Chapter 1

PYXPCS users manual

1.1 System requirements

- Linux PC
- Python 2.6.2 or 2.6.4
- Numpy 1.2.1 or 1.3.0
- Scipy 0.7.0 or 0.7.1
- Matplotlib 0.98.5.1 or 0.99.1.1
- Pyqt3

1.2 Introduction

PYXPCS package is dedicated for calculating correlation functions from the series of 2 dimensional scattering spectra.

$$G(q,\tau) = \frac{\langle\langle I_p(t)I_p(t+\tau)\rangle_p\rangle_t}{\langle I_p(t)\rangle_{p,t}^2} \tag{1.1}$$

$$G(q,t,\tau) = \frac{\langle I_p(t)I_p(t+\tau)\rangle_p}{\langle I_p(t)\rangle_p\langle I_p(t+\tau)\rangle_p} \tag{1.2}$$

The normalised time average intensity correlation $G(q,\tau)$ Eq.1.1 is calculated with multiple-tau and symmetrical normalisation scheme. The time resolved correlation function $G(q,t,\tau)$ Eq.1.2 is calculated only for the first 10000 images due to the memory limitations.

The variance of the $G(q,t,\tau)$ is calculated like:

$$\chi(q,\tau) = \langle G^2(q,t,\tau)\rangle_t - \langle G(q,t,\tau)\rangle_t^2 \tag{1.3}$$

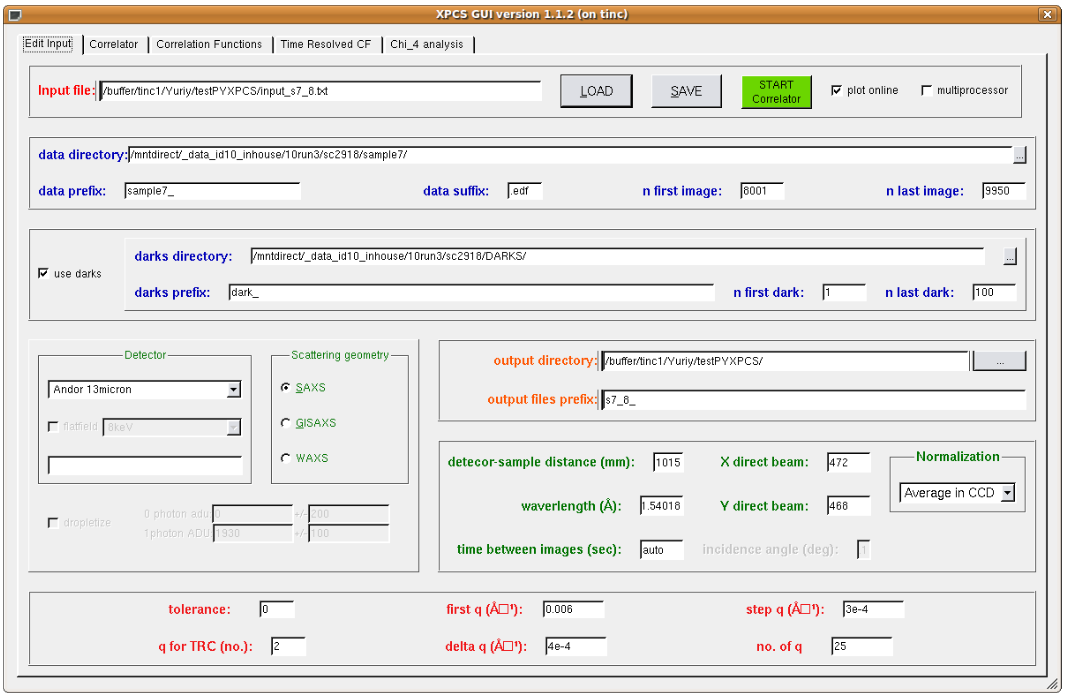

Figure 1.1: Main window.

