Int3D: a data reduction software for single crystal neutron diffraction

Nebil A. Katcho, Laura Cañadillas-Delgado, Oscar Fabelo, Juan Rodríguez Carvajal

Why Int3D?

Status of the software in the single crystal diffractometers of the ILL (D9,D10,D19)

- Outdated software (dates from the 80s, Fortran77, inefficient…)
- Software split in multiple pieces
- Difficult to deal with complex problems (twins, inconmensurability)
- Very limited and low quality data visualization
- Demands high expertise (high workload for local contacts)

The Int3D software

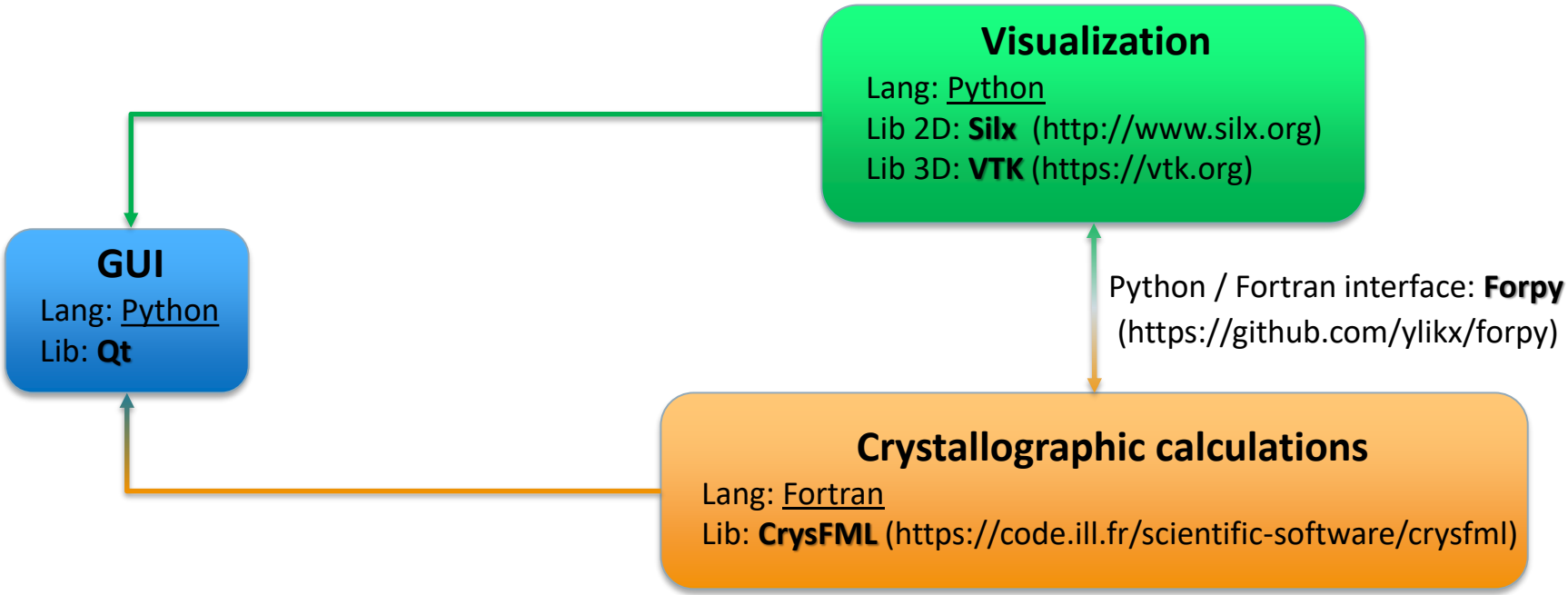
- Integrates in a single application all the required tasks to perform the data reduction:

  - Peaks search
  - Determination of the orientation matrix
  - Integration of the reflections intensity
  - Parameters refinement (sample, instrument)

- It provides a graphical user interface that allows users:

  - Run crystallographic calculations
  - Visualize and interact with the data

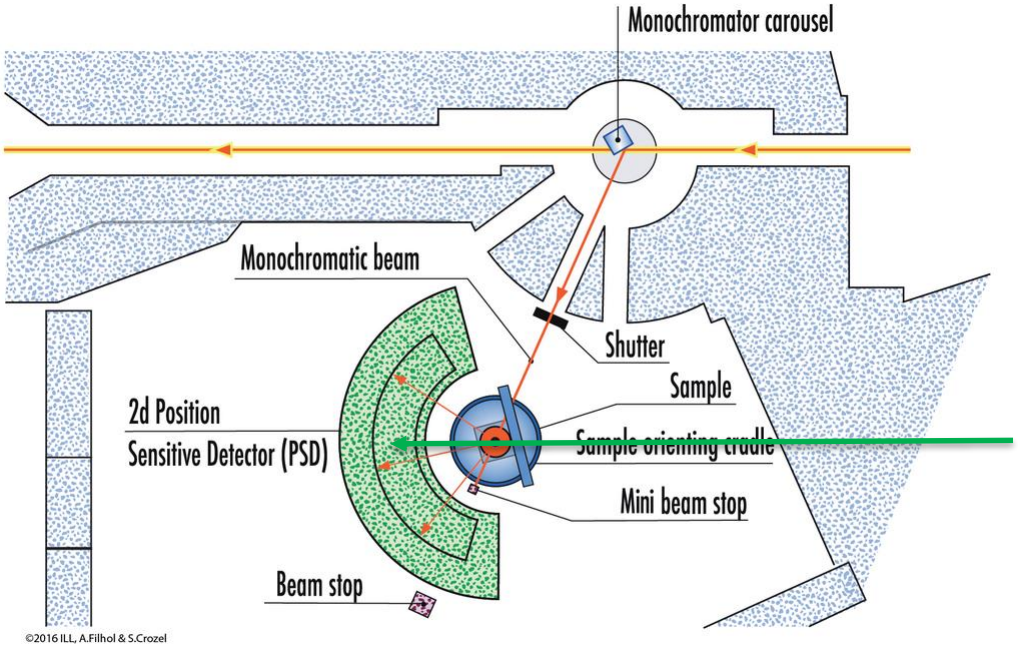
Int3D: languages and libraries



Int3D: current status

Instrument	Status
D9	Ongoing, ready for next ILL cycle, January 2021
D10	Not started yet, but straightforward extension from D9
D19	Fully developed, ready to use

