



# Lookup program for the instrumental resolution function of beamline P02.1

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## Abstract

The Instrumental Resolution Function of the P02.1 beamline was investigated. The measurements were done on a set of  $\text{LaB}_6$  and  $\text{CeO}_2$  *standard* samples at different *thicknesses* (0.5, 1, 1.5 and 2 mm), at various *sample-to-detector distances* (SDD, 380 - 1380 mm with 50 mm steps) and different *beam-sizes* (square cross section, side lengths 0.2, 0.5, 1, 1.2 mm). Program *IRF P02.1 lookup* for the retrieval of the instrumental resolution function was created. User can input desired experimental parameters, and the program then returns the plot of the experimental *full width at half maximum* (FWHM) as a *Caglioti function of the diffraction angle*, its parameters and the experimental points used in its fitting. If the user input parameters differ from the parameters of realized measurements, the program calculates an interpolated resolution function as an average of several nearby datasets. If the user enters the *number of a peak* instead of the sample-to-detector distance, the program looks up the FWHMs at every distance measured, of said peak. In every case, the resulting figure is exported as a *\*.pdf file* into folder “figures” and its name contains all the input parameters.

# Contents

<b>1</b>	<b>Introduction</b>	<b>3</b>
<b>2</b>	<b>Goals</b>	<b>3</b>
<b>3</b>	<b>Experimental part</b>	<b>4</b>
<b>4</b>	<b>Results, discussion</b>	<b>9</b>
<b>5</b>	<b>Attachments</b>	<b>13</b>

# 1 Introduction

X-ray diffraction (XRD) and its variations is a crucial method employed widely in condensed matter physics, biophysics, medicine and nanoscience. Between 1958 and 1962, Caglioti, Paoletti and Ricci published three fundamental papers describing the derivation of analytical expressions for the *instrumental resolution function* (IRF) of monocrystal and powder neutron diffractometers, using the Gaussian approximation [1, 2, 3]. Several other studies have been devoted to the determination of the instrumental resolution and profile shape functions [4, 5, 6, 7, 8, 9, 10, 11].

The Caglioti method is used to fit the dependence of FWHM on the diffraction angle, for the given set of experimental parameters. It changes with photon energy, beam size, thickness of the sample and the SDD. For the beamline P02.1, the photon energy is *fixed at 60 keV*. Thus, only three degrees of freedom remain.

## 2 Goals

My task is to create a program where the user can input the experimental parameters:

- standard
- sample thickness
- beam size
- sample-to-detector distance.

The program then returns:

- plot of experimentally acquired FWHMs
- plot of the instrumental resolution function given by the Caglioti formula
- the parameters of the fitted function.
- when input parameters are different from the experimental, an interpolated Caglioti resolution function using several nearby datasets.

Alternatively, instead of the SDD, the user can input the number of a peak (0–9) and the program then returns the FWHMs of this peak for all measured distances. Finally, export the figures as \*.pdf images.

### 3 Experimental part

The XRD standards  $\text{LaB}_6$  and  $\text{CeO}_2$  were prepared for the purpose of measurement in the form of samples in the photograph, the figure 1. They are also schematically shown from the side in the figure 2. The figure 3 shows the bottle containing the standard  $\text{CeO}_2$ .  $\text{LaB}_6$  was also originally in the form of a bottled powder of violet color, but at the time of writing this report the  $\text{LaB}_6$  bottle was no longer available.