1.3 Getting started

The program can be started from terminal by typing PYXPCS. If you use it at you work machine you need to run mygui.py from /mutlitau_new directory. The window Fig.1.1 will appear on the screen. The first step is to define all input parameters necessary for the program to run. For this you need to feel the form on the **Edit Input** tab. The parameters have to be saved into the input file. You can also load already existing input file by pressing the button **Load** or by providing the input file in the terminal for example PYXPCS /buffer/tinc1/Yuriy/testPYXPCS/input_s7_8.txt at the start up.

1.4 Calculating correlation functions

Once the input parameters are defined and saved to the input file you can proceed to analysis of the data taken. Switch to the tab **Correlator**. First of all you need to produce a dark image by pressing **Make Dark** button. The resulting dark image will be saved to the file indicated in the field **dark file:**. After a static scattering pattern have to be calculated. For this press the button **Make Quick Static**. The program will read first 20 images and produces an average image Fig.1.2. It is saved to the file in the field **static data file:**. The static image is used to make the mask. Press the button **Make Mask**. The extra window will be opened Fig.1.3. Select a range of interest (ROI) by clicking on the image. If you want to mask this ROI press **m**, to unmask ROI press **u**. When you finish press **w** to save the mask then press enter in the terminal to exit. The masked image will be drawn Fig.1.4. The mask file is saved to the file in the field **mask file:**. If you want to use a different mask or dark image you can load them by pressing the right putton after the field. Now it is reasonable to produce iso-Q region for the calculation. For this just press the button **Make Qs**. The iso-Q regions will be visible on the figure Fig.1.5. You can modify the iso-Q regions according to your need by playing with the parameters at the top right corner. Press the button **Make Qs** to recalculate the iso-Q regions. You can see the radial average of the 2D static image by using the button **Show I(q)**. The red dots show the center of each iso-Q region while the blue curve is the radial average of the intensity Fig.1.6. When the mask is produced and the iso-Q region is defined you can press the button **Start correlator** to beging the calculation. An extra window will be opened Fig.1.7. This window displays the current correlation function and the trace for the 2 selected Q regions. When the calculation is finished the extra window is closed automatically. To see the results of the calculation use the tabs **Correlation Functions** to see the $G(\tau)$ Fig.1.8, **Time Resolved CF** to see the $G(t, \tau)$ Fig.1.9 and **Chi_4 analysis** to see the χ_4 function Fig.1.10. The $G(t, \tau)$ and χ_4 functions are calculated only if the parameter **q for TRC (no.)** is valid number of the iso-Q region. In the tab **Correlation Functions** you can define **q number** that you want to display and press **PLOT**. This field also accepts the following keys **all** to plot the correlation functions for all Qs, **1:15** to plot only the correlation functions from 1 till 15. Any correlation function can be removed from the graph by pressing the button **REMOVE**

