Lauetools

A software package for Laue microdiffraction data analysis

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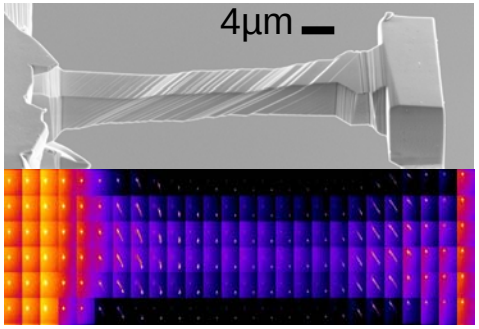
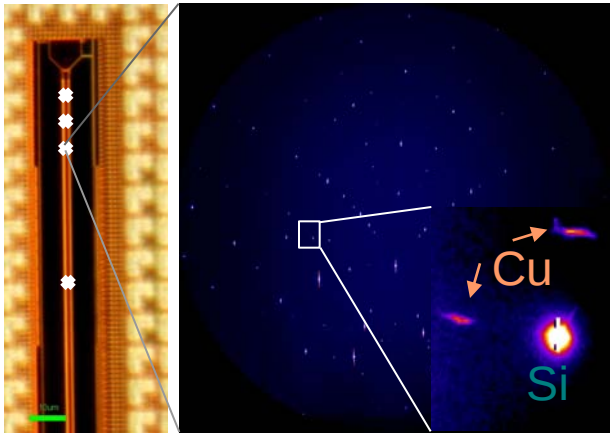
Browse and download codes at: https://sourceforge.net/projects/lauetools/

Scientific objectives

Scientific trends:
- towards Micro-Nano object (applied and fundamental physics)
- size and strain effect on properties (+ distribution)
- real-life, packaged and complex materials (polycrystal), in operando
- reliability & strain engineering in microdevice



Need of structural characterisation
- Accurate strain measurement
- Small probe with high spatial resolution



Local (<1µm) Accurate &No sample preparation (x-ray)
volumic probe (x-ray) Fast (white beam)

Wanted: characterisation tool ~ EBSD, TEM

Laue diffraction assets

- $\sum_{\lambda}$ **(mono-λ diffraction)** at the same time
- No sample rotation
- (All λ are unknown)

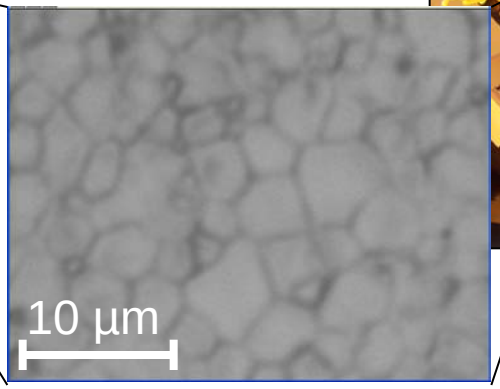
=> Angular unit cell distorsion (b/a,c/a,α,β,γ)

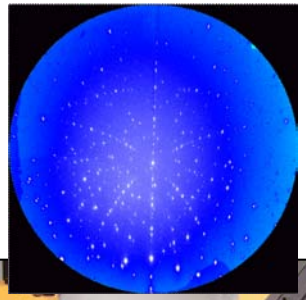
Bragg's law

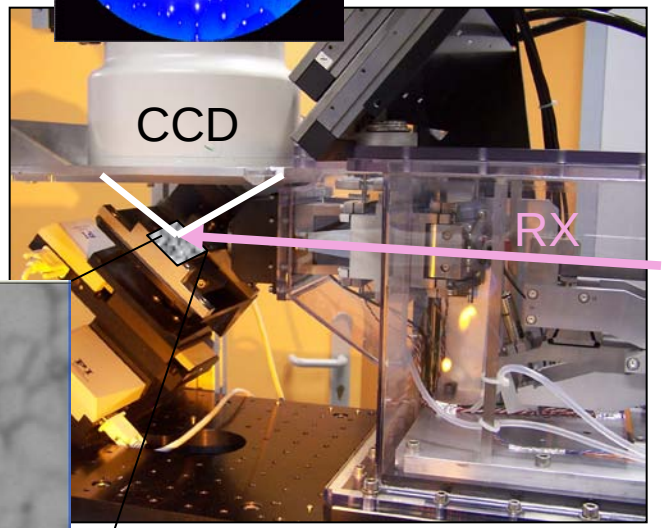
$$2\,d\sin\theta=\lambda$$

Instrumental objectives

Make Laue diffraction where you want …



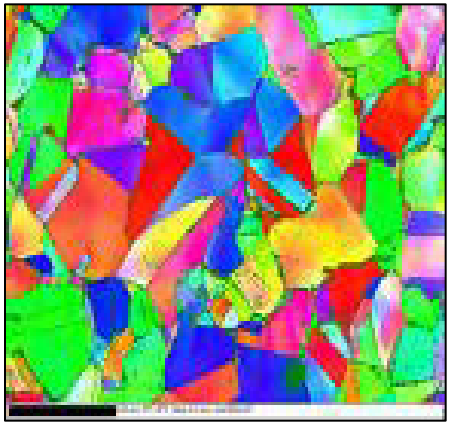




2D Laue Diffraction Microscopy:

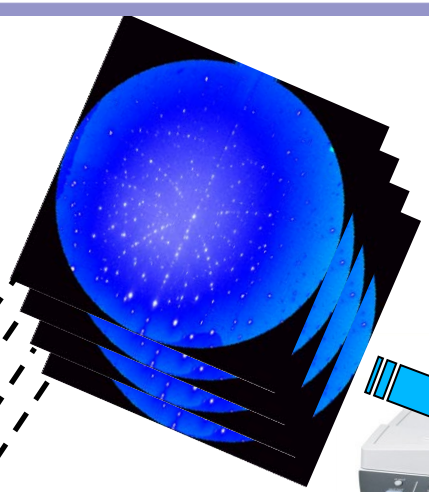
- **Location**
- **Orientation**
- **Strain**