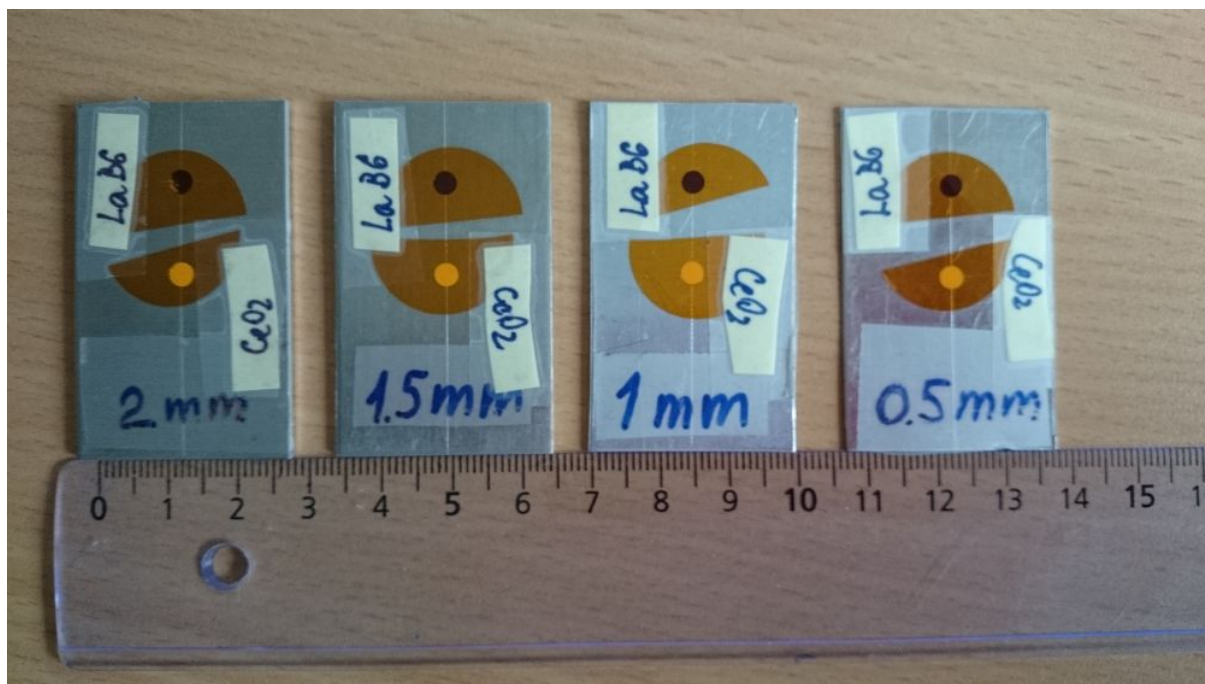


Figure 1: Photograph of the real samples. Each strip of Al contained both the  $\text{LaB}_6$  and  $\text{CeO}_2$  standard, and had its given thickness from 0.5 mm to 2 mm in 0.5 mm steps. The powders are covered from both sides by kapton (polyimide) tape. The units of the ruler in the bottom are centimeters, for comparison.

The experiments were carried out using the experimental setup schematically represented in the figure 4. The figure 5 shows an actual photograph of the beamline.

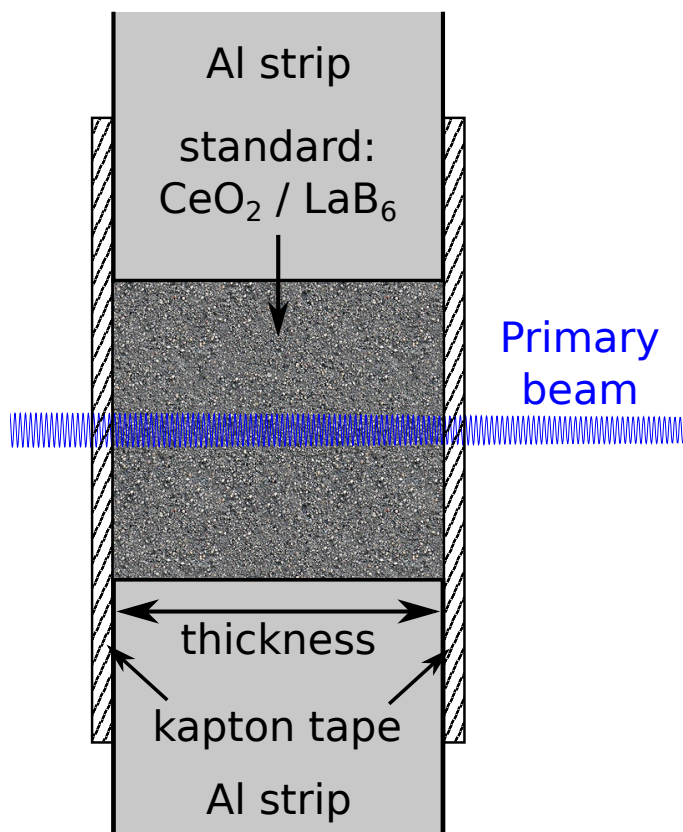


Figure 2: Schematic representation of the used samples, side view. An aluminium strip with a drilled hole filled with the standard material powder. The hole was sealed from both sides by a kapton tape.