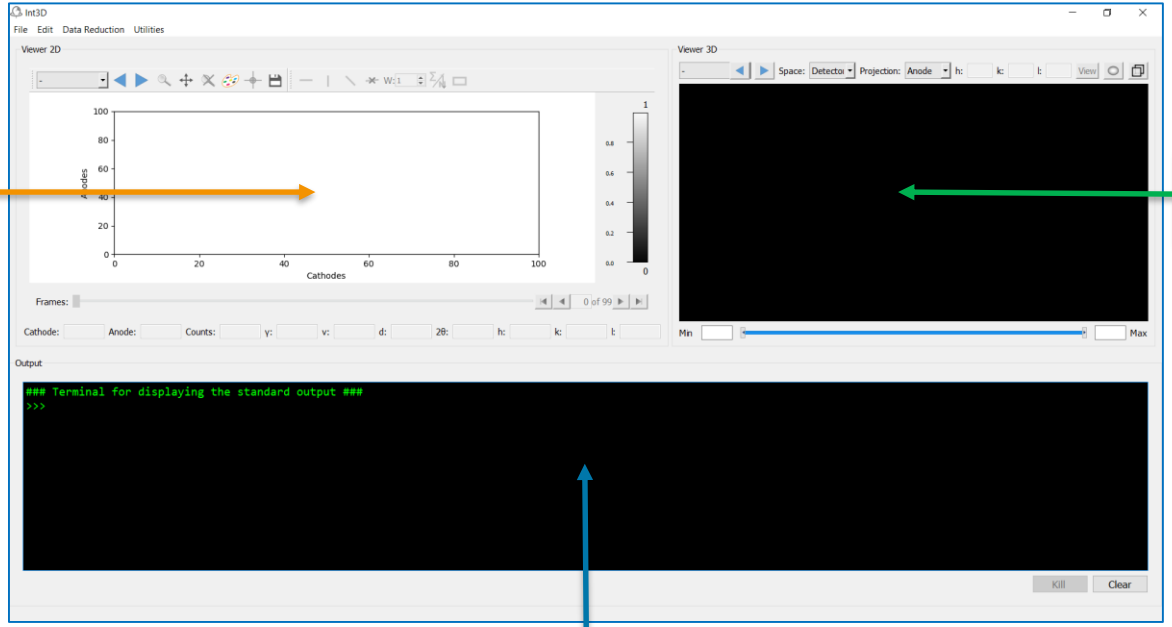
D19 single crystal diffractometer



Very large “banana” position sensitive detector (120° × 30°)

