be displayed. This image is taken using an old CCD-camera with no ant-blooming capability. The yellow areas are overexposed and contain no reliable pixel intensities.



Select “Standard Steps->All Steps” from the menu-bar. The following steps will be performed successively:

-Determination of the position of the central beam (origin). This position is marked by a blue cross.

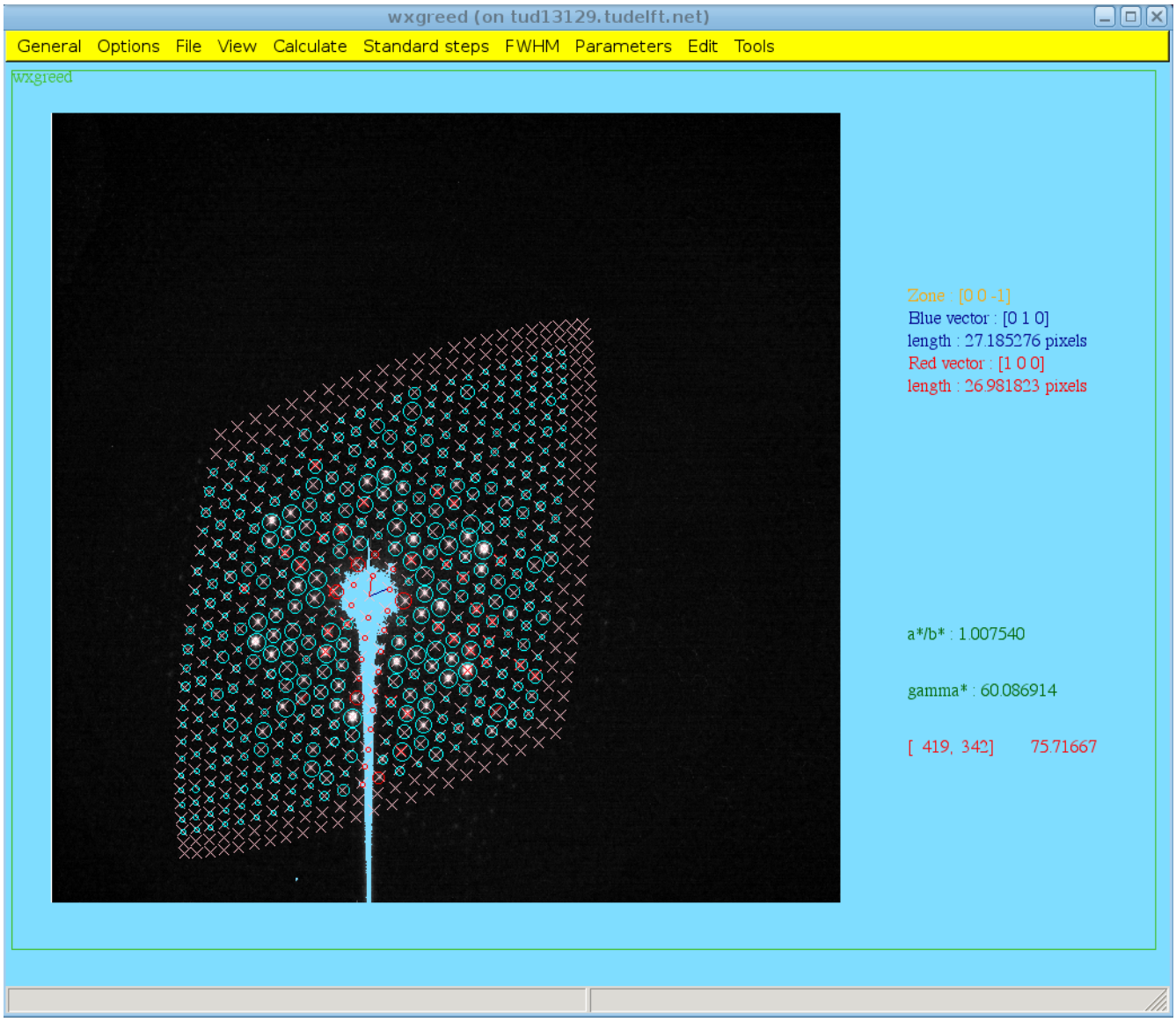
-Determination of the areas which are not to be used, i.e. Due to blooming or over-saturation. These areas are marked blue.