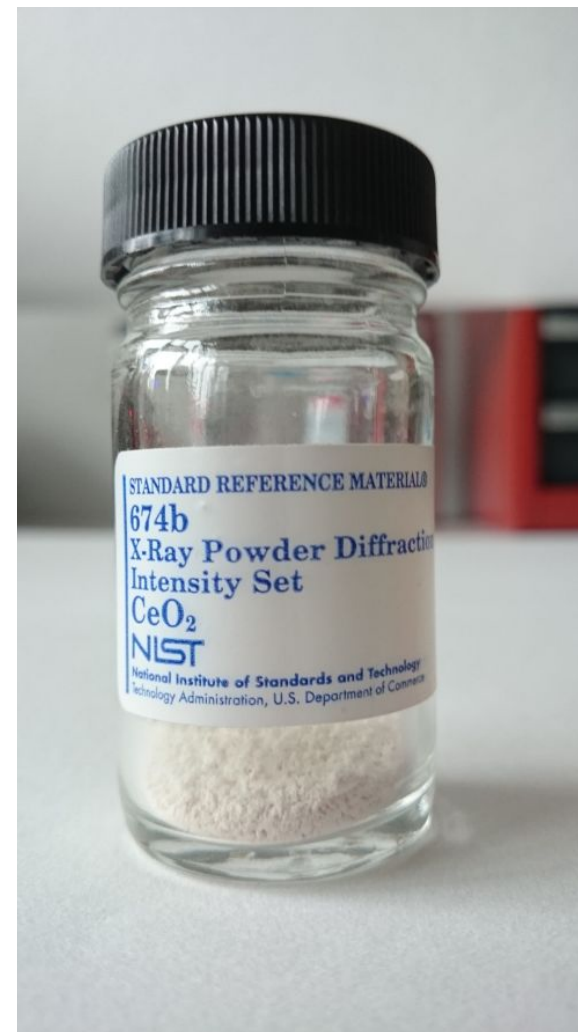


Figure 3: Bottle of the standard  $\text{CeO}_2$  used in creation of the sample.

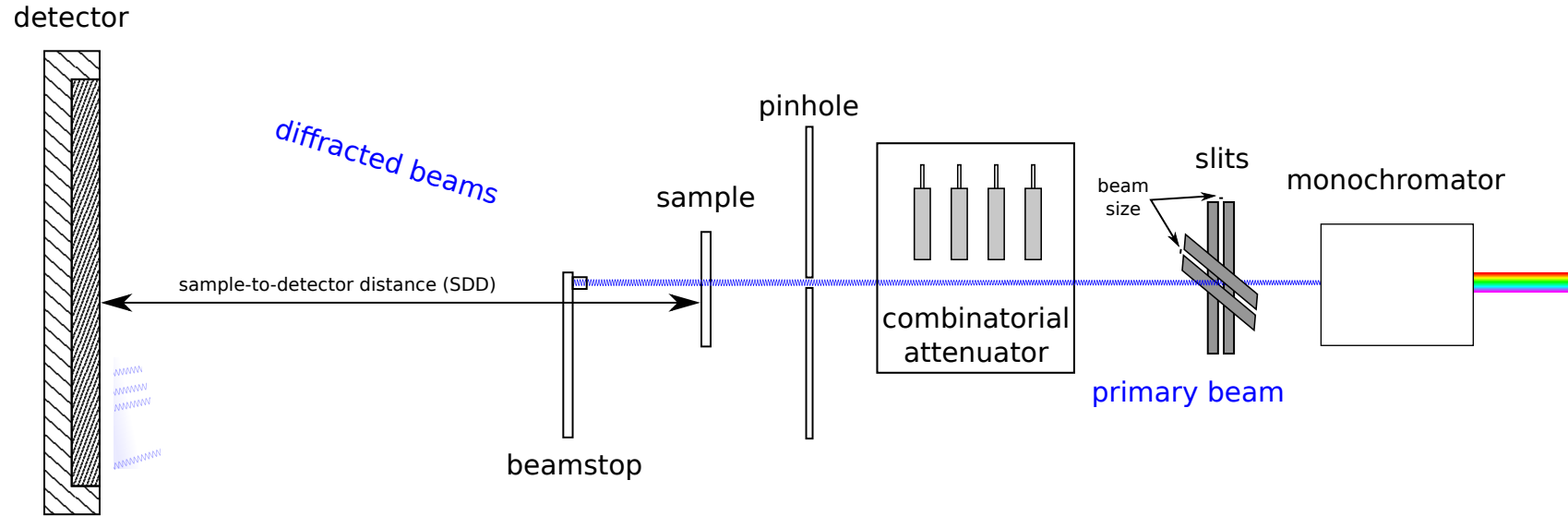


Figure 4: Schematical representation of the experimental geometry used in gathering the diffraction data. After the primary beam passes the monochromator of the P02.1 beamline in PETRA III, its photon energy is fixed at 60 keV, corresponding to the wavelength of 0.2066 Å. The beam then goes through slits, combinatorial attenuator, pinholes and finally the sample. The direct beam is then dumped into a beamstop. The diffracted beam is recorded by a detector. Slits set the beam size and pinholes reduce the air-scattered photon background. The measurements were done at sample-to-detector distances 382–1382 mm with 50 mm steps, and beamsizes 0.2 mm, 0.5 mm, 1 mm and 1.2 mm. The free cross-section of the slits was always a square.