Int3D: the GUI

Scan 2D viewer
Frame by frame visualization

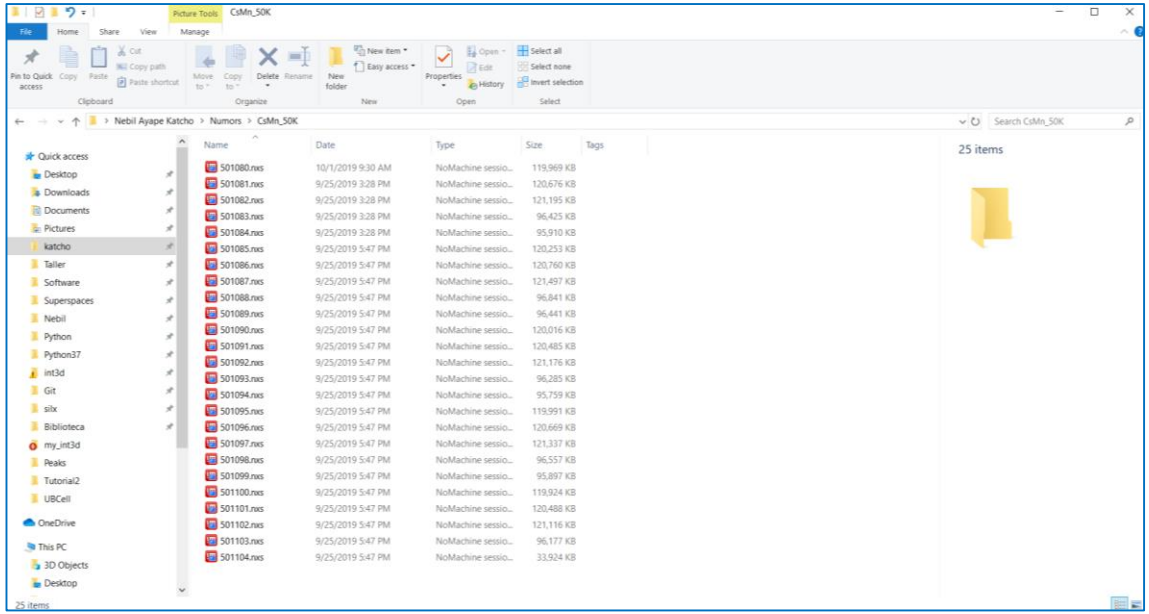


Scan 3D viewer
Detector / reciprocal spaces

Terminal
Output of crystallographic calculations

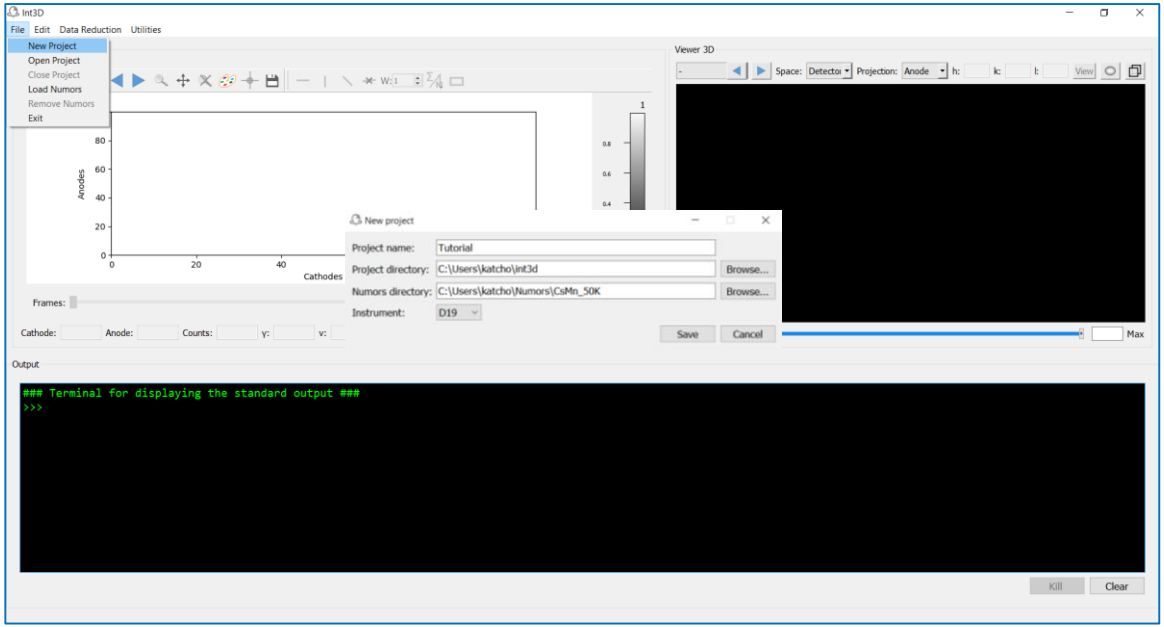
Int3D: the raw data

- The raw data for Int3D consists of a series of nexus files, called numors.
- Every numor corresponds to a given scan, usually an omega scan.