maps



Data Analysis objectives

Fast
Laue pattern
recording …



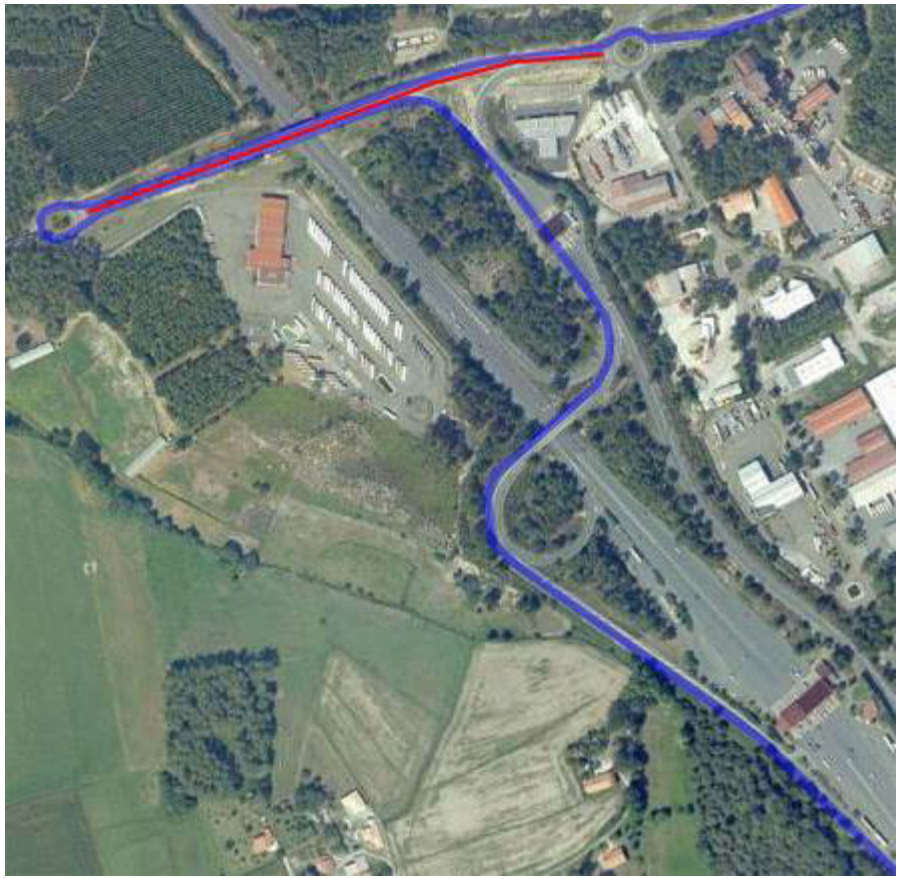
Grains'
facebook

- Orientation
- Strain state
- Location
- phase
- mother, children

…

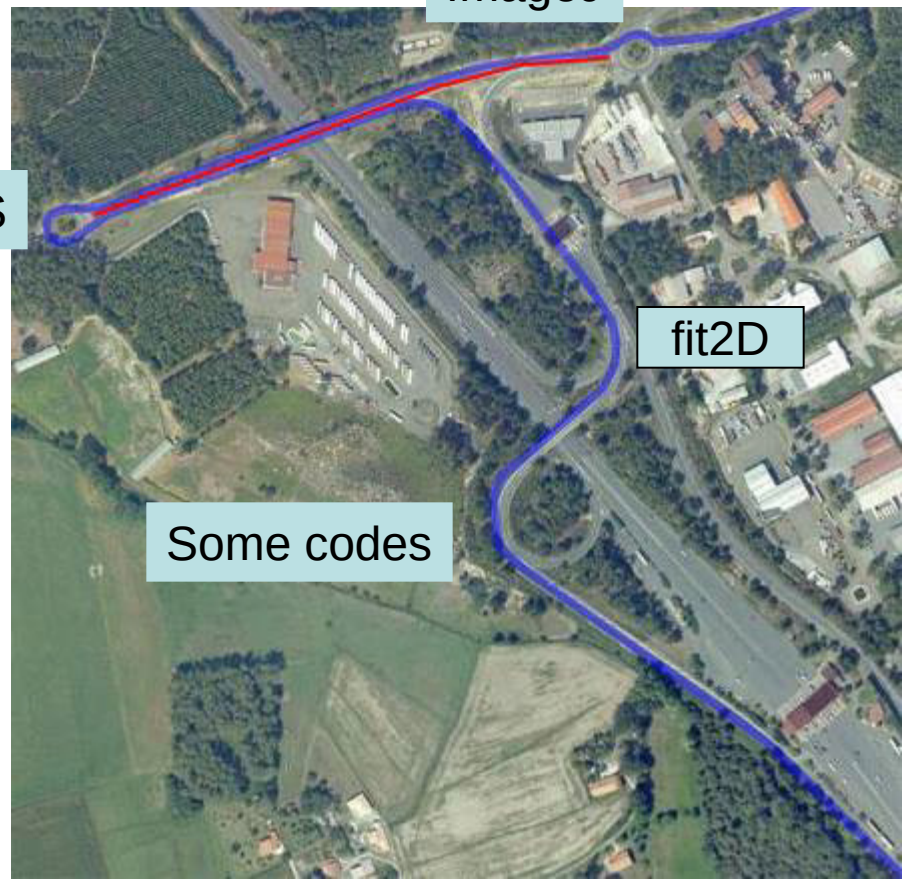
… but efficient analysis is lacking

Data Analysis challenges



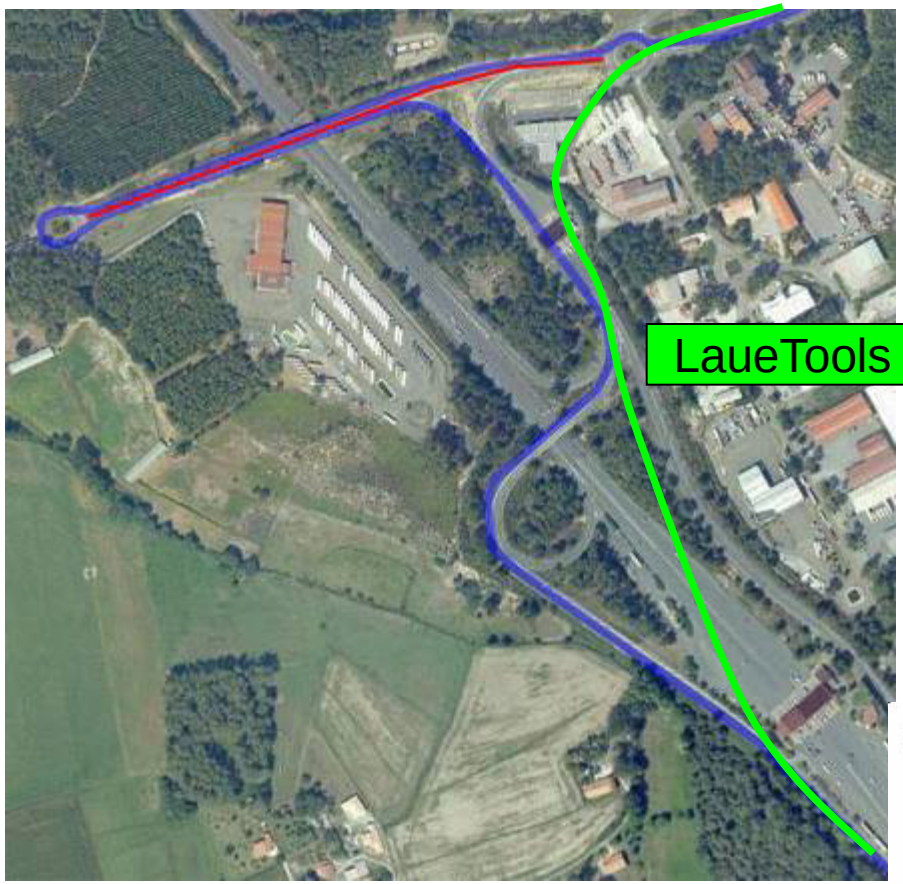
Data Analysis challenges

LAUE raw data



Data Analysis challenges

LAUE raw data



makes data flow easier …

Data Analysis challenges

LaueTools is for increasing scientific throughput of µLaue

- Online/offline analysis

- Help on data acquisition strategy

- GUI, command line, bashable

- Open-source:

stimulate development and maintenance

user control of codes and models

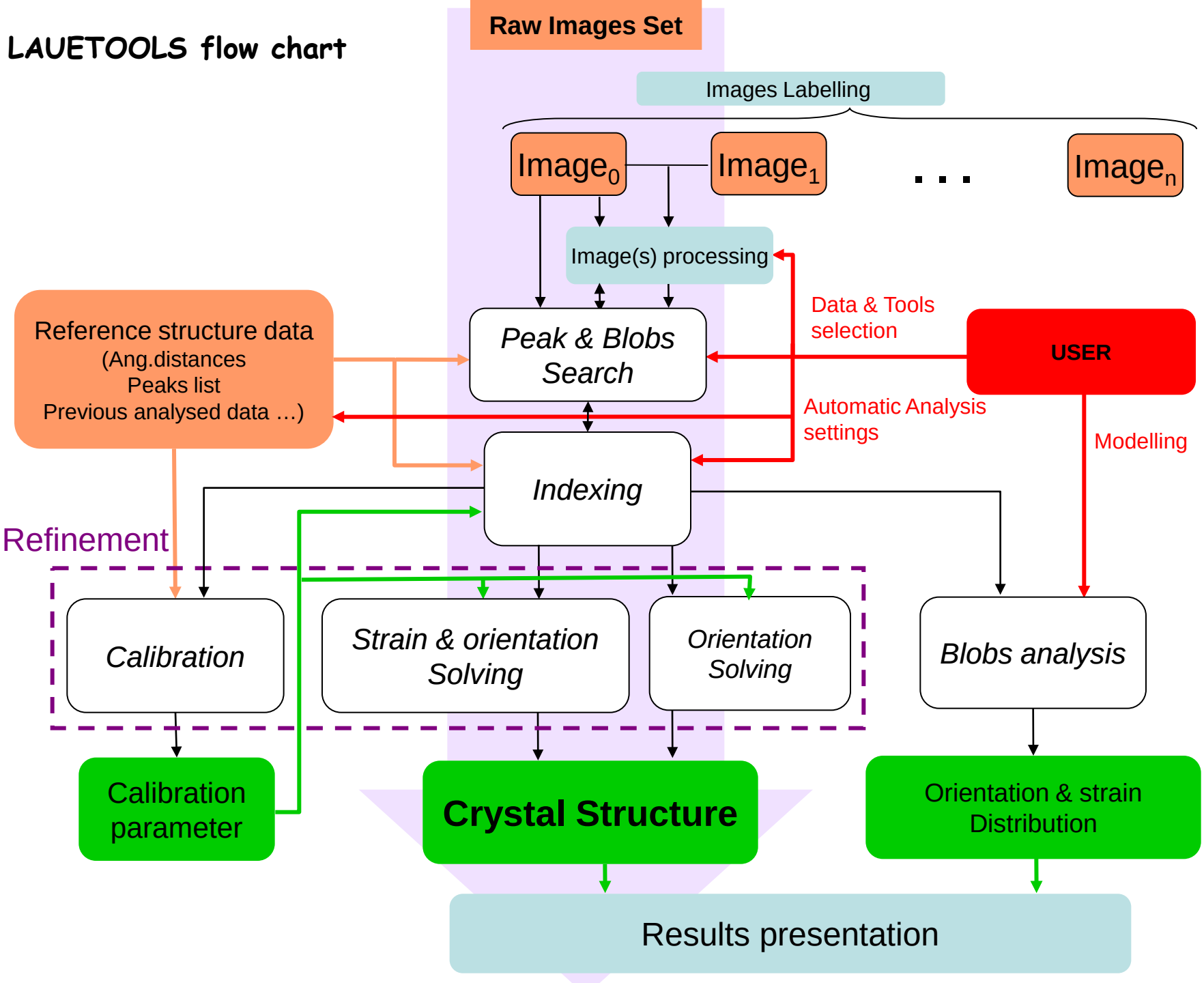
interactions: mechanics, physics, Xtallographers, programmers…

Lauetools

Codes in python

-high level programming language
-OO, script, easy prototyping
-open-source
-multi-platform
-scientific and graphical libraries
(pylab,Image, numpy, optimisation,wxpython)

Modularity,Separated routines, classes
Interactive python
interface with C, JAVA, Fortran


LAUETOOLS flow chart
Raw Images Set
Images Labelling
Image0
Image1
. . .
Imagen
Image(s) processing
Reference structure data
(Ang.distances
Peaks list
Previous analysed data …)
Peak & Blobs Search
Data & Tools selection
USER
Automatic Analysis settings
Modelling
Indexing
Refinement
Calibration
Strain & orientation Solving
Orientation Solving
Blobs analysis
Calibration parameter
Crystal Structure
Orientation & strain Distribution
Results presentation

LAUETOOLS package

readmccd.py image data reading
digital processing, numerical operations

fit2dintensity.py 2D intensity profile fitting

gnomon.py projection on to gnomonic plane
Hough transform
data and reference images matching

laue.py Laue pattern simulation

graingraph.py cliques finding

find2thetachi.py date coordinates transforms

recognition.py spot and zone recognition

findorient.py orientation matrix from indexation

fitOrient.py Orientaton&Strain&Calibration refinement

GUIs in wxpython

LaueTool.py

Data representation
Indexation
Refinement
Results visualisation

MapCanvas.py

Images dataset
Navigator and
Analysis

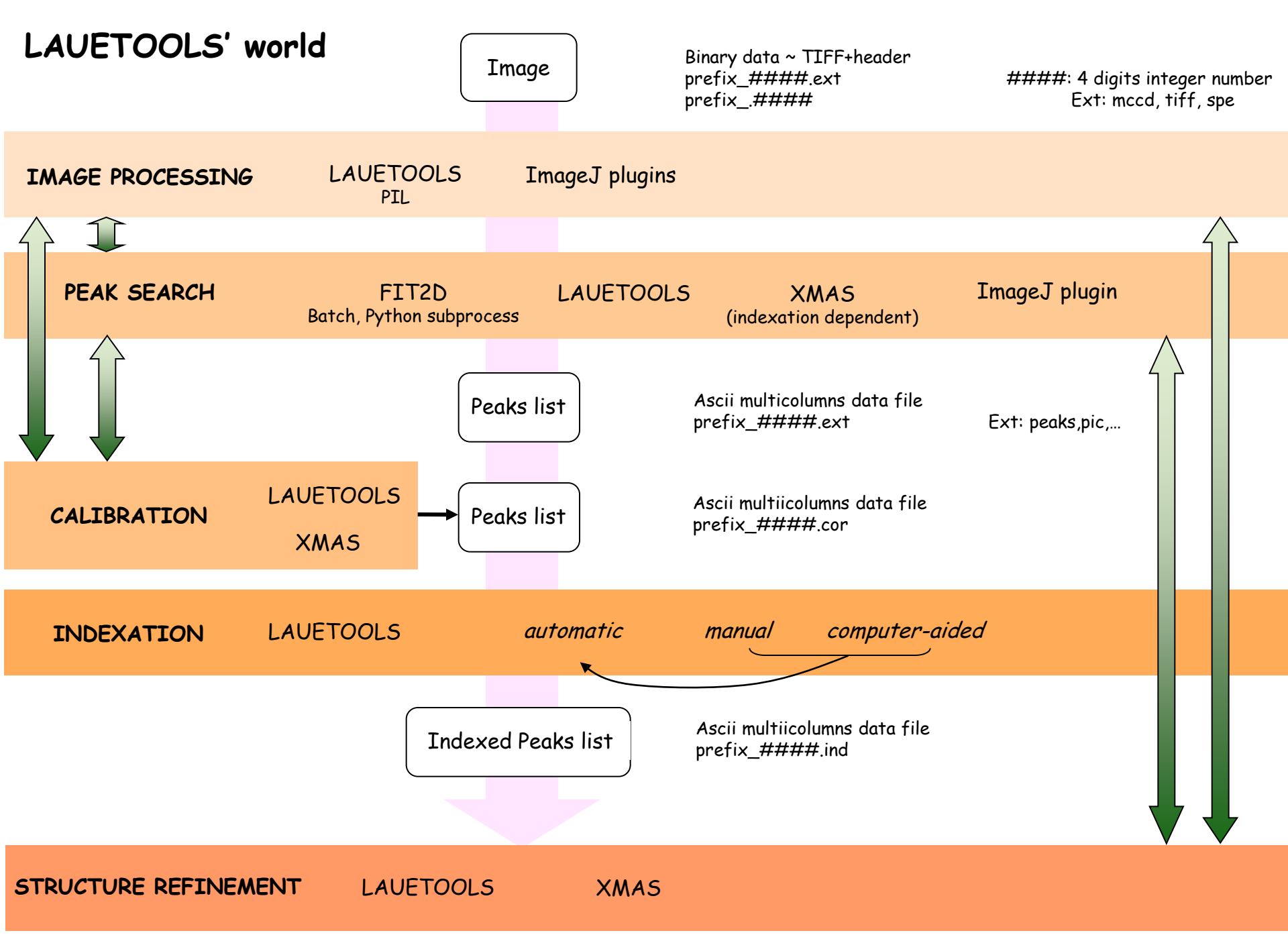
3D Laue pattern visualisation in PyOpenGL

laue3D.py

Data representation
Quick U estimation
Strain & Energy effect

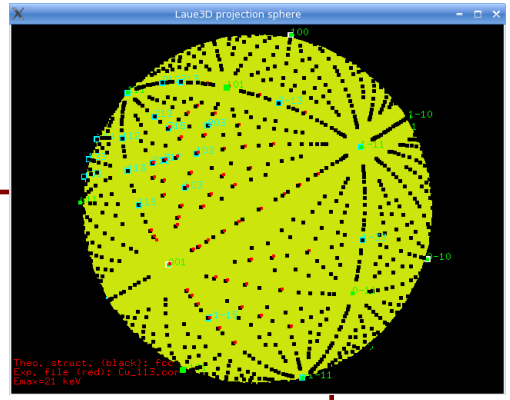
Online tools

Plotmeshspec.py 2D scan plot
Mosaic.py 2D mosaic plot


LAUETOOLS' world
Image
Binary data ~ TIFF+header
prefix_####.ext
prefix_.####
####: 4 digits integer number
Ext: mccd, tiff, spe
IMAGE PROCESSING
LAUETOOLS
PIL
ImageJ plugins
PEAK SEARCH
FIT2D
Batch, Python subprocess
LAUETOOLS
XMAS
(indexation dependent)
ImageJ plugin
Peaks list
Ascii multicolumns data file
prefix_####.ext
Ext: peaks,pic,...
CALIBRATION
LAUETOOLS
XMAS
Peaks list
Ascii multiicolumns data file
prefix_####.cor
INDEXATION
LAUETOOLS
automatic
manual
computer-aided
Indexed Peaks list
Ascii multiicolumns data file
prefix_####.ind
STRUCTURE REFINEMENT
LAUETOOLS
XMAS