-Correction for the different sensitivity of each pixel on the CCD-chip (Flatfield-correction)
-Search for significant peaks. The are marked by red crosses

-Indexing the peaks. This means that the 2 spanning vectors of the zone (and some correction terms are determined, The vectors are marked red and blue. Than all locations where reflections are expected are marked with pink crosses. For a successful indexing for red cross (found peak) a pink cross should be at the same position. A guess for the actual zone-orientation is given at the right-hand site of the diffraction pattern.

-Determine the integrated indexed intensities by putting blue circles around each reflection position. The integrated intensity is the sum of the intensities of the pixels inside a circle corrected for the background using the pixels on the circles. Reflections in red circles are ignored because they contain pixels in excluded regions of the CCD.



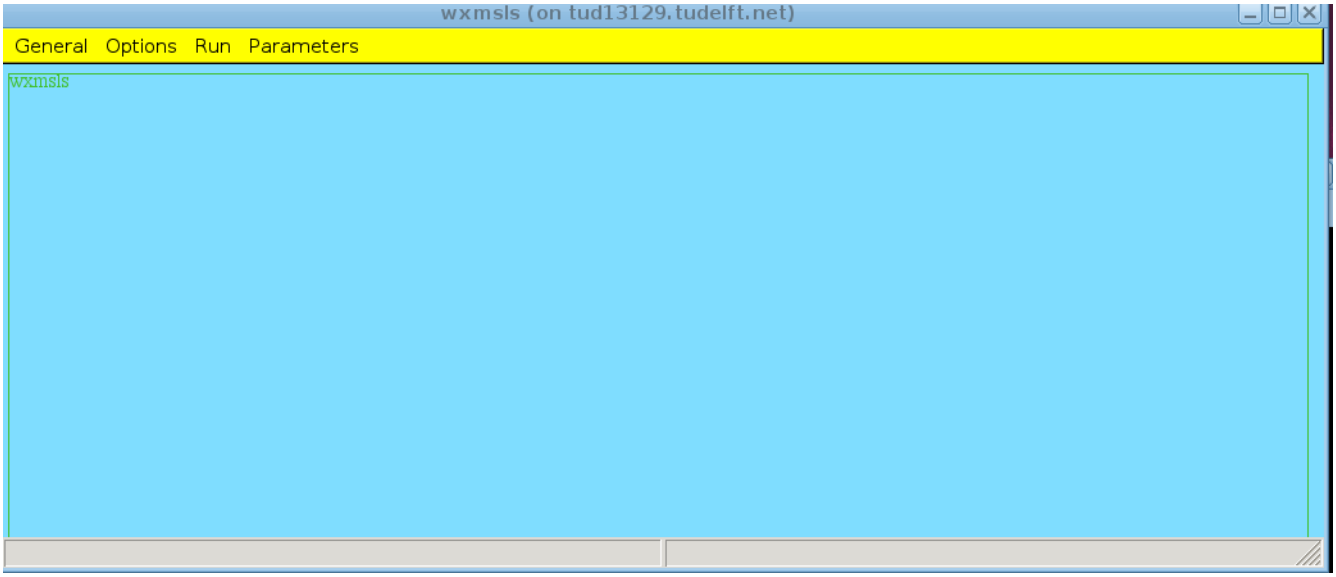
The most important file the program created is call 30jun95_016.ii and contains the indexed integrated intensities.

By selecting *"general->exit"* from the top-menu you can leave the program.