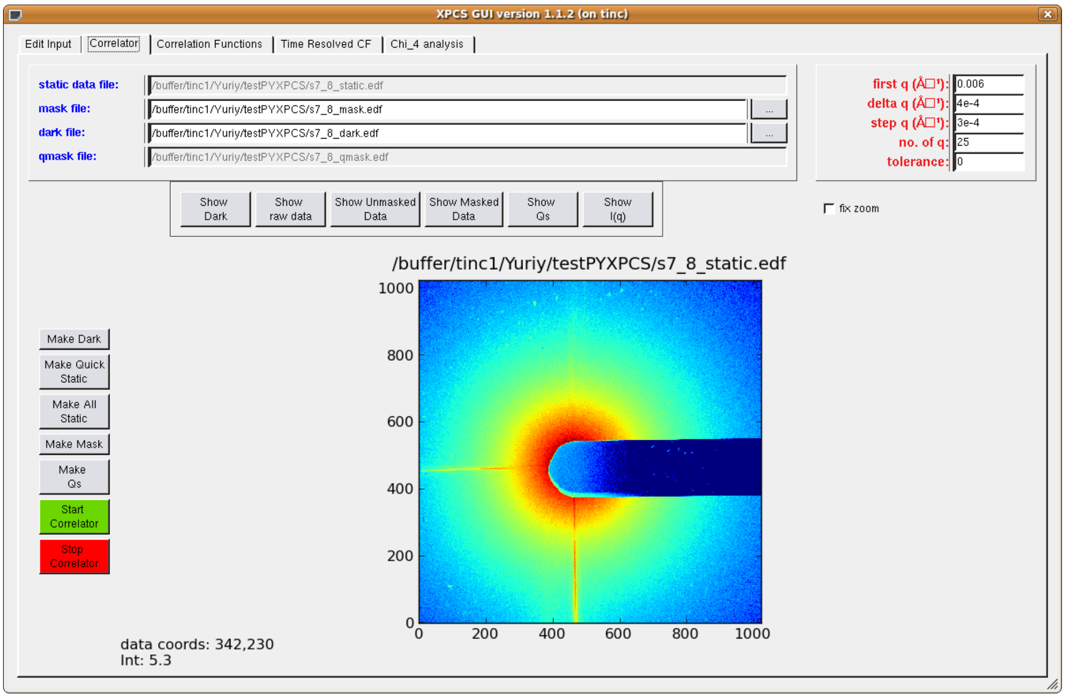

Figure 1.2: Static image.

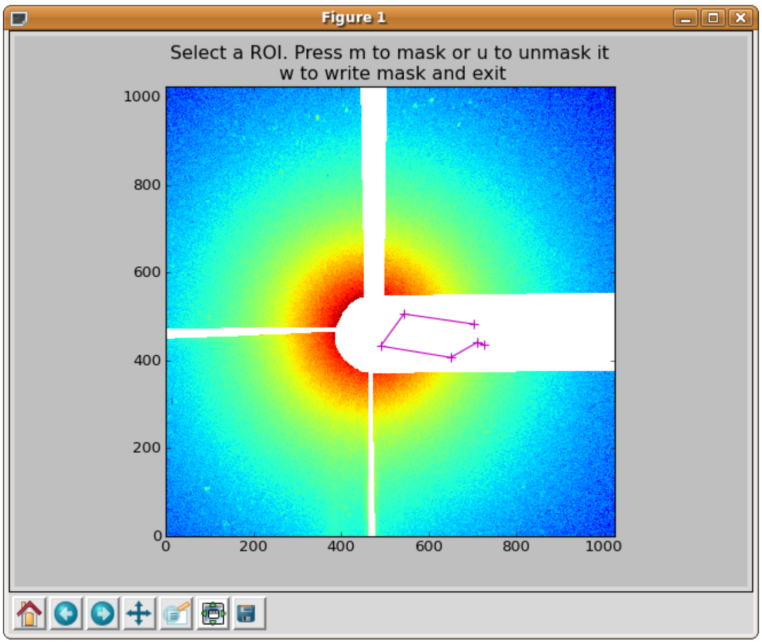

Figure 1.3: Masking window.