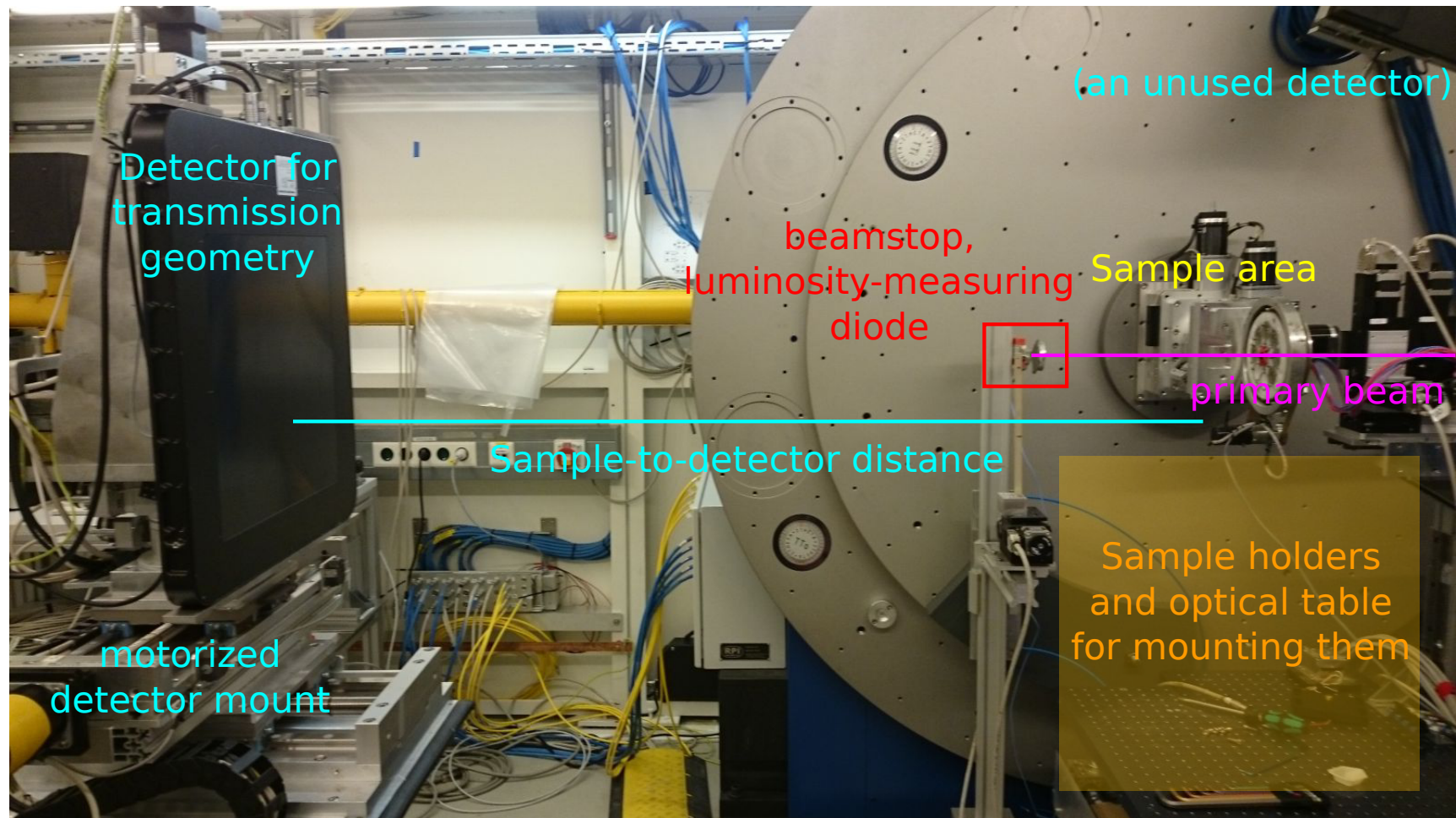


Figure 5: Photograph of the P02.1 beamline. The measurements were done at sample-to-detector distances 382-1382 mm with steps of length 50 mm and beamsizes 0.2 mm, 0.5 mm, 1 mm, 1.2 mm.