LAUETOOLS current status

- Simulation



ü General and pedagogical tool (laue3D)

Input:

ü Detector geometry: transmission, backreflection, side, top
ü Spectral Range

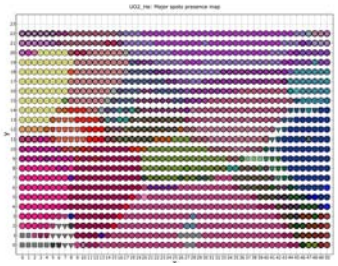
Materials parameters

ü multigrains
ü orientation matrix (U)
ü lattice matrix (B)
ü some transforms on U,B: twins, mosaicity, strain gradient

Output:

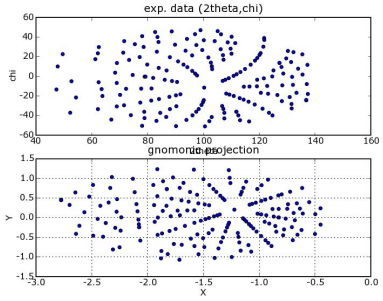
ü Ascii file
ü Spot objects list
ü Plot

LAUETOOLS current status



Data pre-processing

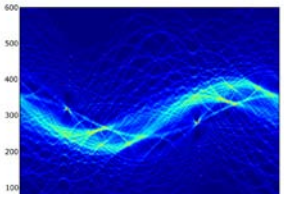
- ü Basic Grain mapping (most intense peak)
- ü Peak search (basic, digital processing)

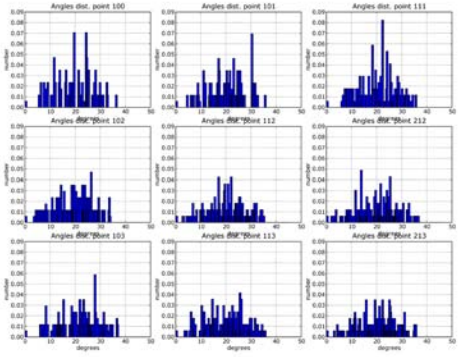


Indexing

- ü manual -> automatic
- ü brute force (trials and errors)
- ü image matching (in Hough space) (~ no peak search)
- ü information selection (Human-computer collaboration)

gnomonic projection
hough space
cliques
spot & zone axis recognition

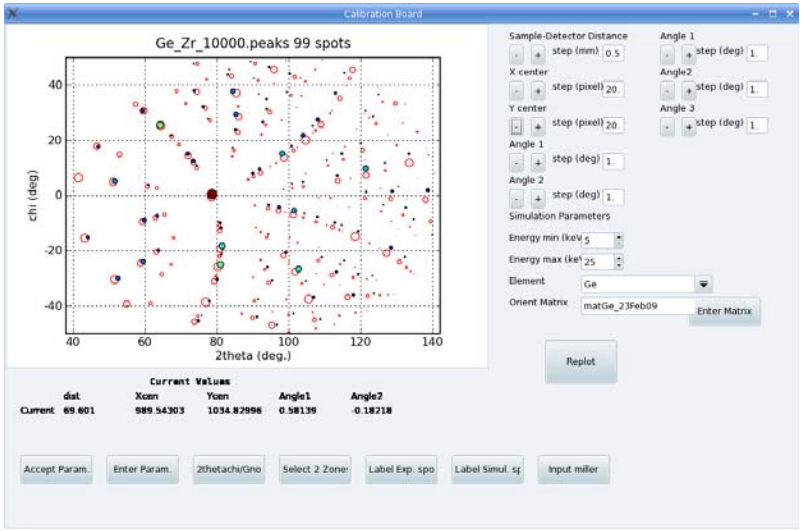




LAUETOOLS current status

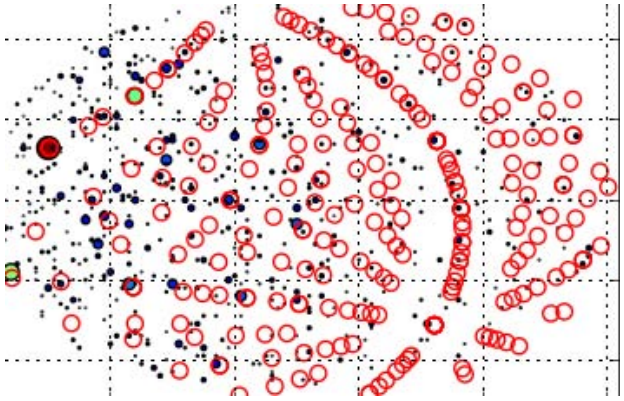
- Structure solving

ü Detector calibration: refinement, methods
ü Strain Refinement



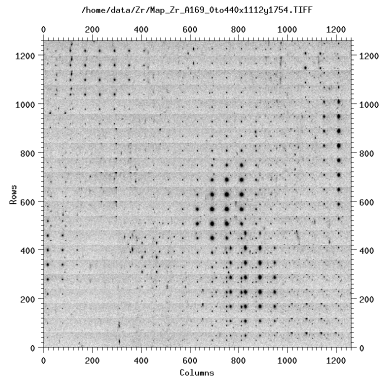
- Visualisation

ü Data representation & manual indexing
ü Graphical User Interface: data visualisation & indexing
ü Only ideas and trials for results visualisation

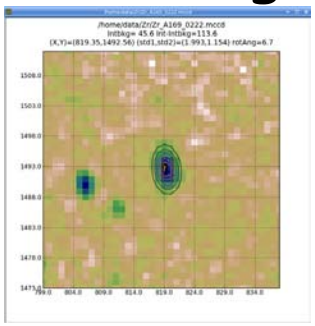


Data analysis and visualisation tools

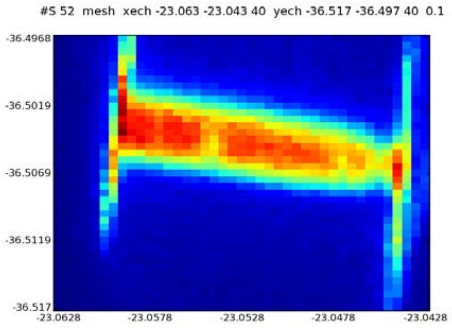
- mosaic

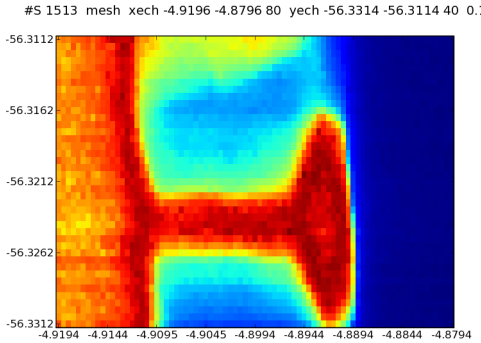


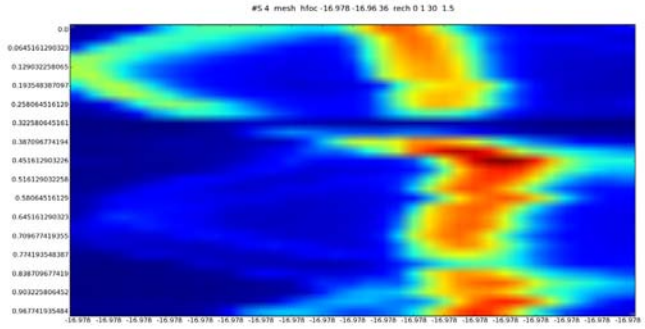
- Images set navigator & processing



- plotmesh







LAUETOOLS perspectives

- **Complete the entire treatment chain of One image**: from raw data to orientations&strains
- Implement efficient peak search (C, java …)
- Improve calibration method (peak shape modelling + optimisation)
- Improve strain determination (refinement, statistics on peaks set)

- **Get more users and developers**

Improve Distribution & simplify installation (webserver? Migrate to fortran, java, matlab?)
Build clean documentation
Compose tutorials
? Build laboratory single crystal Laue Pattern analysis software ?

- **Automatic** indexing & structure determination of **file series** and real-life data:
- manage peaks overlaps
- separate linked grains (twins, phase transform)
- 2D/3D data visualisation

- **Improve and Add functionnalities**:
- Smarter refinement methods (global optimisaton, constraints,…)
- more physics & Xtallography & metallurgy models input
- More experts for indexing (evaluate performances and scopes)
- on-line tools
- Parallel computing
- …

Upcoming techniques

- 3D microLaue Diffraction
- Laue spot tomography
- intensity harvesting

Opening-up to other softwares

-TotalCryst & Fable (algorithms & Laue plugins)

- ILL laue software, LaueGen, CrysFML, cctbx …

Acknowledgements

- CRG-IF BM32 Beamline staff
O. Robach, O. Ulrich, X. Biquard, F. Rieutord,

- Nice supporting users:

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B. Devincre, G. Daveau …	ONERA, Paris
T. Hoc, B. Chiron…	ECP, Paris
O. Sicardy, J. Villanova…	CEA-Grenoble/LITEN
P. Goudeau, G. Geandier…	CNRS Phymat, Poitiers, France
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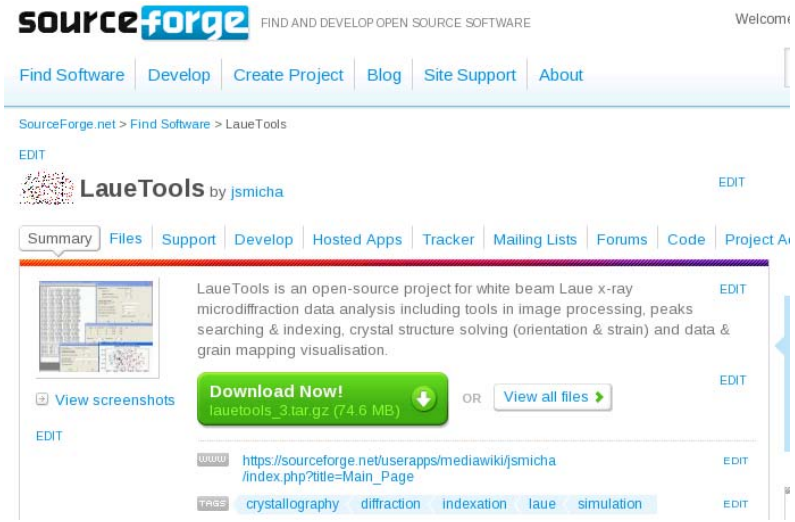
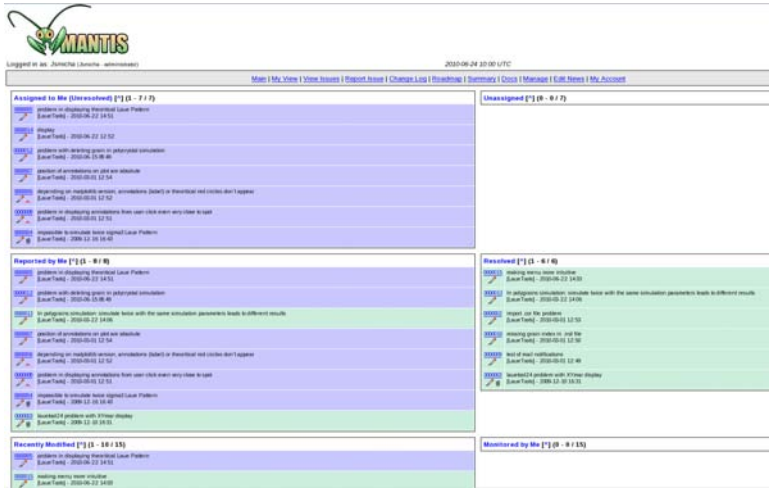
P. Lamontagne, L. Doyen …	ST microelectronics
H. palancher, A. Richard, P. Martin…	CEA-Cadarache/DEN
GDR Mecano	

…

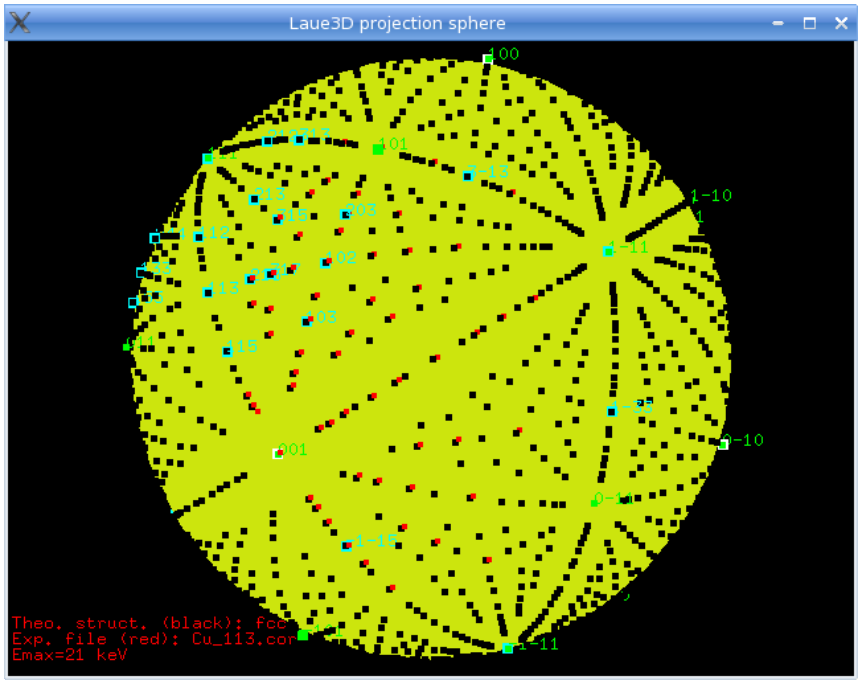
Need support…

python packages distribution
- Using existing functionalities/libraries
- Codes refactoring
- bugs / new functionalities
- Linking to existing framework/similar projects
- Software development
-…

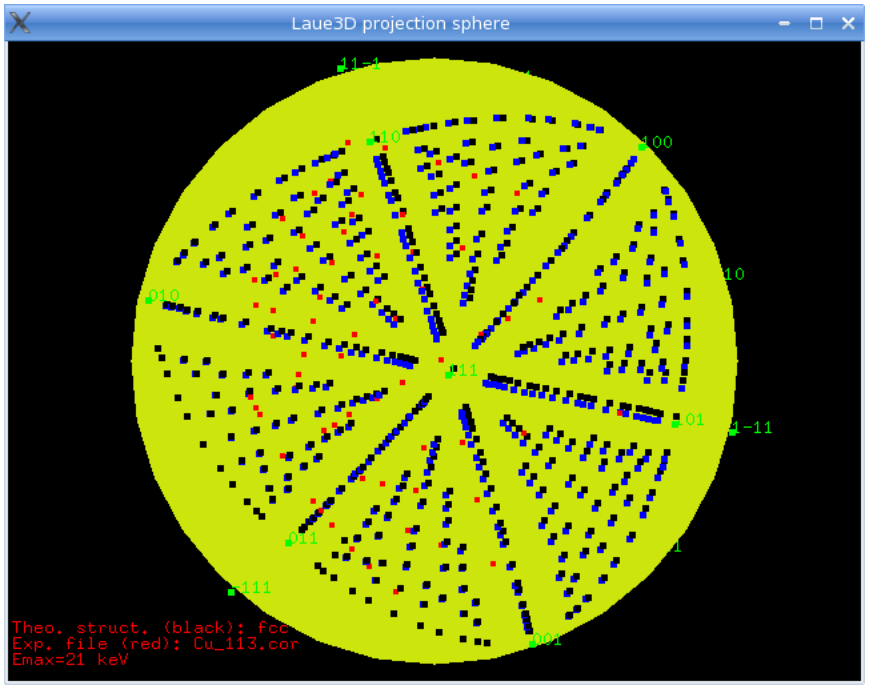




https://sourceforge.net/projects/lauetools/

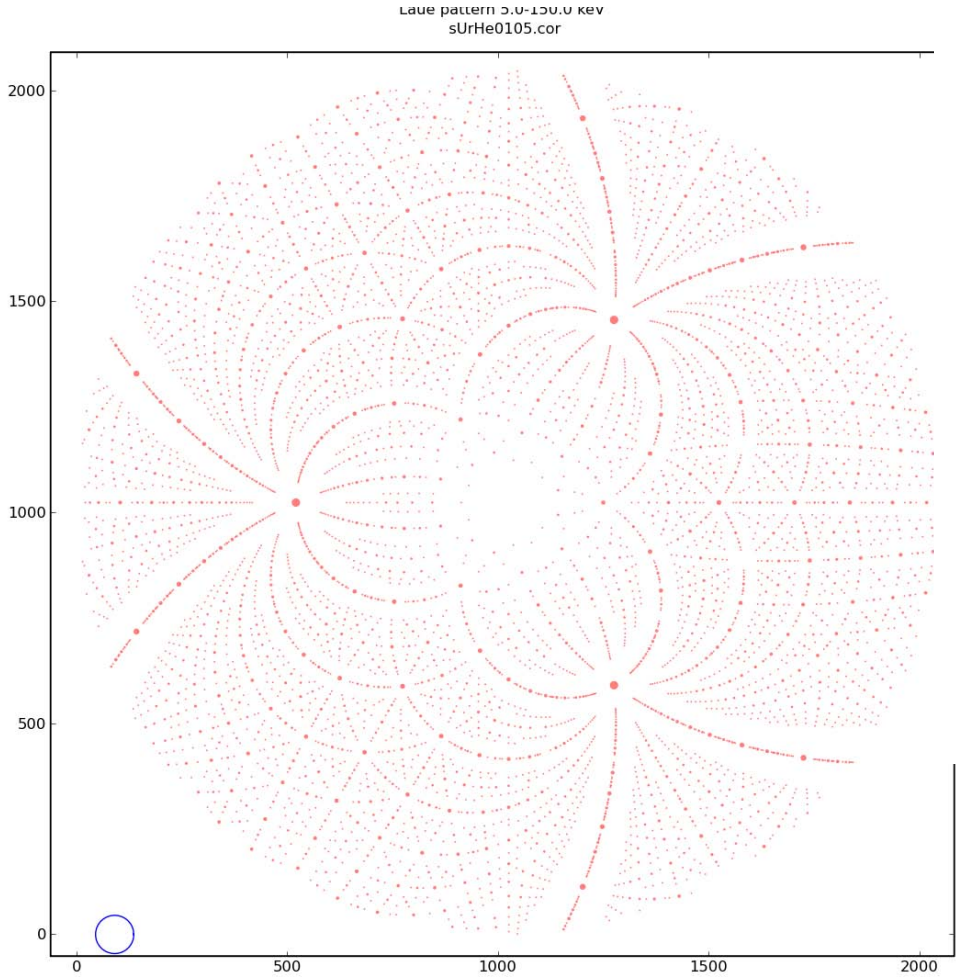


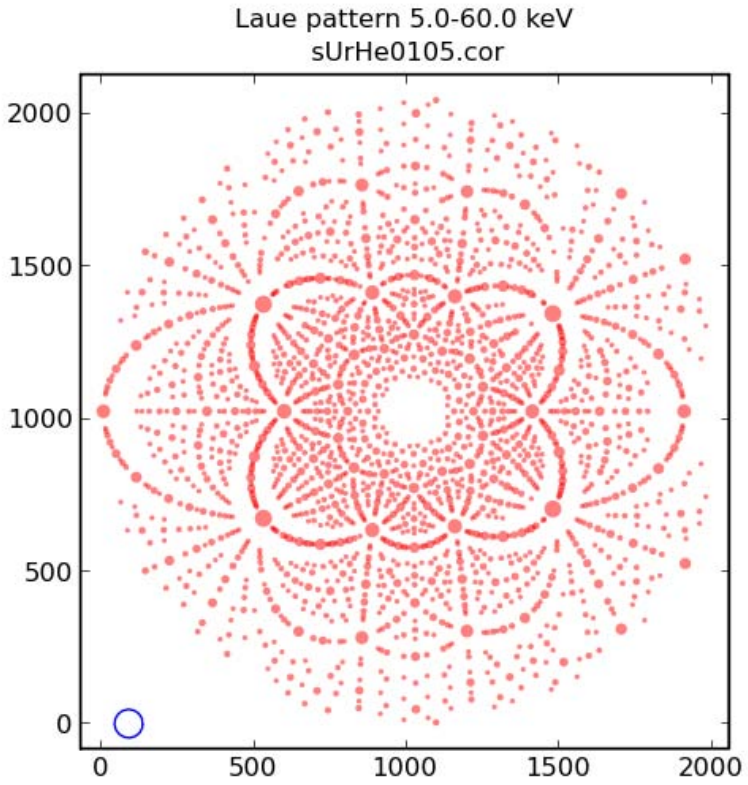
Orientation matrix found by pattern matching