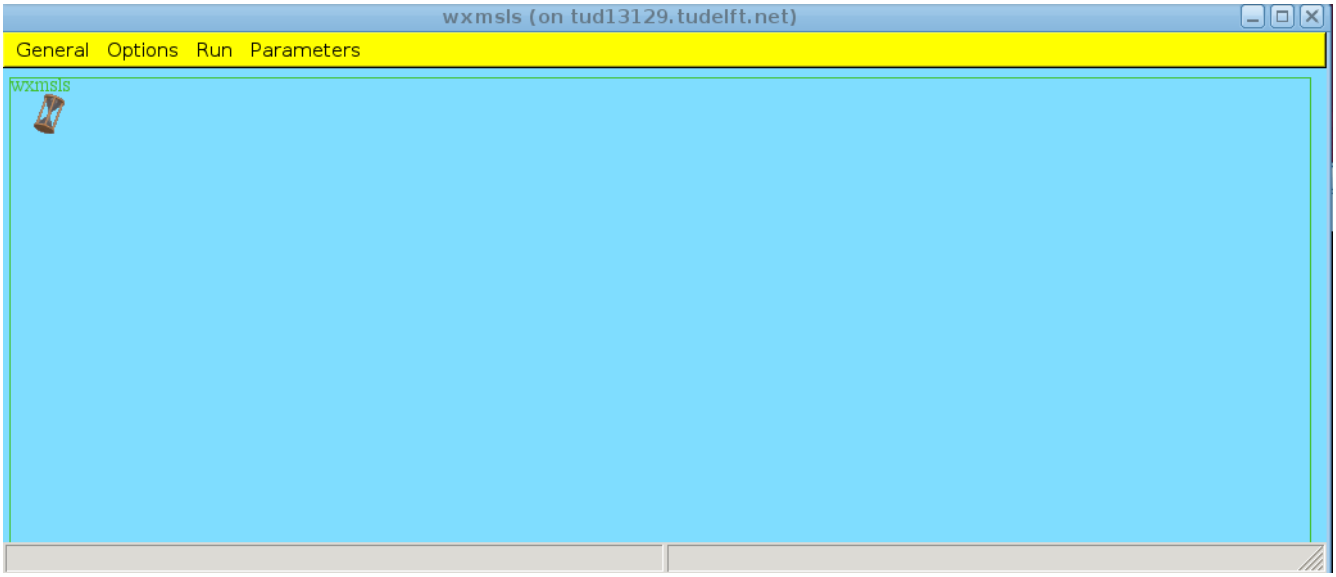
The final program to test is the Least-Squares-Multi-Slice (MSLS) refinement program. To start the program type the following command in the terminal window

$defdir/wxmsls.exe

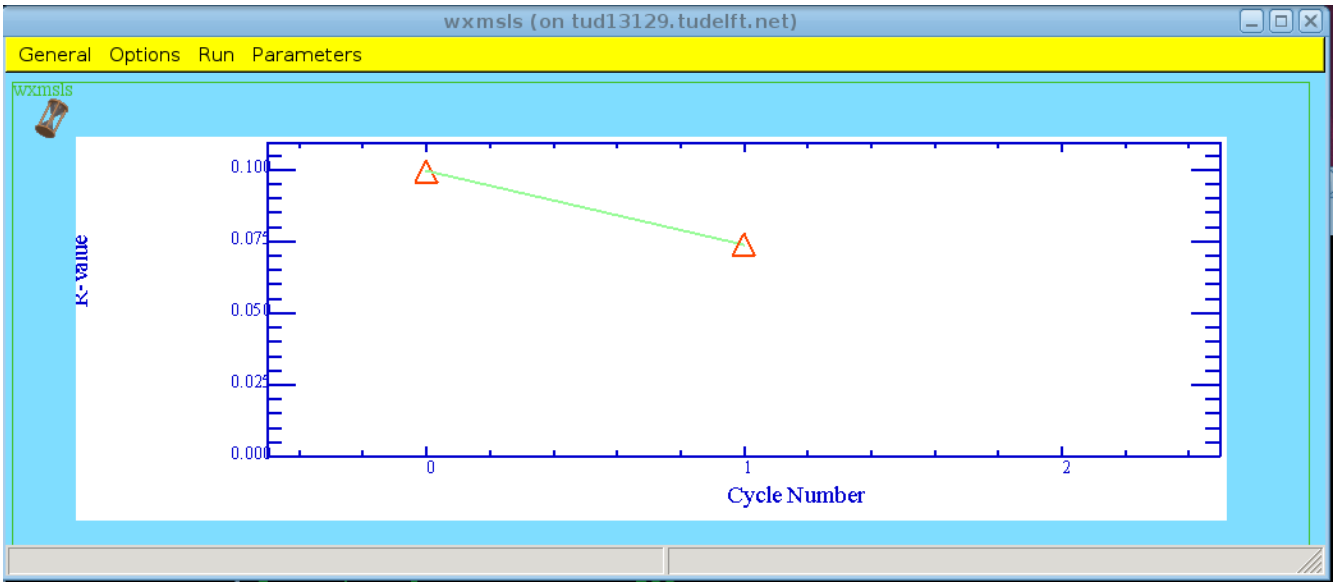
The following window pops-up.