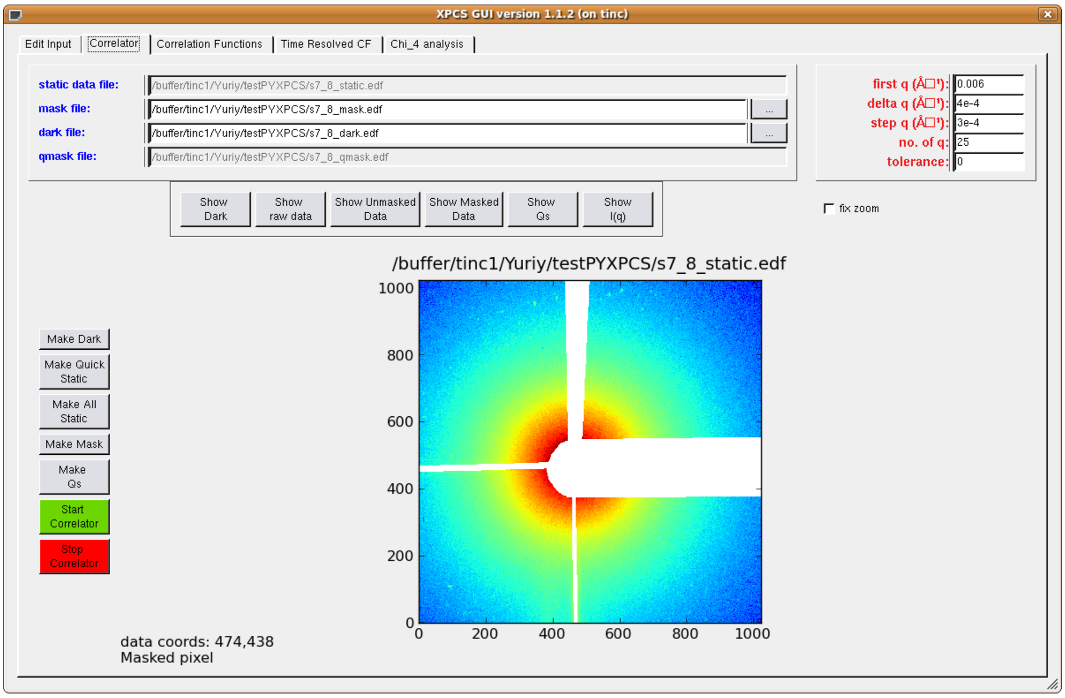

Figure 1.4: Masked image.

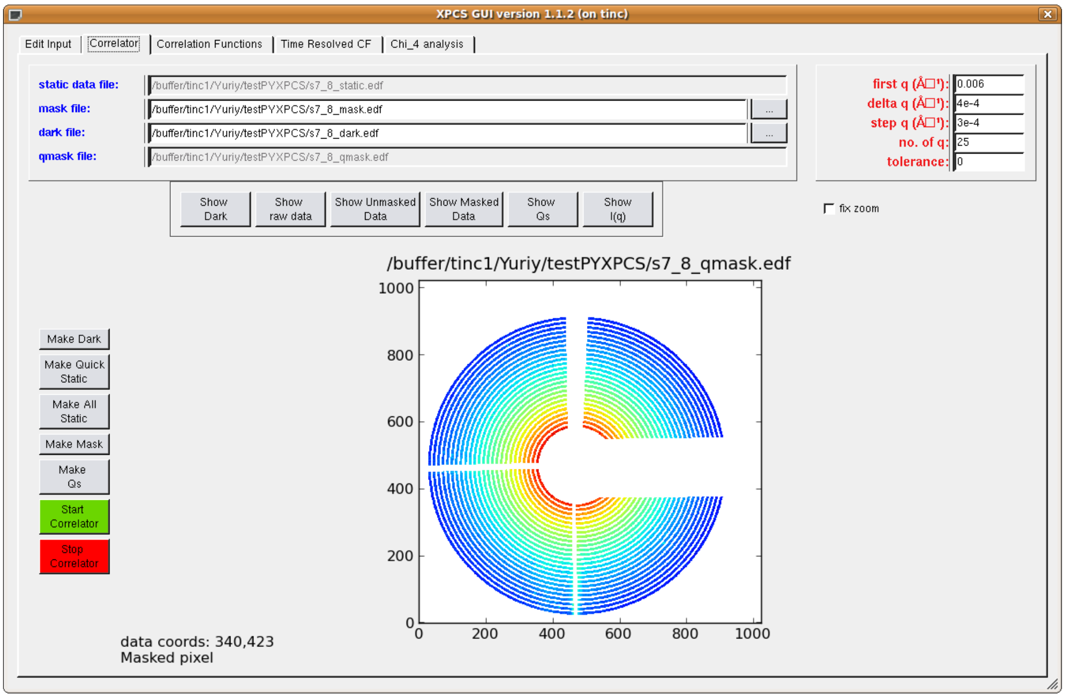

Figure 1.5: Iso Q regions.