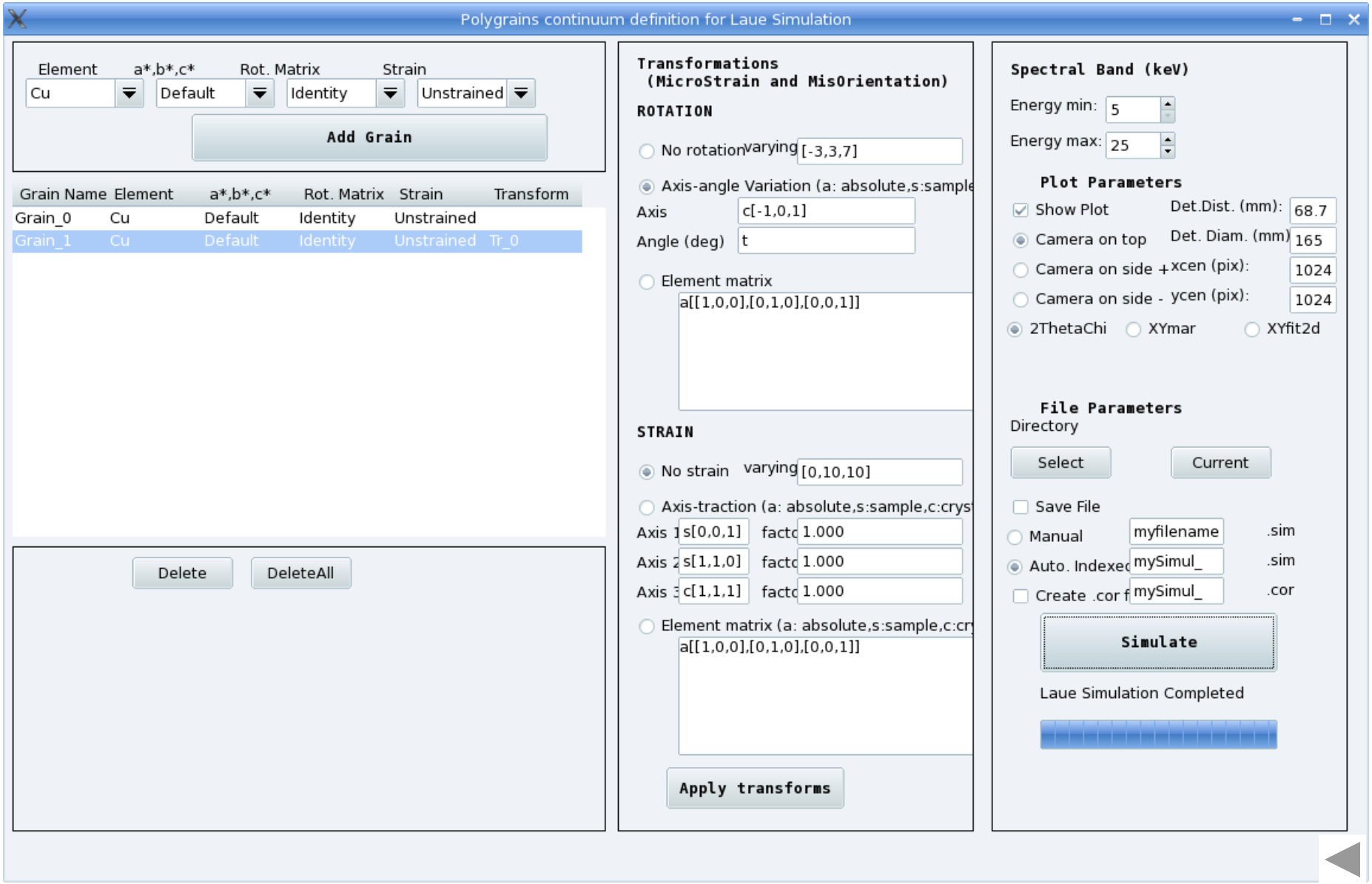
Strain simulation

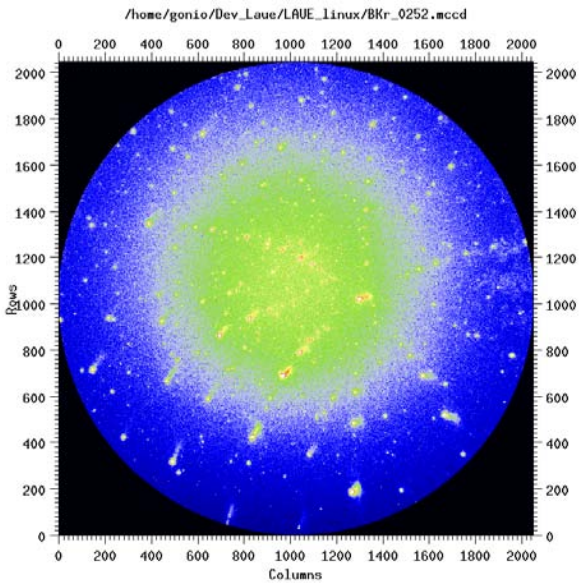
Transmission

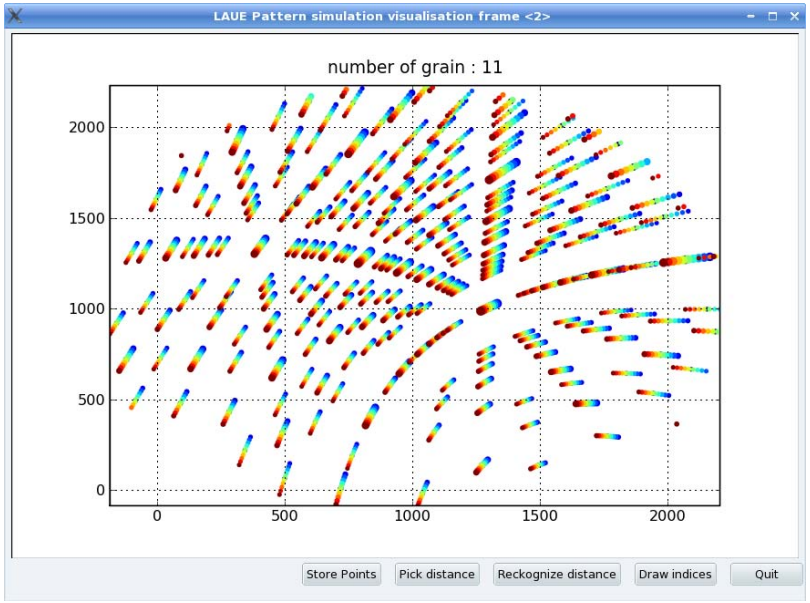




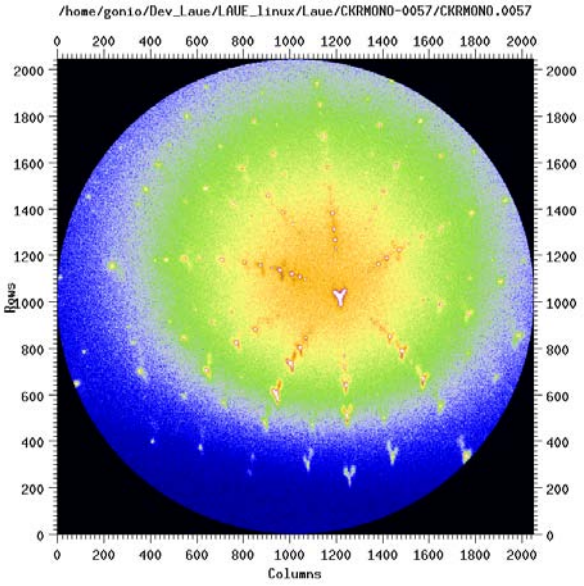
Back-reflection

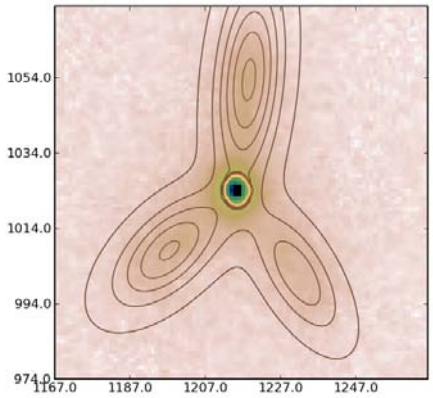

Polygrains continuum definition for Laue Simulation
Element
a*,b*,c*
Rot. Matrix
Strain
Cu
Default
Identity
Unstrained
Add Grain
Grain Name
Element
a*,b*,c*
Rot. Matrix
Strain
Transform
Grain_0
Cu
Default
Identity
Unstrained
Grain_1
Cu
Default
Identity
Unstrained
Tr_0
Delete
DeleteAll
Transformations
(MicroStrain and MisOrientation)
ROTATION
No rotation
varying
[-3,3,7]
Axis-angle Variation (a: absolute,s:sample
Axis
c[-1,0,1]
Angle (deg)
t
Element matrix
a[[1,0,0],[0,1,0],[0,0,1]]
STRAIN
No strain
varying
[0,10,10]
Axis-traction (a: absolute,s:sample,c:crys
Axis 1
s[0,0,1]
facto
1.000
Axis 2
s[1,1,0]
facto
1.000
Axis 3
c[1,1,1]
facto
1.000
Element matrix (a: absolute,s:sample,c:cr
a[[1,0,0],[0,1,0],[0,0,1]]
Apply transforms
Spectral Band (keV)
Energy min:
5
Energy max:
25
Plot Parameters
Show Plot
Det.Dist. (mm):
68.7
Camera on top
Det. Diam. (mm)
165
Camera on side +
xcen (pix):
1024
Camera on side -
ycen (pix):
1024
2ThetaChi
XYmar
XYfit2d
File Parameters
Directory
Select
Current
Save File
Manual
myfilename
.sim
Auto. Indexed
mySimul_
.sim
Create .cor f
mySimul_
.cor
Simulate
Laue Simulation Completed





Slip system activated !