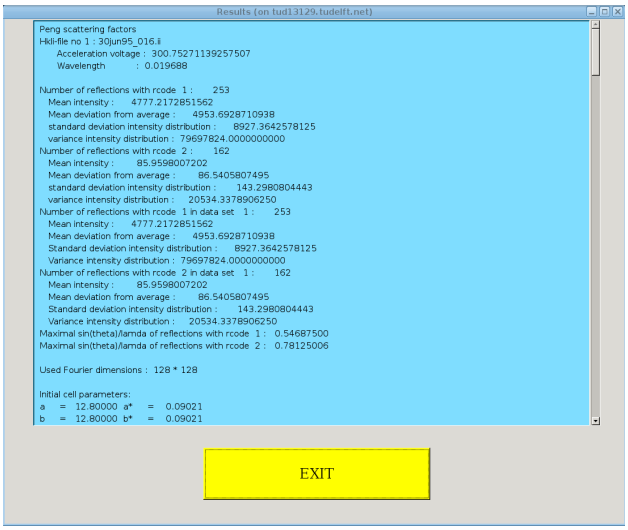
For the testing all parameters are already set to their correct values. So we can start running immediately by selecting “Run->Run MSLS” from the menu bar. An hourglass will tell you that a calculation is in progress.

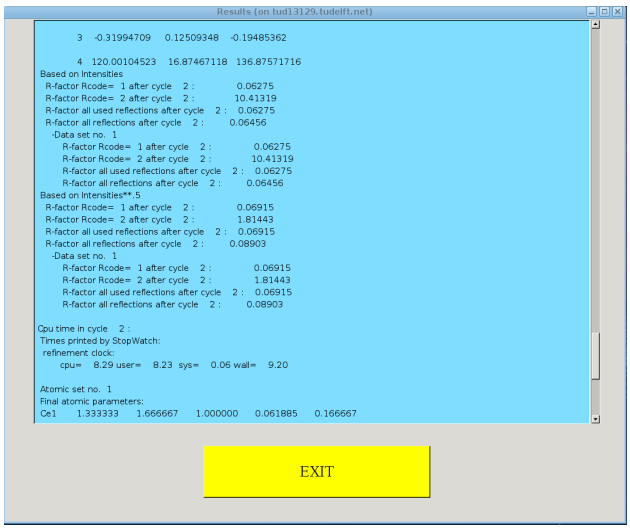


When the first R-values are calculated a graph will appear showing the current status of the R-value.

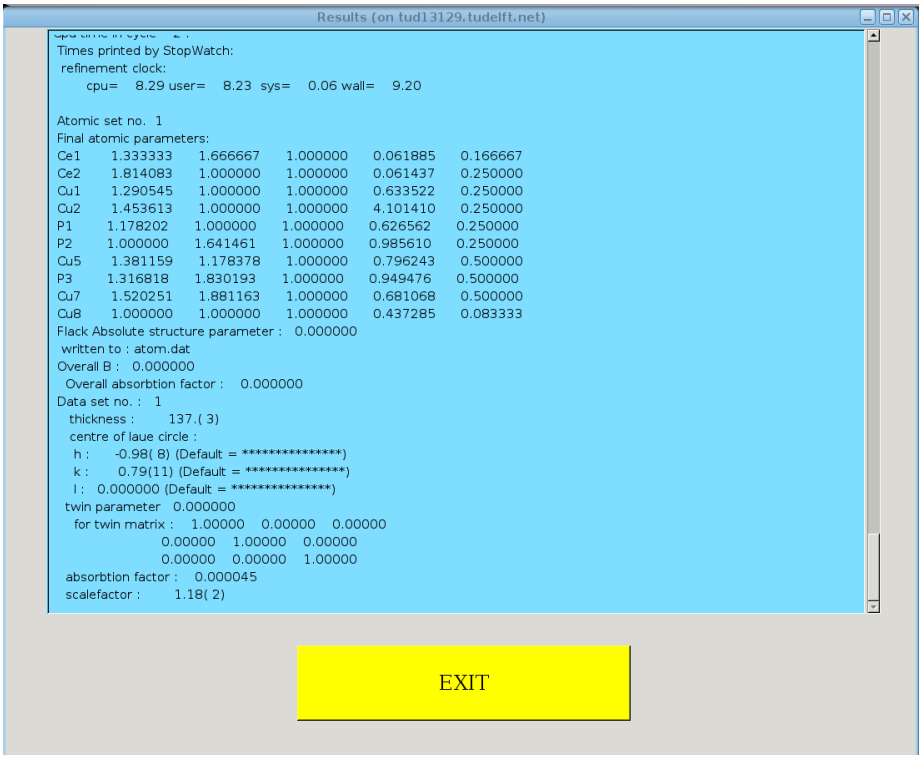


The plot is updated for each refinement cycle. When the refinement is finished a window containing the results pops-up.