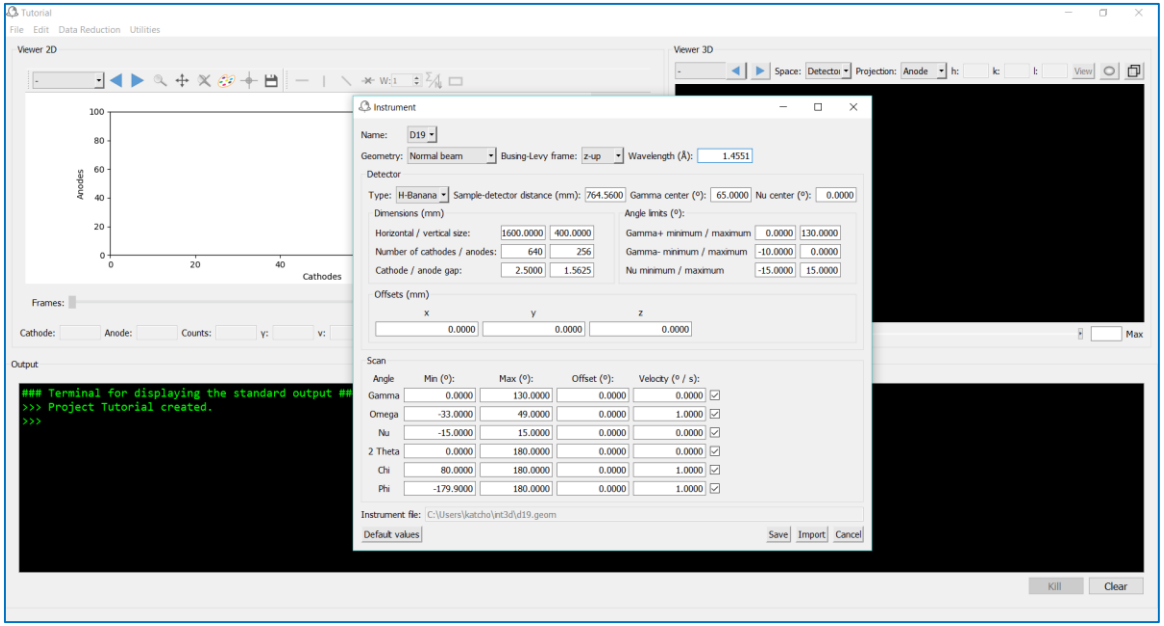
Data reduction step by step

1. Create a project and configure the instrument

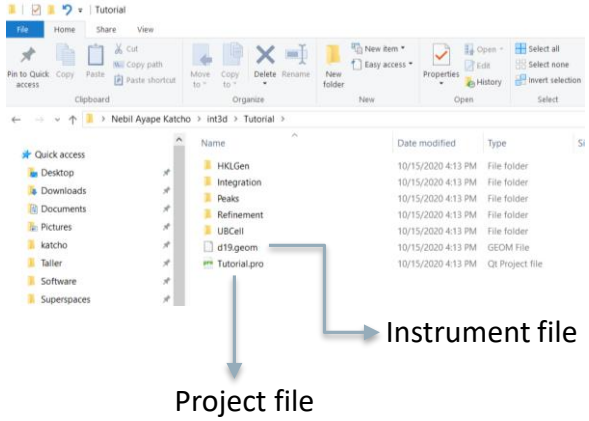


Data reduction step by step

1. Create a project and configure the instrument

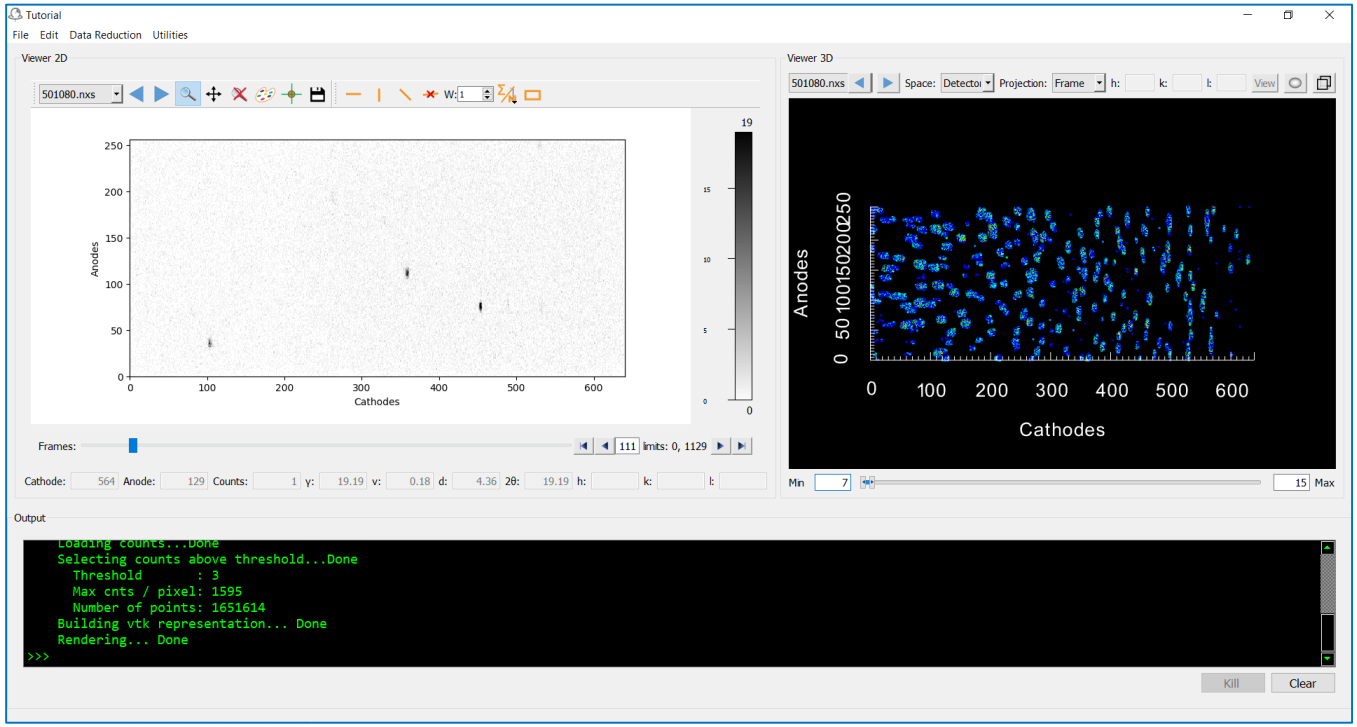


Project structure



Data reduction step by step

Appearance of D19 data

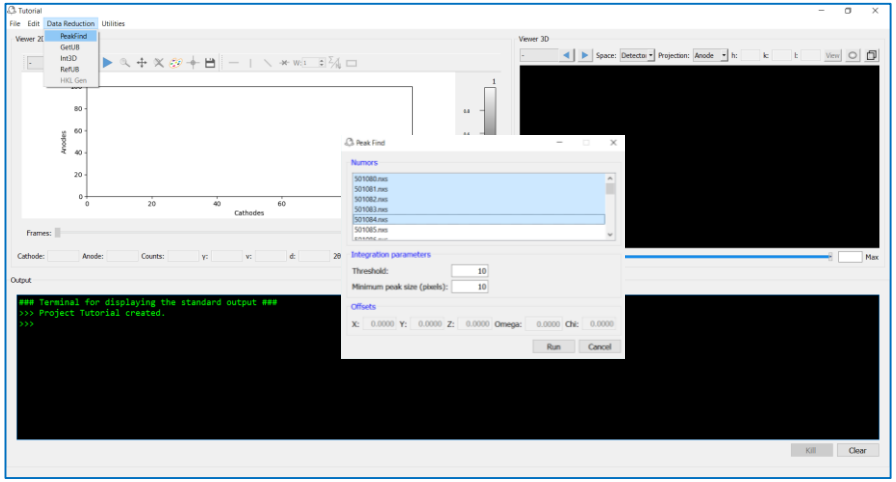


Data reduction step by step

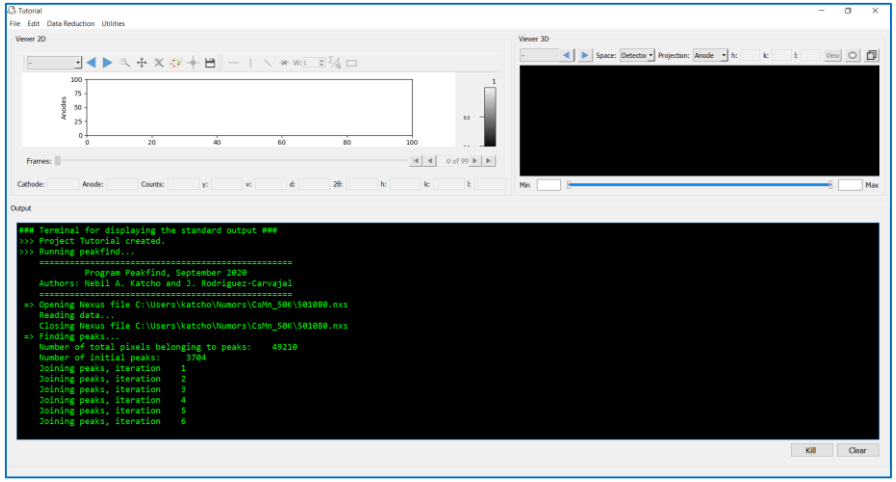