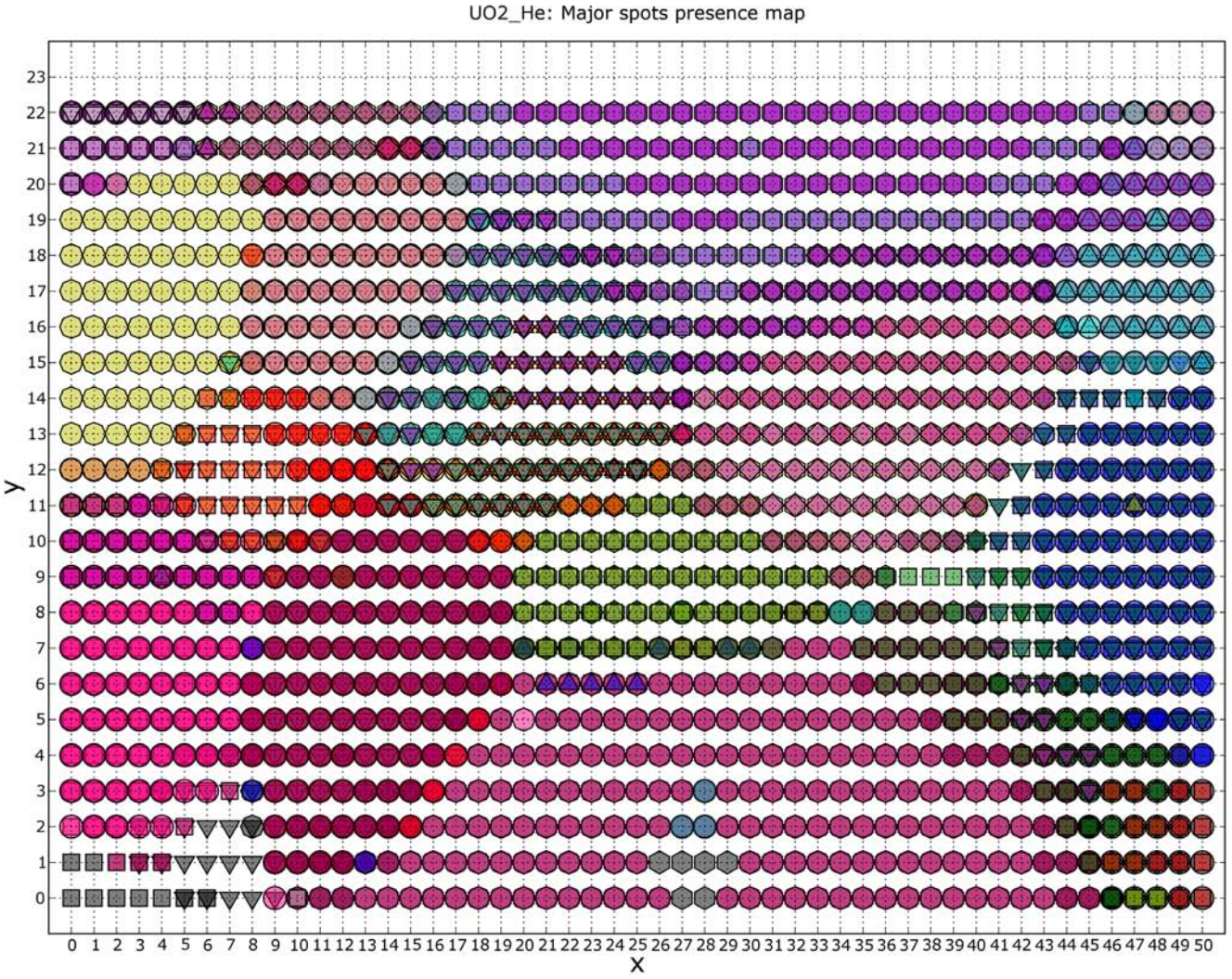
3% tetragonal strain along a*,b*,c*

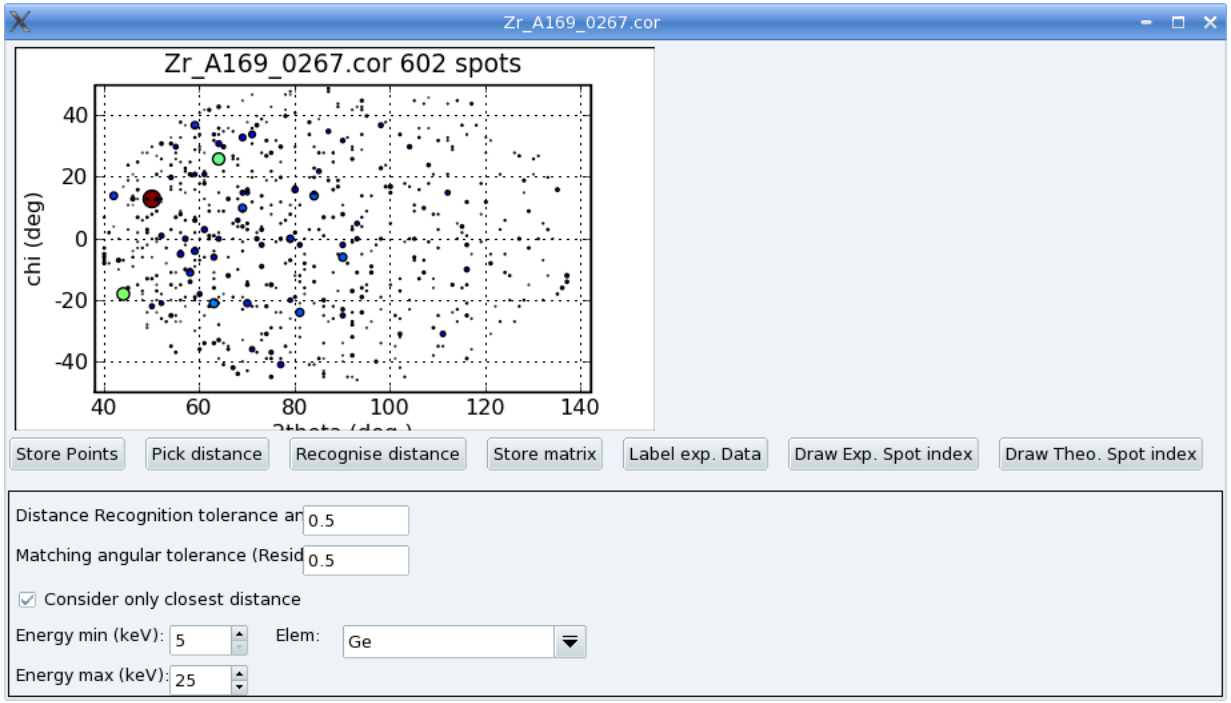
LaueTools Simulation & Indexation Program v1.0 2009 Zr_A169_0267.cor

File Plot Calib. Tools Indexation Sequence Simulation Parameters About

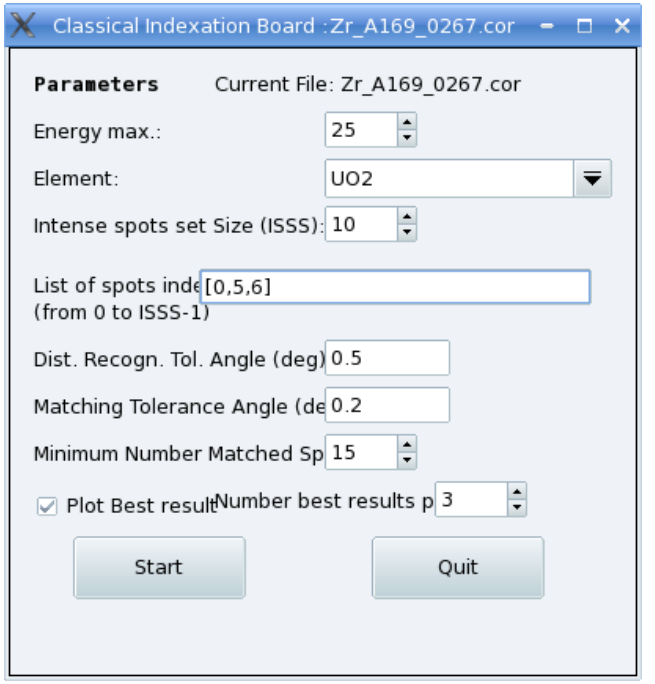
Simulation Data from LAUE Pattern Program v1.0 2009
spot# h k l E 2theta chi X Y
#G 0 Grain_0 0 956

0	-28	-10	-8	58.30012	130.8445	-128.6598	2730.1702	944.0748
1	-9	-11	-9	54.14559	64.6871	-129.2894	2745.6740	-521.1022
2	-11	-7	-1	26.76841	114.5322	-98.1301	2169.8161	393.1338
3	-17	-9	-9	45.68217	106.3555	-135.0000	2900.7127	353.9036
4	-3	-7	3	38.45676	43.0009	-66.8014	1682.5517	-994.8315
5	-24	-10	8	53.09329	123.8318	-51.3402	1365.8298	731.9118
6	-25	-9	-5	50.34966	135.2338	-119.0546	2521.7293	983.4620
7	-23	-9	-1	45.74383	137.0197	-96.3402	2142.7459	920.6826
8	-28	-10	8	58.30012	130.8445	-51.3402	1365.8298	944.0748
9	-25	-9	5	50.34966	135.2338	-60.9454	1574.2707	983.4620
10	-10	-10	8	45.45933	75.9703	-51.3402	1365.8298	-272.8681
11	-7	-5	-5	24.35321	89.4212	-135.0000	2900.7127	-12.1816
12	-17	-11	5	44.06152	109.1921	-65.5560	1660.4033	326.0372
13	-11	-7	-7	34.28235	96.0285	-135.0000	2900.7127	127.3532
14	-9	-11	1	38.83941	78.3478	-84.8056	1970.4807	-176.5718
15	-17	-13	5	48.92348	101.3433	-68.9625	1720.0336	183.2754
16	-9	-13	1	48.02312	69.2322	-85.6013	1982.4067	-324.3224
17	-24	-14	0	55.38921	119.4871	-90.0000	2048.0000	482.1887
18	-11	-15	3	55.57184	71.4393	-78.6901	1877.4575	-291.9895
19	-19	-7	3	37.97341	136.3152	-66.8014	1682.5517	971.3231
20	-13	-9	5	36.42575	103.2436	-60.9454	1574.2707	229.5765
21	-22	-10	-12	56.98071	109.2488	-140.1944	3071.2553	465.1160
22	-19	-13	11	58.99925	96.2613	-49.7636	1326.4738	122.5559
23	-19	-13	-3	48.84885	109.8475	-102.9946	2244.7799	315.8835
24	-18	-12	4	46.30117	109.8064	-71.5651	1763.7624	323.7150
25	-12	-6	-2	26.40315	124.4174	-108.4349	2332.2376	615.8481
26	-11	-11	-1	38.03932	89.7642	-95.1944	2125.5193	-3.5236
27	-21	-13	5	52.06832	112.8908	-68.9625	1720.0336	385.7510
28	-15	-15	1	51.77313	89.8730	-86.1859	1991.1525	-1.8949
29	-13	-15	5	55.49959	78.8536	-71.5651	1763.7624	-177.1019
30	-18	-12	10	54.33691	98.0967	-50.1944	1337.4061	157.9098
31	-15	-9	-1	35.24246	117.7619	-96.3402	2142.7459	451.6219
32	-8	-14	0	55.96319	59.4898	-90.0000	2048.0000	-502.4914
33	-14	-12	-12	59.53008	79.0424	-135.0000	2900.7127	-233.4809
34	-5	-9	-5	45.11494	51.8064	-119.0546	2521.7293	-767.4415
35	-10	-4	-2	20.66333	131.8103	-116.5651	2474.3564	852.7127
36	-4	-4	2	15.49750	83.6206	-63.4349	1621.6436	-106.5891
37	-19	-7	-5	39.42346	131.2823	-125.5377	2657.0805	920.0322
38	-15	-11	5	42.58943	102.2946	-65.5560	1660.4033	204.1343

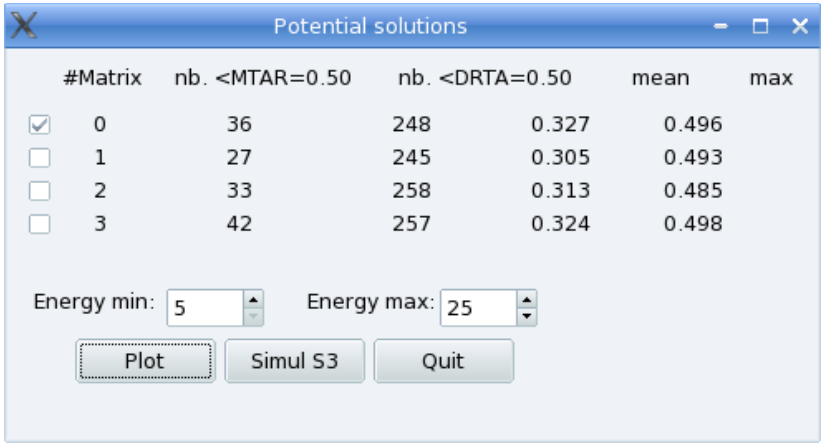

UO2_He: Major spots presence map
y
x
0 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23
0 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39 40 41 42 43 44 45 46 47 48 49 50