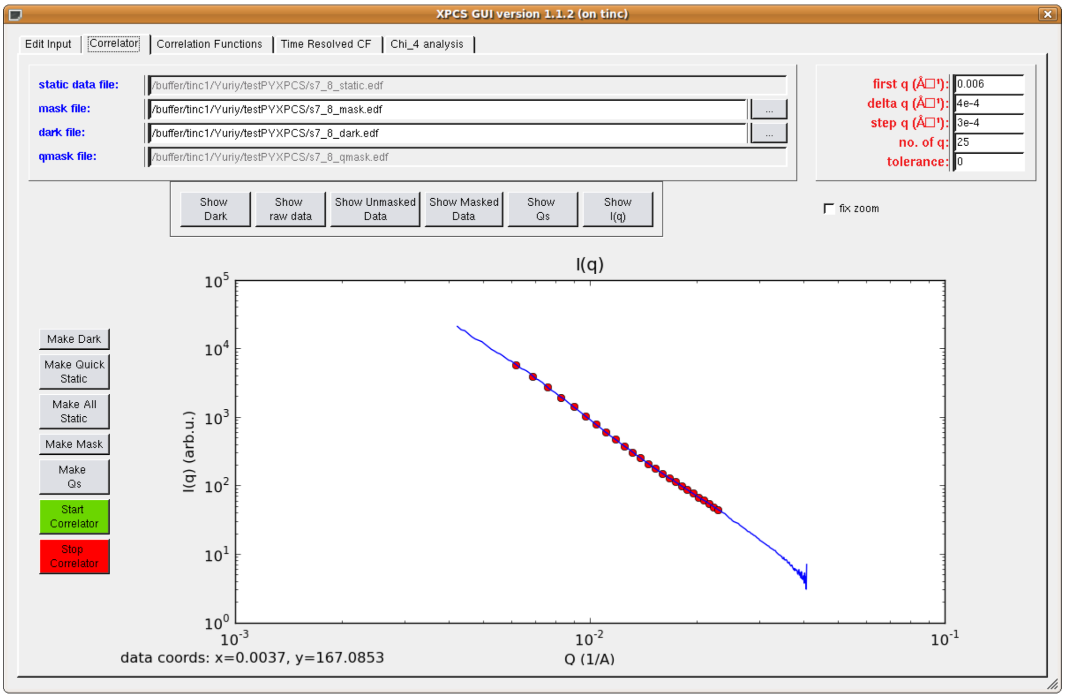

Figure 1.6: Radial average intensity.

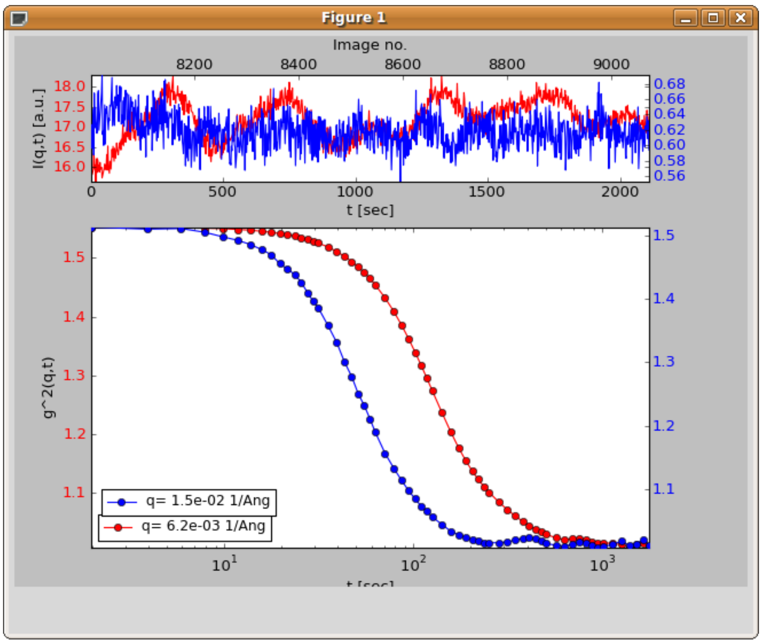

Figure 1.7: Current correlation function.