The samples of thicknesses 0.5 mm, 1 mm, 1.5 mm and 2 mm were put in the way of the beam of the beamline P02.1, the vertical and horizontal slits being 0.2 mm, 0.5 mm, 1 mm and 1.2 mm apart. Diffractograms were measured at approximate distances 382 mm to 1382 mm, with steps 50 mm long. For each measurement, the distance was refined during fitting.

The set of all the combinations of the experimental parameters that I was provided with experimental data for can be thus written as (dataset parameters, DSP)

$$\begin{aligned} DSP &= STD \times TH \times BS \times DIST \\ &= \{\text{CeO}_2, \text{LaB}_6\} \times \{0.5, 1, 1.5, 2\} \times \{0.2, 0.5, 1, 1.2\} \times \{382, 432, \dots, 1382\}, \end{aligned}$$

where all the distances are in millimeters.



## 4 Results, discussion

I managed to create a program that fulfills all the criteria in the Goals section 2. After receiving the input parameters from the user, the program finds the experiment the parameters of which are the closest, and plots both the experimental FWHMs and the fitted Caglioti function for that experiment. Figures with screenshots follow.

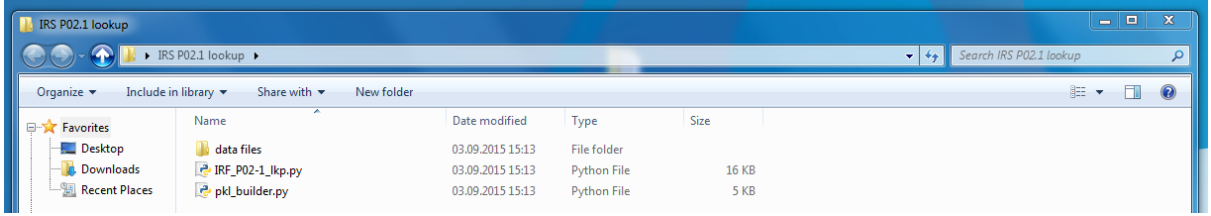


Figure 6: The program directory before running anything. Run “pkl\_builder.py” to create three \*.pkl files. These are three nested list objects that “IRF\_P02-1\_lkp.py” will need to read at each runtime. This step only needs to be done once.

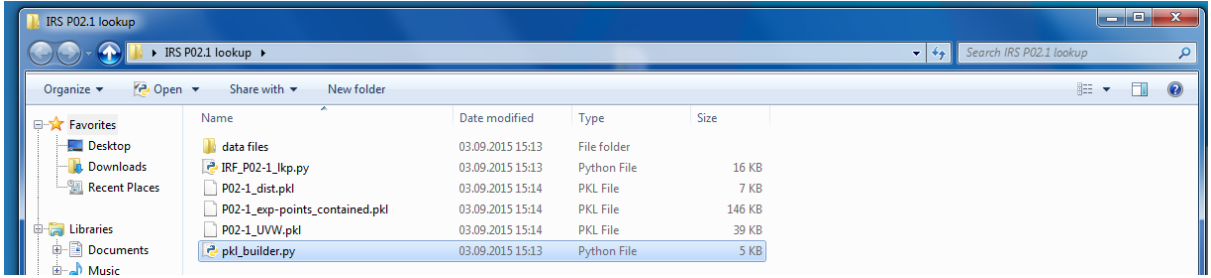


Figure 7: Now that the pickle files were created, it is possible to run “IRF\_P02-1\_lkp.py”. The folder named “data files” is no longer needed.

For cases when the user inputs experimental parameters between the actually measured values, the program calculates the interpolated Caglioti function. The interpolation is linear, and up to three-dimensional – in beam size, sample thickness and sample-to-detector distance. The logic and formula used are shown in the equations 1, 2 and the figure 10.  $f(\vec{0})$  is short for Caglioti function at the closest measured parameters,  $\vec{T}$  is the user input (target).  $\vec{A}$  stands for the measured parameters that differ in thickness,  $\vec{B}$  in beam size,  $\vec{C}$  in SDD.

$$\vec{T} = x\vec{A} + y\vec{B} + z\vec{C} \quad (1)$$

$$f(\vec{T}) \approx f(\vec{0}) + x[f(\vec{A}) - f(\vec{0})] + y[f(\vec{B}) - f(\vec{0})] + z[f(\vec{C}) - f(\vec{0})] \quad (2)$$