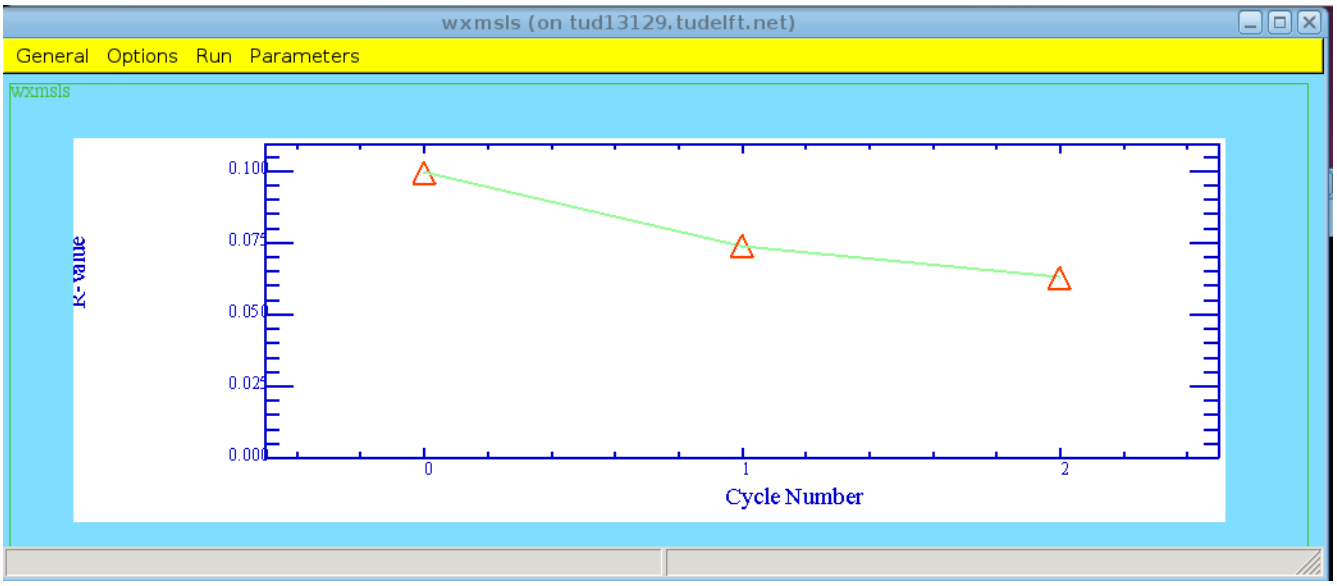




Check now that the values for the crystal thickness, Centre of Lau-circle and scalefactor are close to the values displayed in the sample window below.



Close the window by pressing the “EXIT” button. Check now that the R-value graph is similar to the one displayed here.



Close the program by selecting “general->exit” from the menu bar.
If everything did run correctly, I can congratulate you with a working version of ELSTRU.

3. Obtain a license

Contact Jouk Jansen (joukj@hrem.nano.tudelft.nl) for the license conditions. Once you have a proper license you will be provided with a username/password which is coupled to your E-mail address.
Once you got the username/password you can generate your machine-dependent license file, nodelock, in the following way:

```
$ cd ~
$ mkdir tmp
$ cd tmp
$ cp /opt/local/bin/nodelock ./
$ $defdir/getlicenseinfo.txt
   Username : <fill in username>
   Password : <fill in password>
```

The program now send all the needed information to Delft (see the licinfo.txt file to see what is actually sent). Within a working day an E-mail should be returned containing a nodelock file. This file can be placed in one of the following locations:

/usr/lib/netls/conf/ (For an installation of all users on the machine)
~ (=the home directory of the user using ELSTRU)

Once yo have done this all the programs of the ELSTRU package should be functioning with all the available options.

4. asking questions and making remarks

The ELSTRU software and documentation improves by your comments. So, do not hesitate to ask what is not clear and make comments on what you (dis)like about the software and the documentation. Please, send your questions and remarks to Jouk Jansen (joukj@hrem.nano.tudelft.nl).