2. Peaks search

From Data Reduction menu, open the Peakfind program

Input



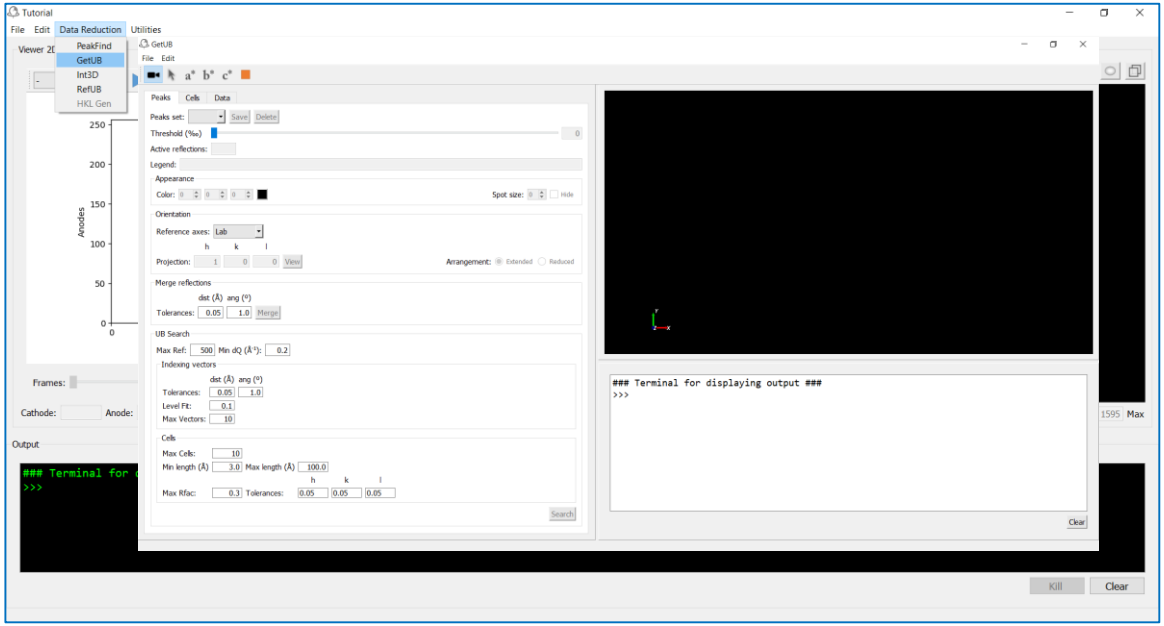
Output



Data reduction step by step

2. Determine the orientation matrix

From Data Reduction menu, open the GetUB application



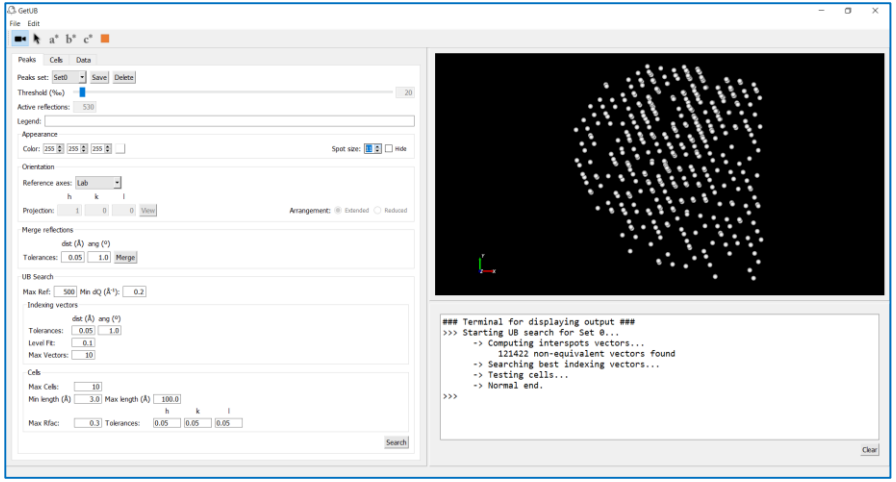
GetUB

- Determination of the orientation matrix
- Visualization of reciprocal space
- Orientation
- Interaction with the data:
  - Classification
  - Filtering
  - Deletion