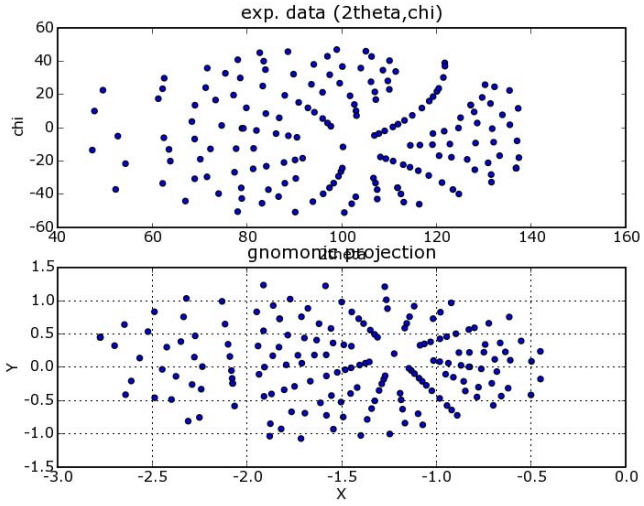


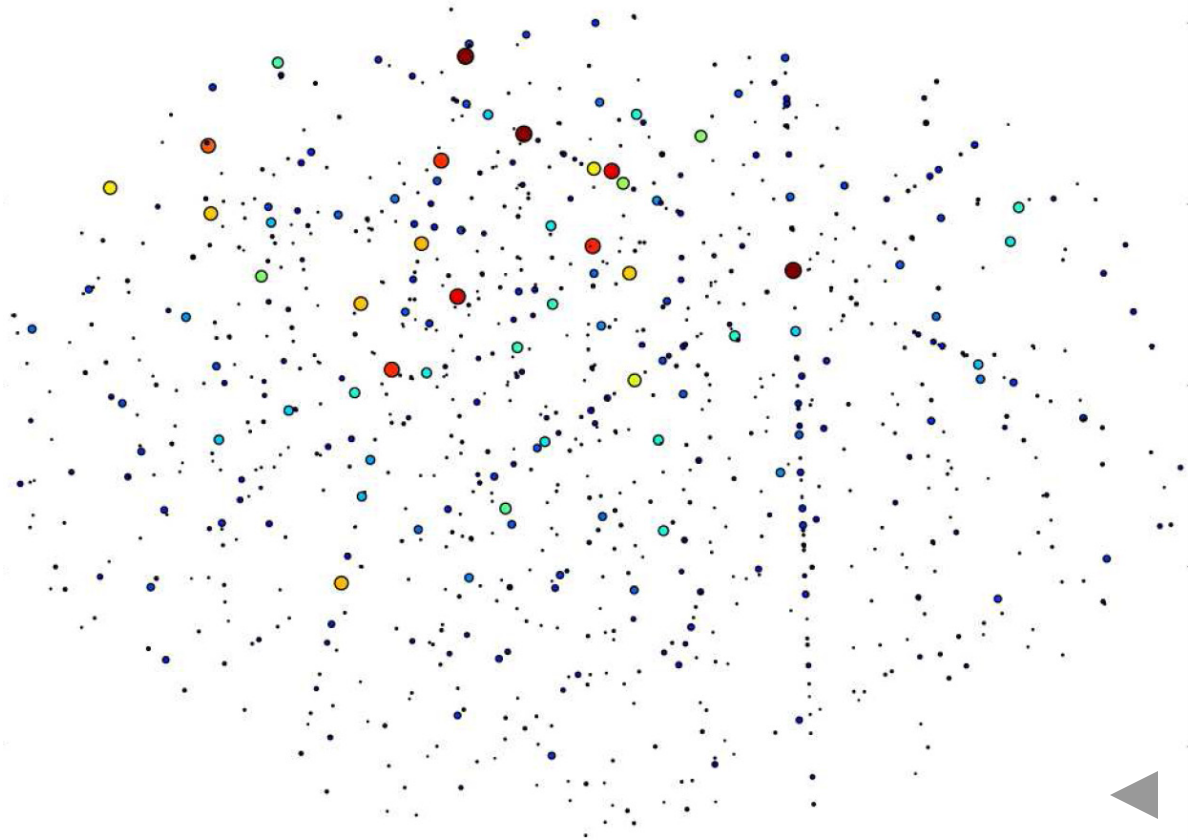
Human-aided indexing



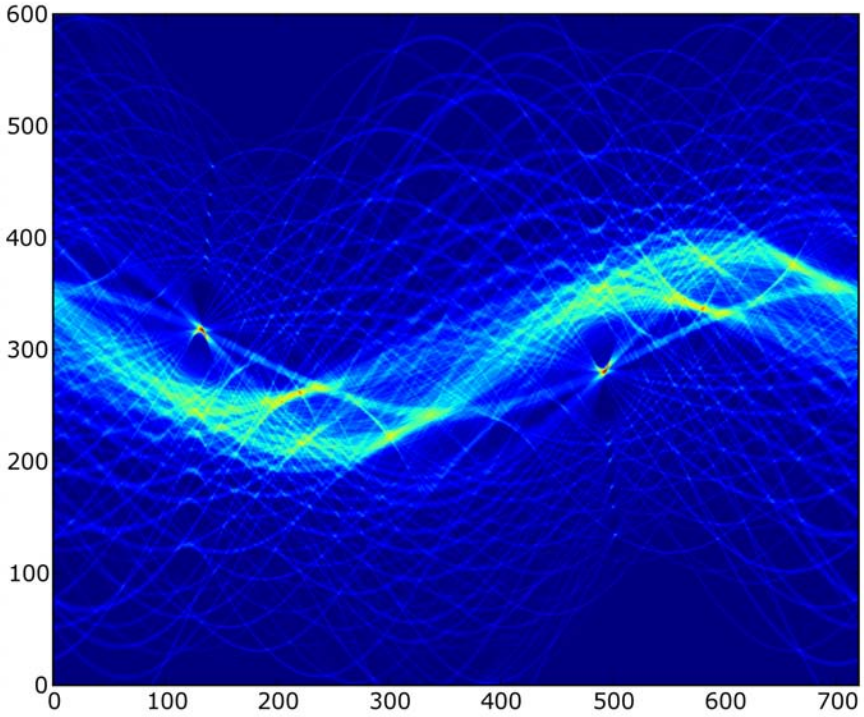
Automatic indexing




exp. data (2theta,chi)
chi
60
40
20
0
-20
-40
-60
40
60
80
100
120
140
160
gnomonic projection
Y
X
1.5
1.0
0.5
0.0
-0.5
-1.0
-1.5
-3.0
-2.5
-2.0
-1.5
-1.0
-0.5
0.0