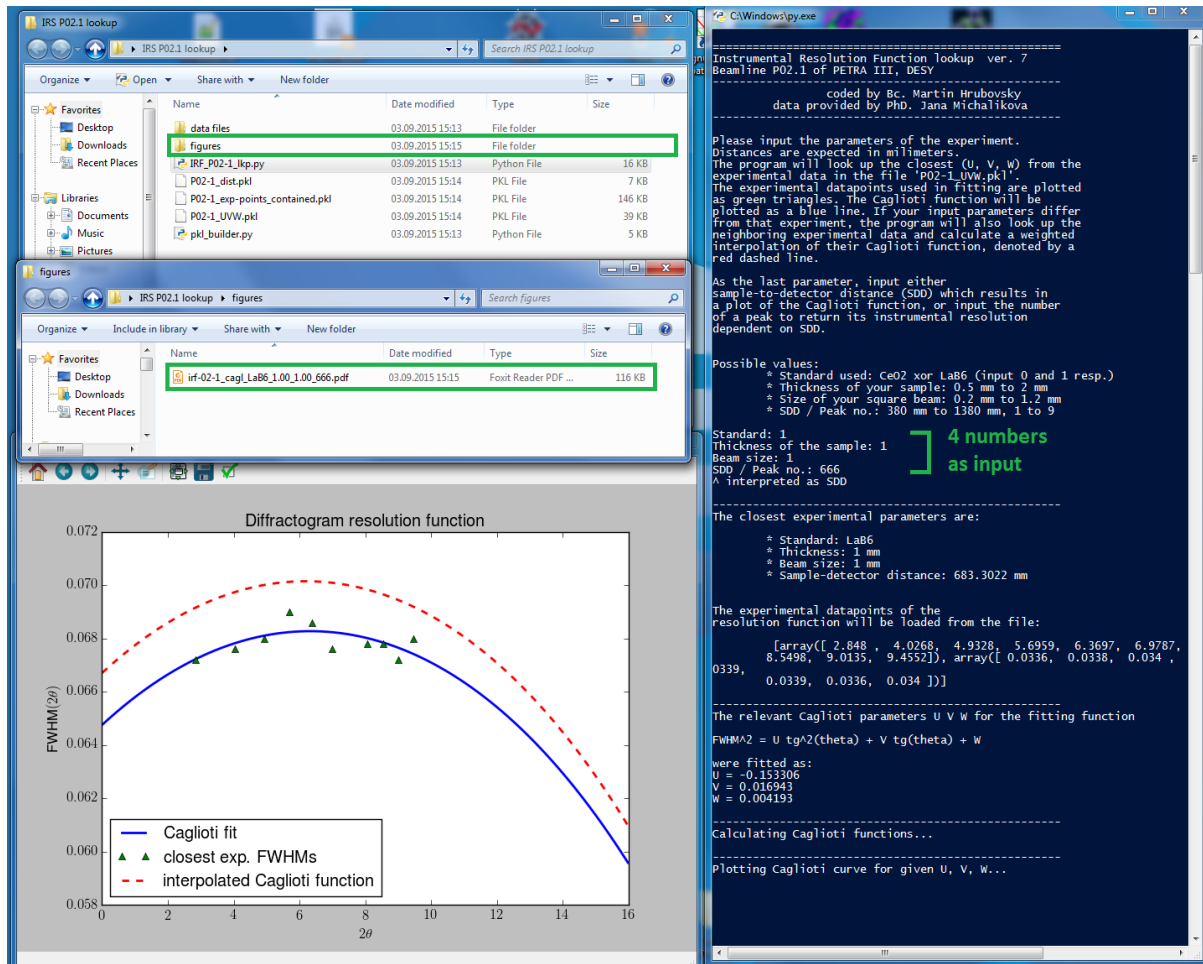


Figure 8: The result of running the main program, “IRF\_P02-1\_lkp.py”. The user is given an explanation of the program and possible input values. The user inputs 4 numbers and the program then looks up the closest measured dataset and plots experimental FWHMs and the fitted Caglioti function. The closest experimental parameters and the Caglioti parameters are also explicitly given. Then the plot window shows and the appropriately named figure file is created.