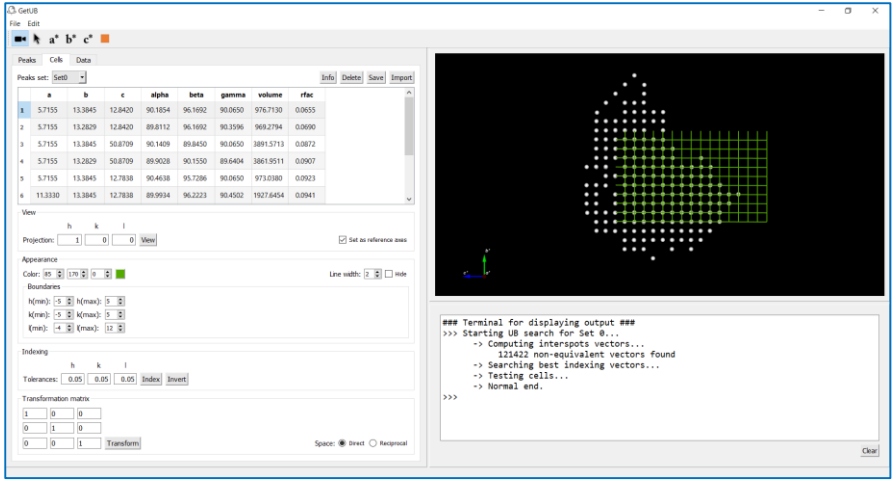
Data reduction step by step

2. Determine the orientation matrix

Load peaks found by peakfind and search the UB matrix

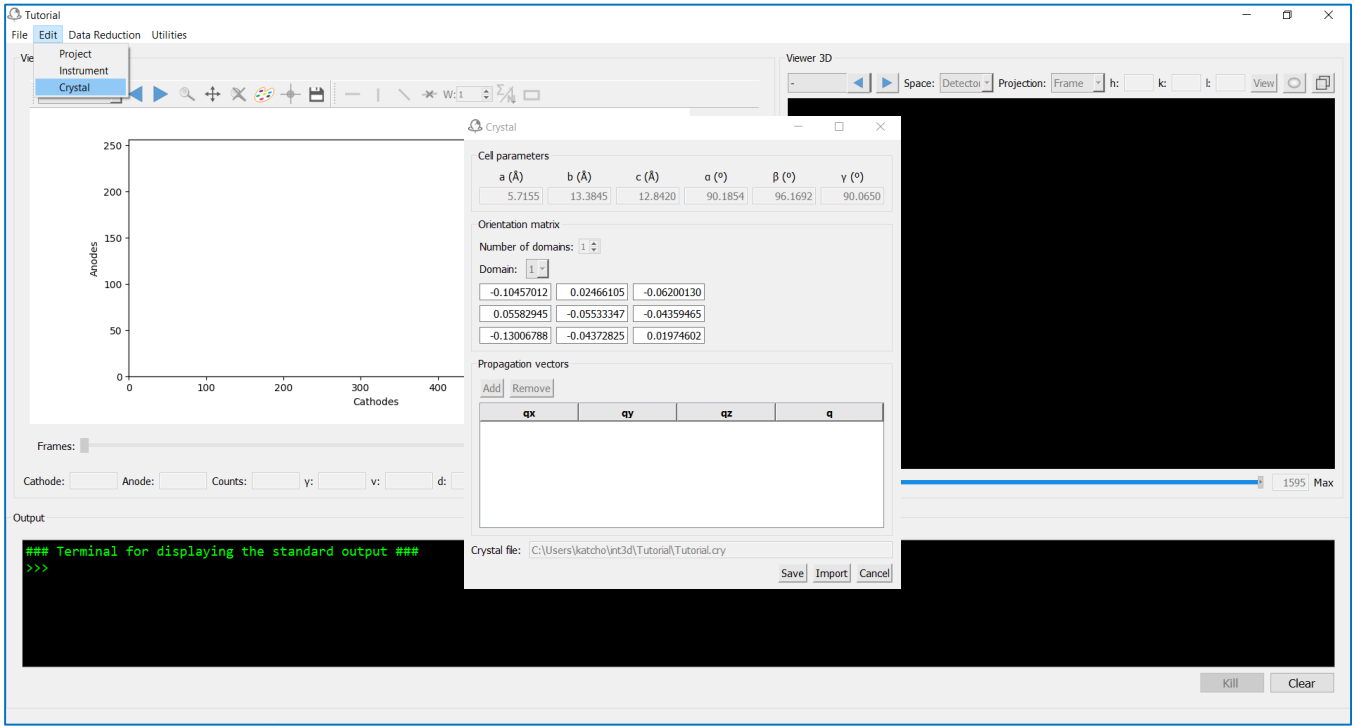


Check proposed cells



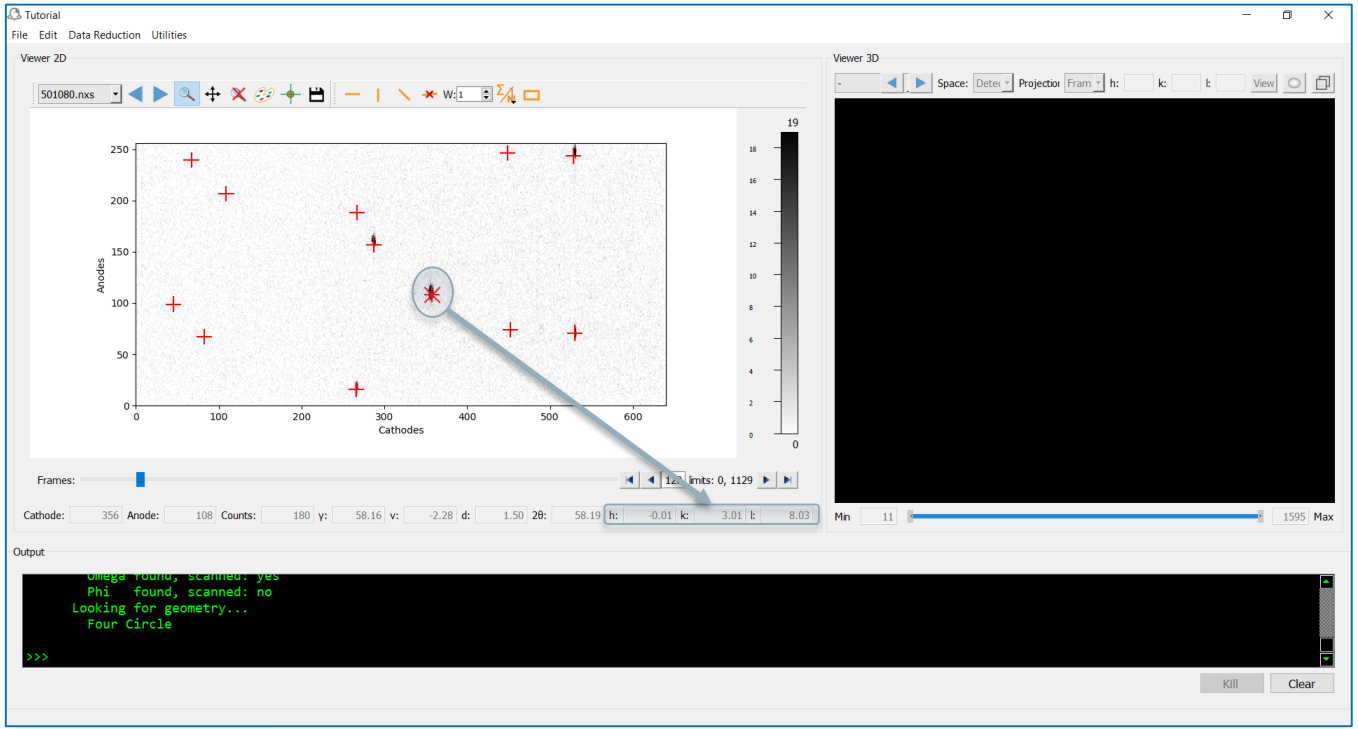
Data reduction step by step

Load the UB matrix



Data reduction step by step

Get the data indexed

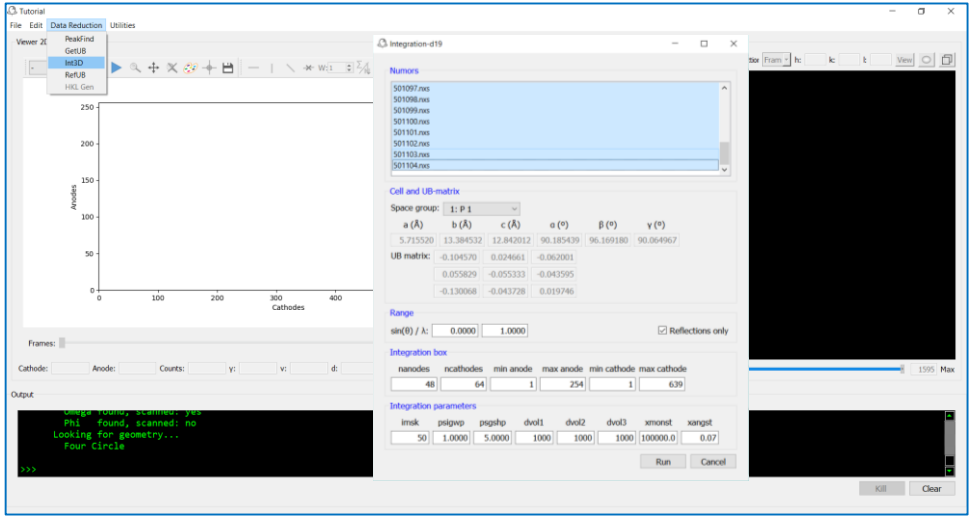


Data reduction step by step