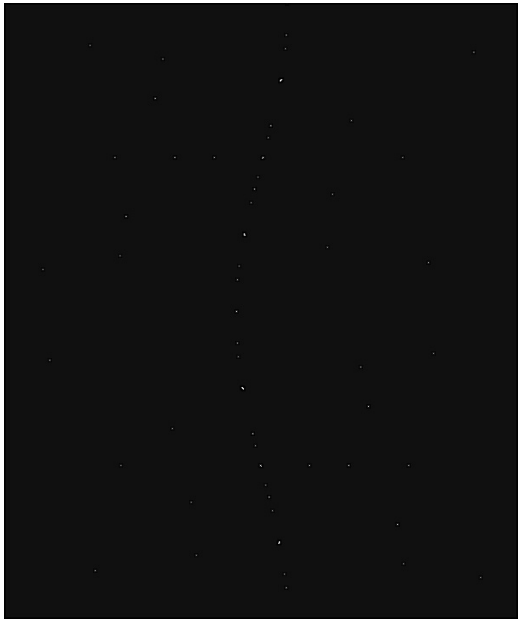
Hough space



Data 27000 most intense pixel

matching

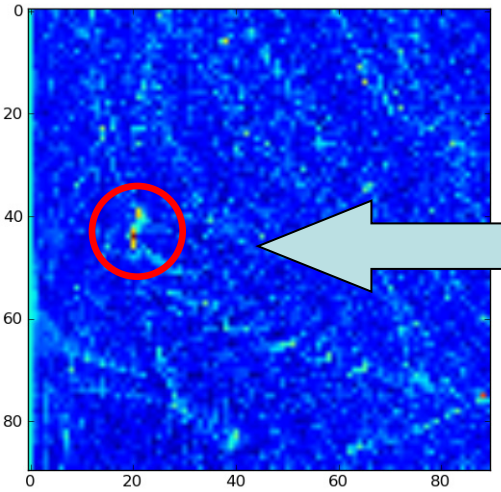
Databank of …

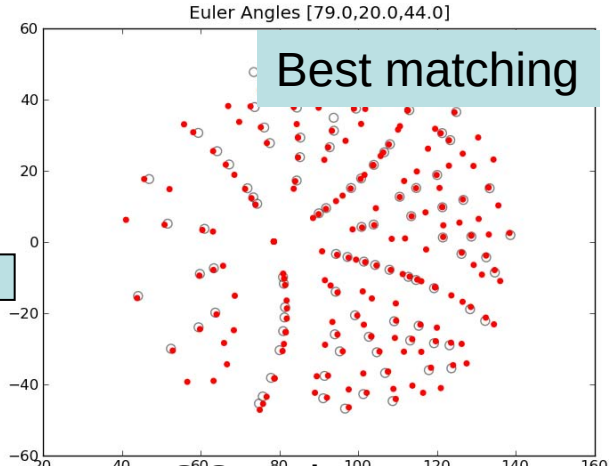


… Fingerprint of each crystal orientation:
$\phi 1, \phi 2, \phi 3$

Only few non zeros pixels

Euler space
Matching intensity solution

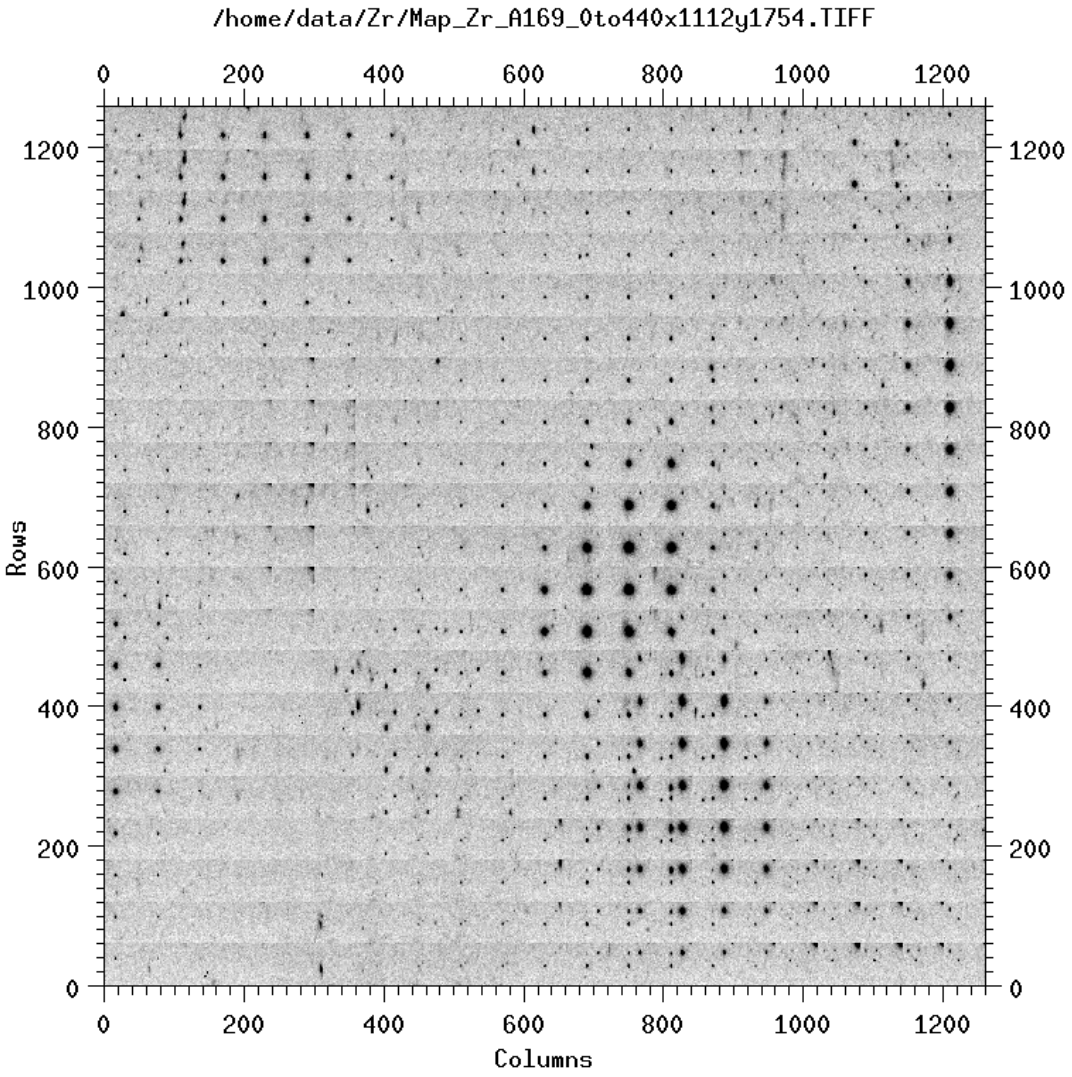




Best matching

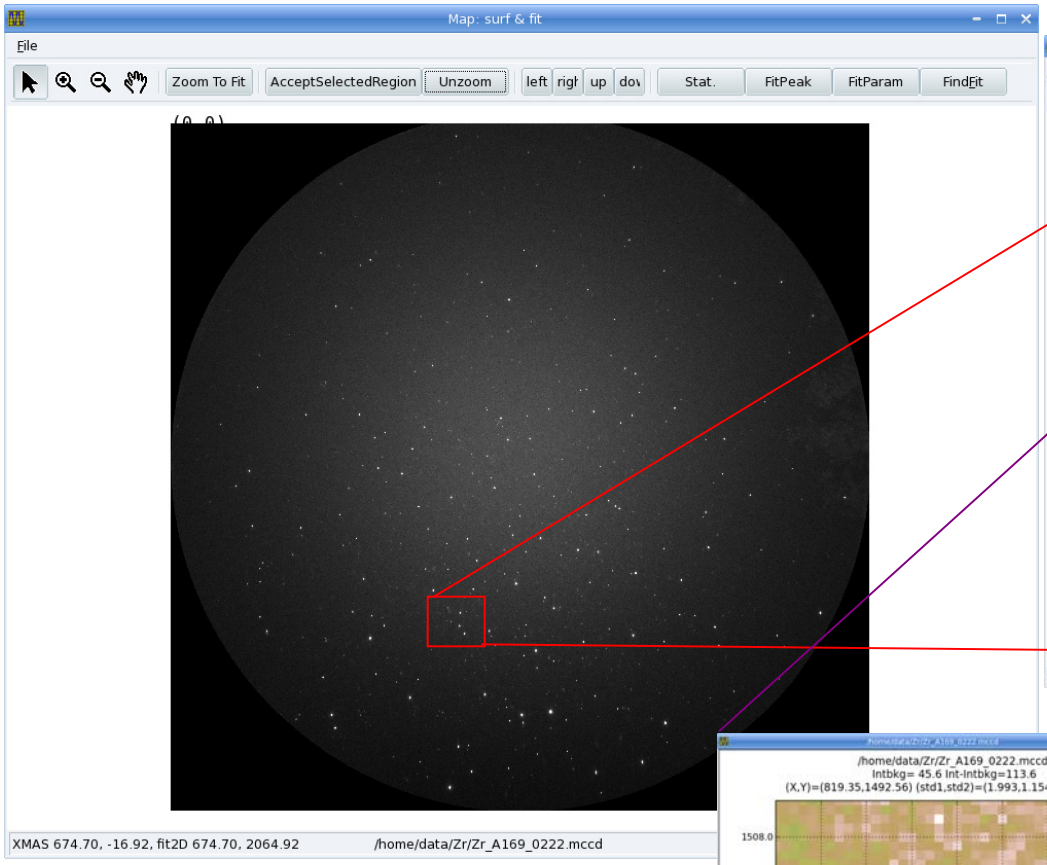
CCD plane space

mosaic

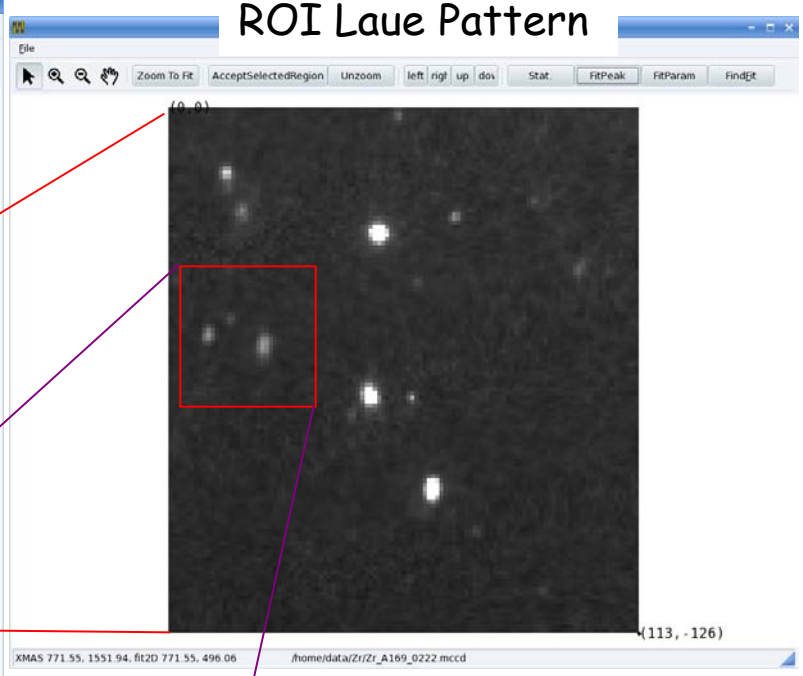


2D microLaue pattern ROI
Grain mapping

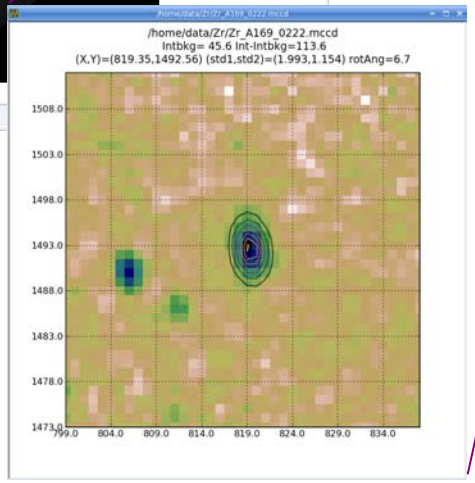
Images set navigator & processing



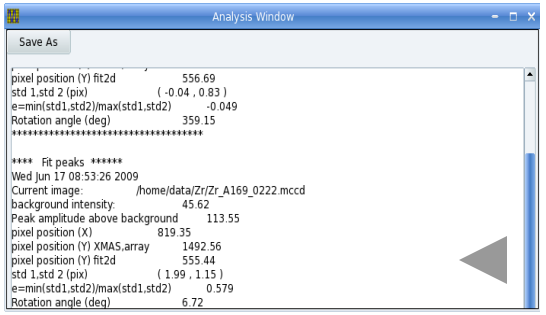
ROI Laue Pattern



2D intensity fitting



results, batchable



Navigation on images dataset : Full Pattern

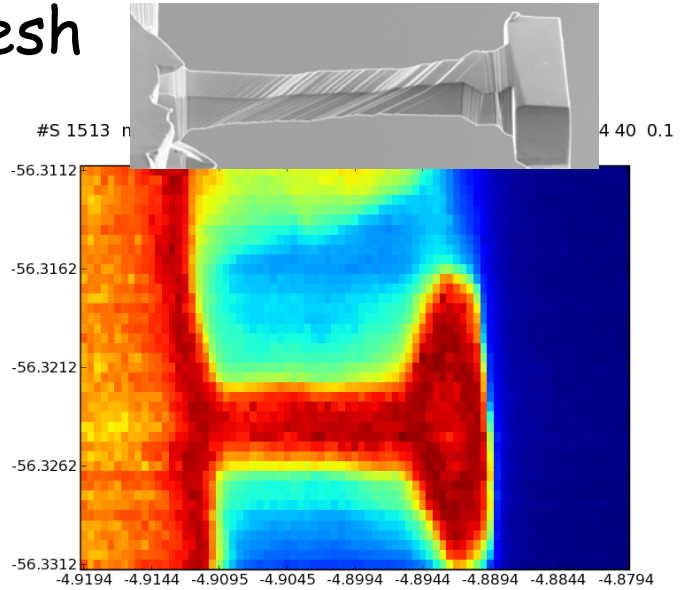
Mapcanvas.py

fit2Dintensity.py

Plotmesh

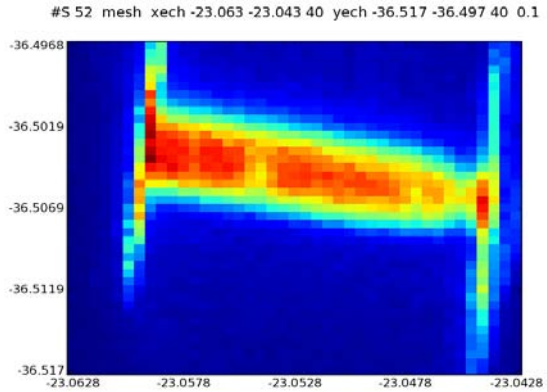
2D fluorescence mapping visualisation

(sub)Micropositioning



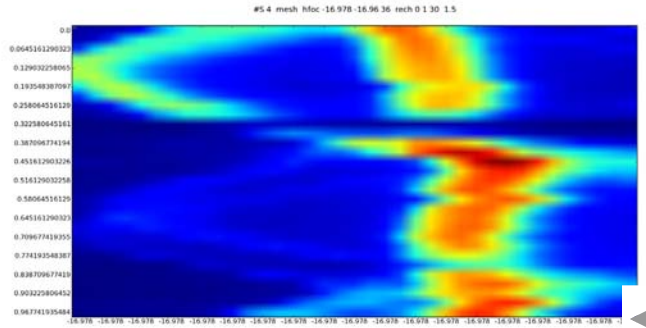
Data from J. Keckes on BM32

Sample alignement
Chemical element localisation



Data from P. Bleuet on BM32

Tomography's sinogram



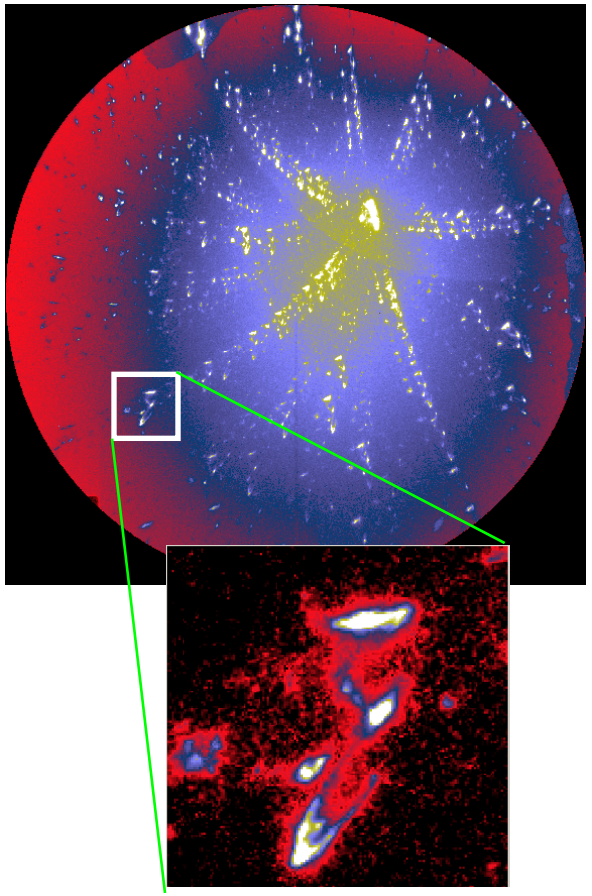
µLaue Perspectives on BM32

Better instruments

- more flux, smaller beam (fixed-curvature KB)
- Faster CCD camera
- Energy-resolved detection

Smarter and more automated Analysis

- software development
- peak shape analysis/modelling



µLaue Perspectives on BM32

Better instruments

+

Smarter and more automated Analysis

=

3D grain mapping
- full strain tensor
- micrometric resolution