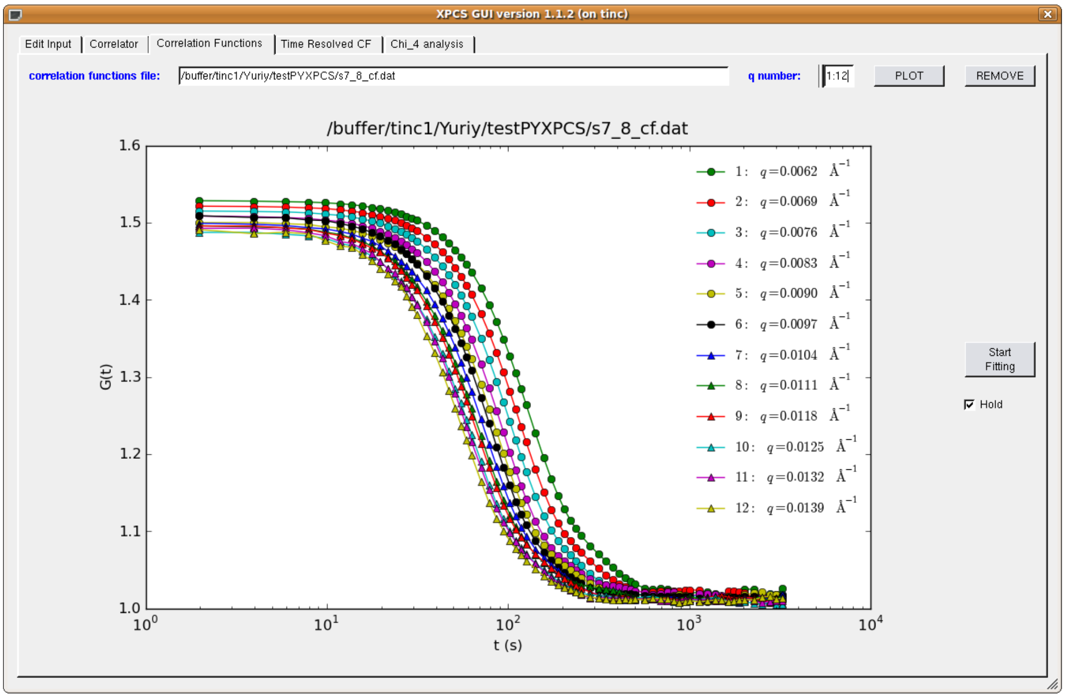

Figure 1.8: Correlation functions.