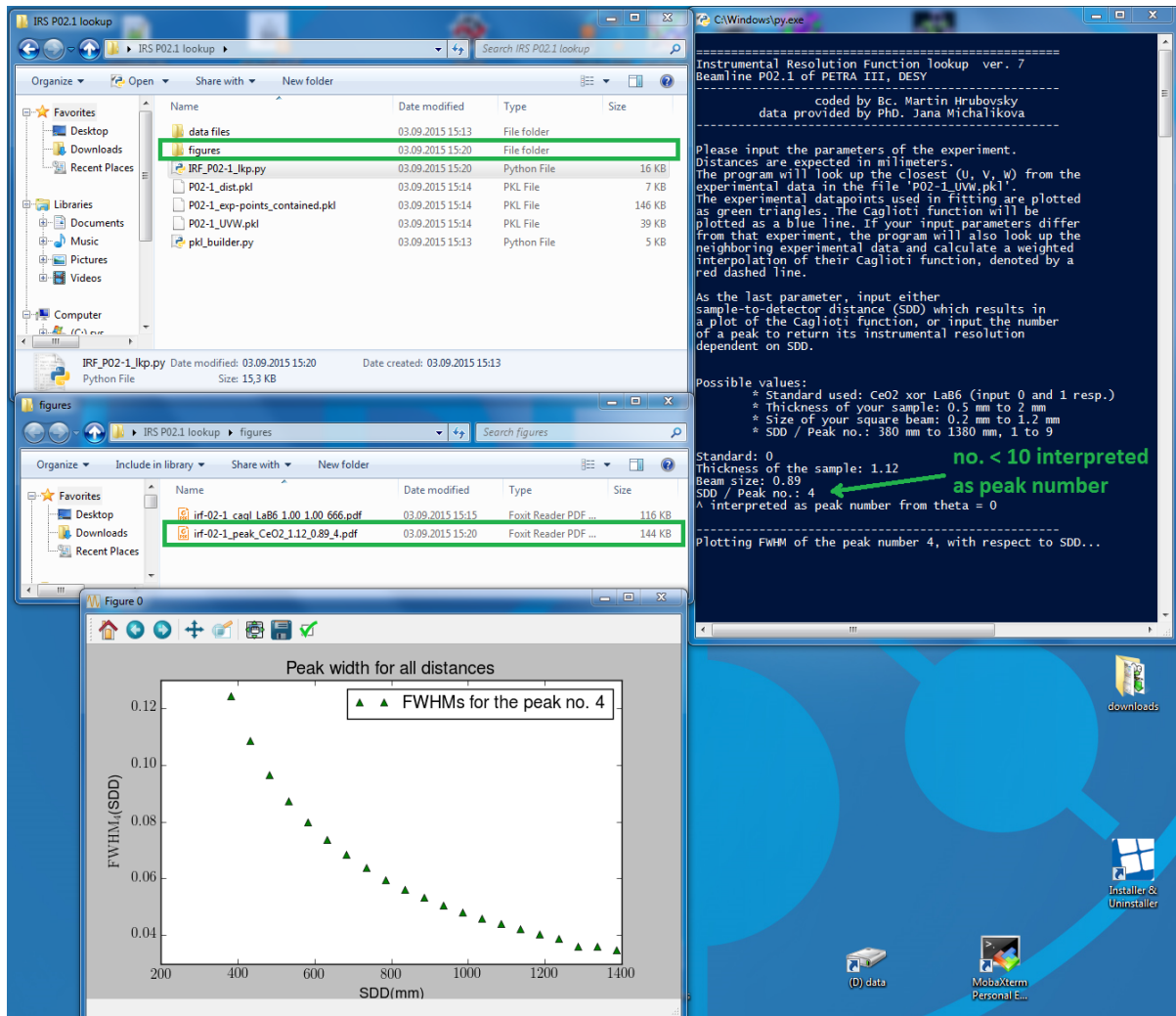


Figure 9: The alternative mode of the program. If the input number for sample-to-detector distance is smaller than 10, the program interprets it as a peak number 1–9. The program then looks up all FWHMs for that peak at given thickness, beam size and standard, at various distances.