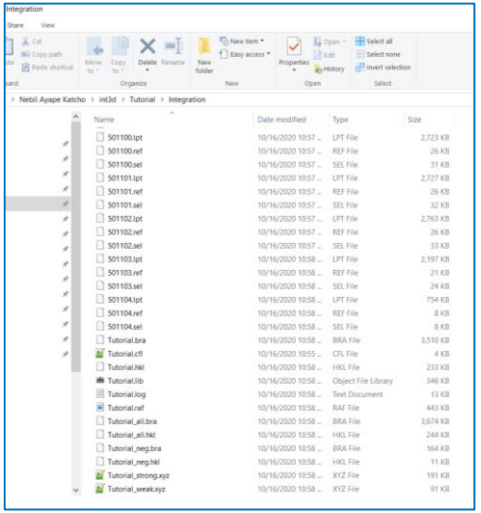
3. Integration

From Data Reduction menu, open Int3D

Input



Output

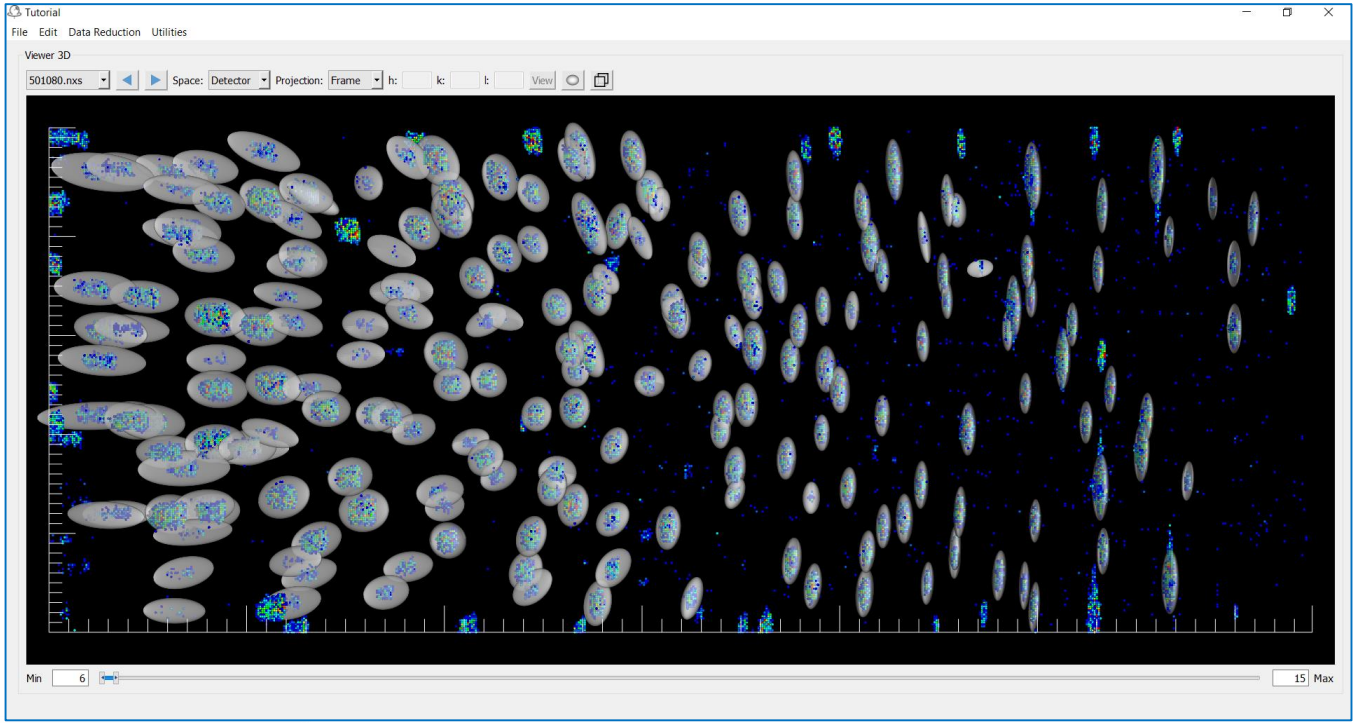


Files

.lpt : integration details
.ref : peak centroids
.sel : integration ellipsoids
.hkl : integrated intensities
.lib : library for weak refl
.raf : used for refinement

Data reduction step by step

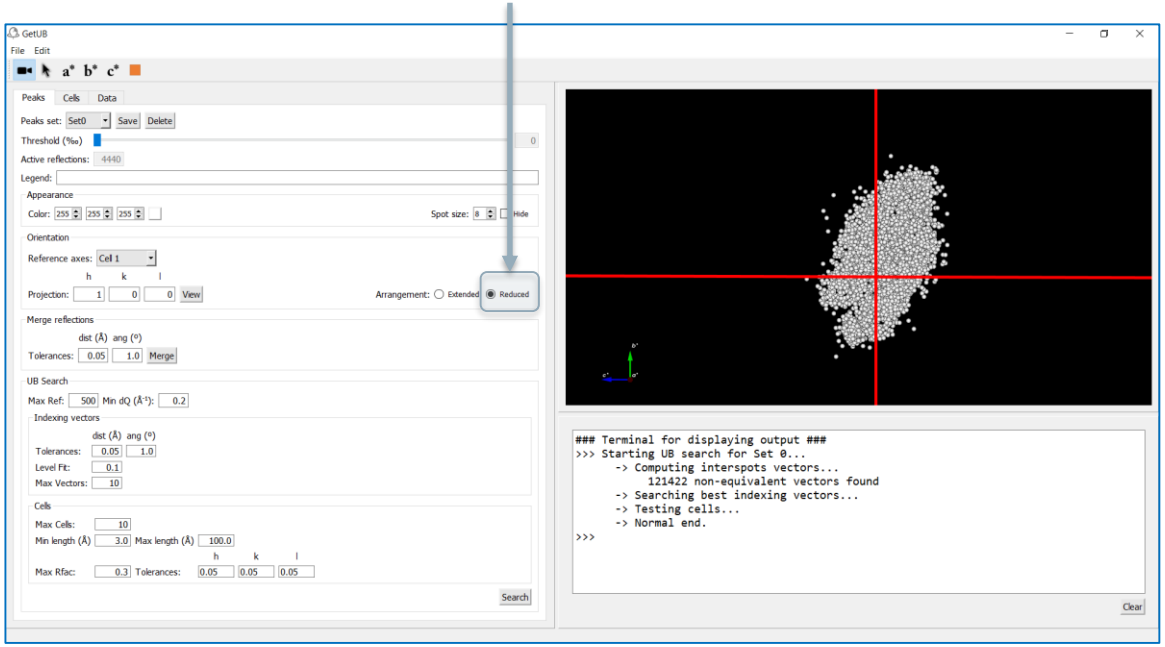
Check integration ellipsoids by visual inspection