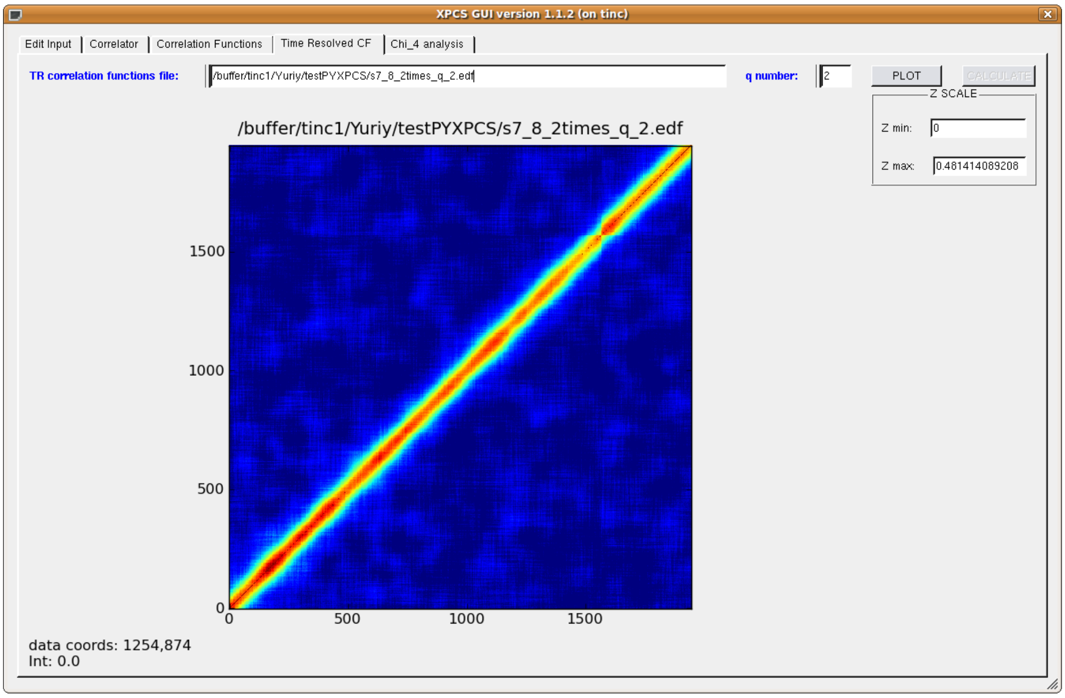

Figure 1.9: Time resolved correlation function.

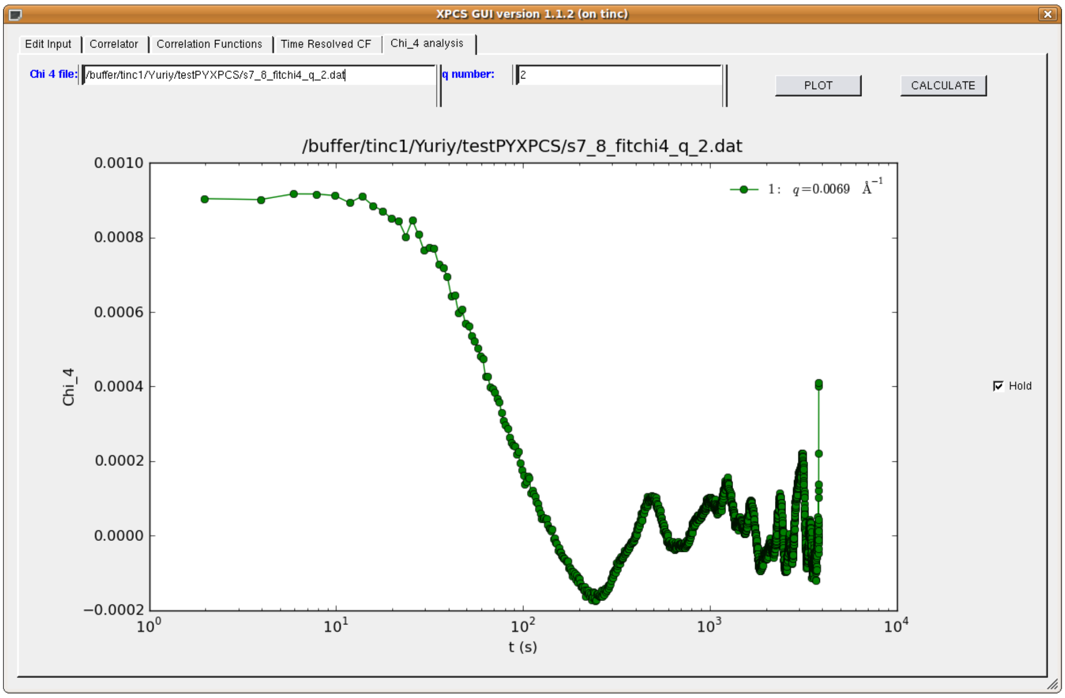

Figure 1.10: Variance $\chi(q, \tau)$ of $G(q, t, \tau)$.