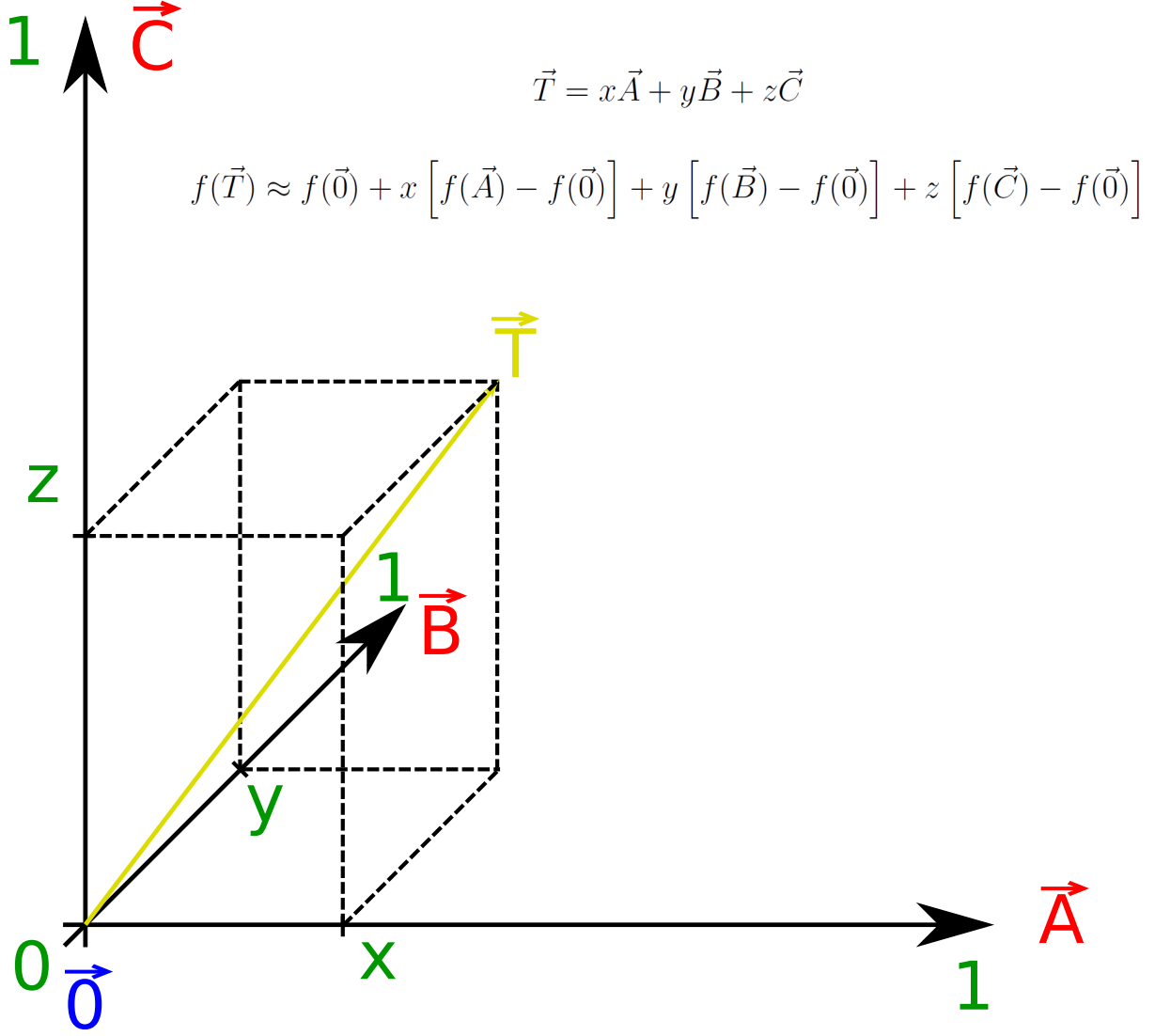


Figure 10: The Caglioti function for the closest experimental parameters sits at  $\vec{0}$ . The user entered the parameters at  $\vec{0} + \vec{T}$ . The user parameters are between the closest set and the  $\vec{0} + \vec{A} + \vec{B} + \vec{C}$  (which may not have been measured). The dataset at  $\vec{A}$  has sample thickness different from  $\vec{0}$ ,  $\vec{B}$  has different beam size and  $\vec{C}$  has different SDD. The program then finds the coefficients  $(x, y, z)$ . Each of these takes values  $[0, 0.5]$ . Finally, the interpolated function  $f(\vec{T})$  is put together as a linear combination of the closest (up to) 4 Caglioti functions.

The program is coded in the programming language Python v3.4 and Python v2.7. To create the program, I used Notepad++ and the scientific Python distribution Anaconda, by Continuum Analytics. The vector images used in this report were drawn using Inkscape v0.91.

## 5 Attachments

### The full program, with all the required experimental data

To run, it requires Python 3 with modules “numpy”, “matplotlib”, “math” and “pickle” installed.

1. Link to the .zip archive attached inside this document:
  - a)  
for Python v3.4 (does NOT work in Adobe Reader without registry hacks; safe reading needs to be disabled in other .pdf readers)
  - b)  
for Python v2.7 (neither this works in Adobe, due to Adobe’s safety philosophy)
2. Alternatively, a link to my personal Dropbox, where the same .zip-s are hosted:
  - a) IRF\_P02-1\_lkp\_distr.zip  
(for Python v3.4, requires internet connection)
  - b) IRF\_P02-1\_lkp\_py27\_distr.zip  
(for Python v2.7, requires internet connection)

To use:

1. unzip anywhere on the disk
2. run “pkl\_builder.py”. This should generate three \*.pkl files.
3. run “IRS\_P02-1\_lkp.py”. Input your desired experimental parameters and watch.

The results should resemble the screenshots in the previous section 4.

## References

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