Data reduction step by step

Check offsets

Use GetUB to translate all reflections to the origin



Not well centred
Anisotropy

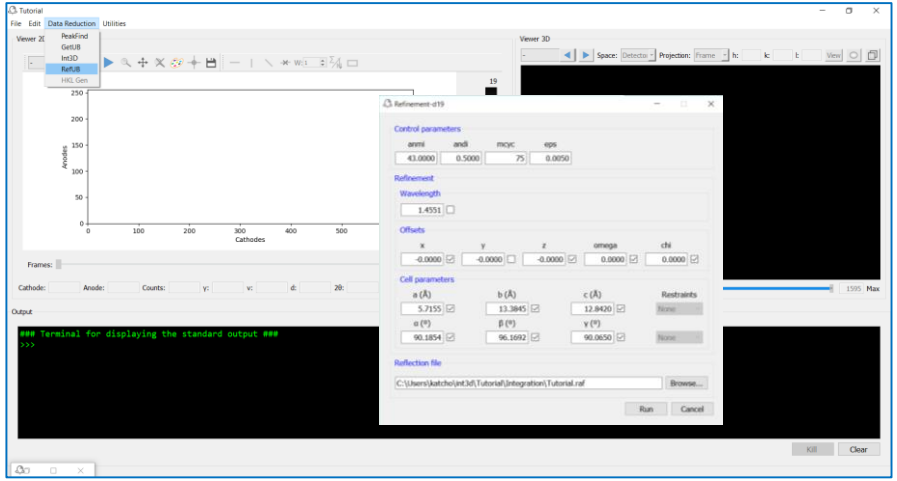
Refine!

Data reduction step by step

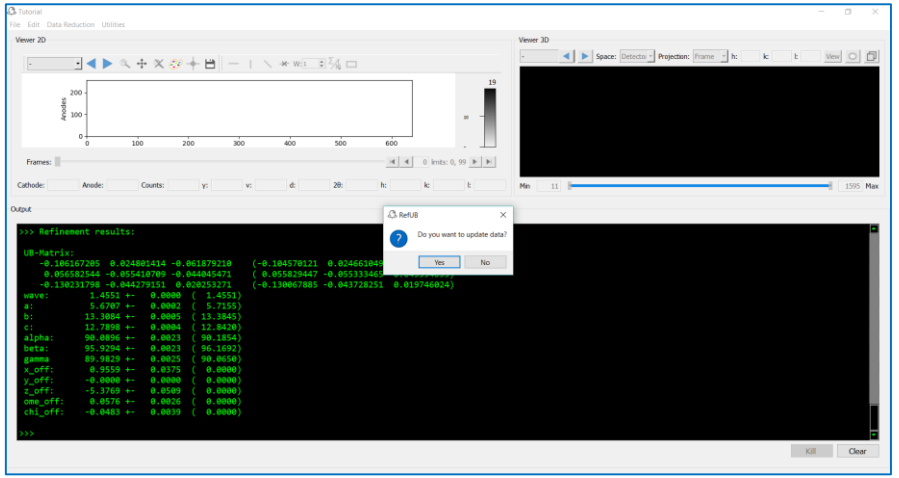
4. Refinement

From Data Reduction menu, open RefUB

Input

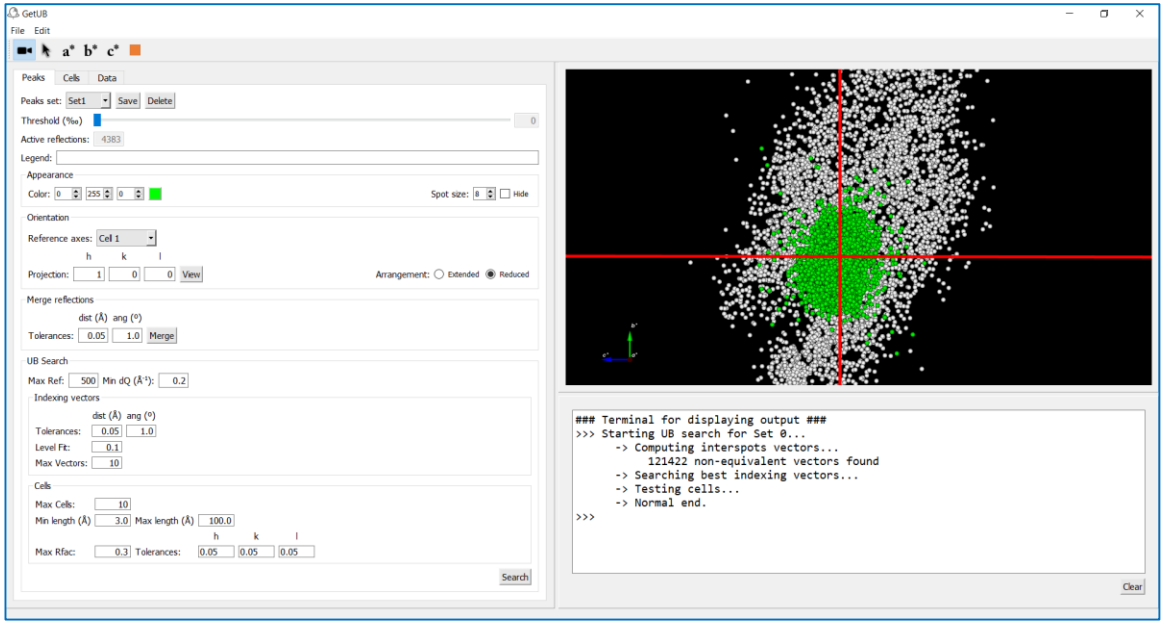


Output



Data reduction step by step

Check offsets



Well centred
Isotropy
Less dispersion

Summary and conclusions

- We have integrated in a single application all the required tasks for performing the data reduction in single crystal neutron diffraction experiments.

- Int3D provides powerful graphical tools and suggest reasonable parameters for the different steps of the data reduction process, which makes it accessible to users without demanding high expertise.

- The application is distributed as a single folder containing all required libraries and executables. No installation of libraries or python is required.

- Video tutorial: www.int3d.fr

- Future improvements: absorption correction, complete visualization of data in reciprocal space, users demands…


INSTITUT LAUE LANGEVIN
NEUTRONS
FOR SOCIETY