

FABLE – TotalCryst –  
And some ideas on how to  
“remove all possible causes why  
the user shouldn’t publish data  
collected at a synchrotron”

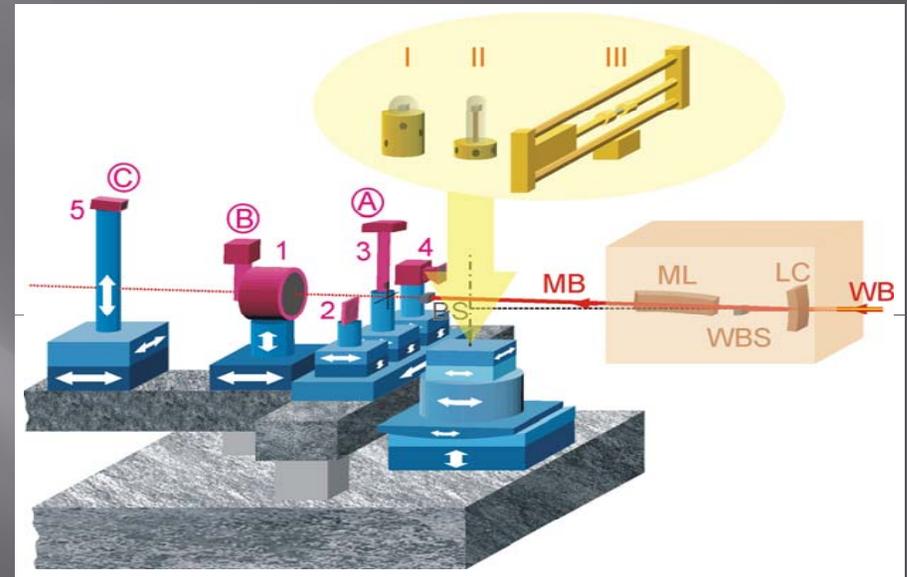
Søren Schmidt

# Outline

- ▣ FABLE
- ▣ TotalCryst
- ▣ (McXtrace)
- ▣ ... and some ideas

# Outline

- ▣ FABLE
- ▣ TotalCryst
- ▣ (McXtrace)
- ▣ ... and some ideas



3DXRD, ID-11 ESRF

# FABLE

## Fully Automatic BeamLines and Experiments

More than 10 developers: From ESRF, Risø DTU, Copenhagen University and APS

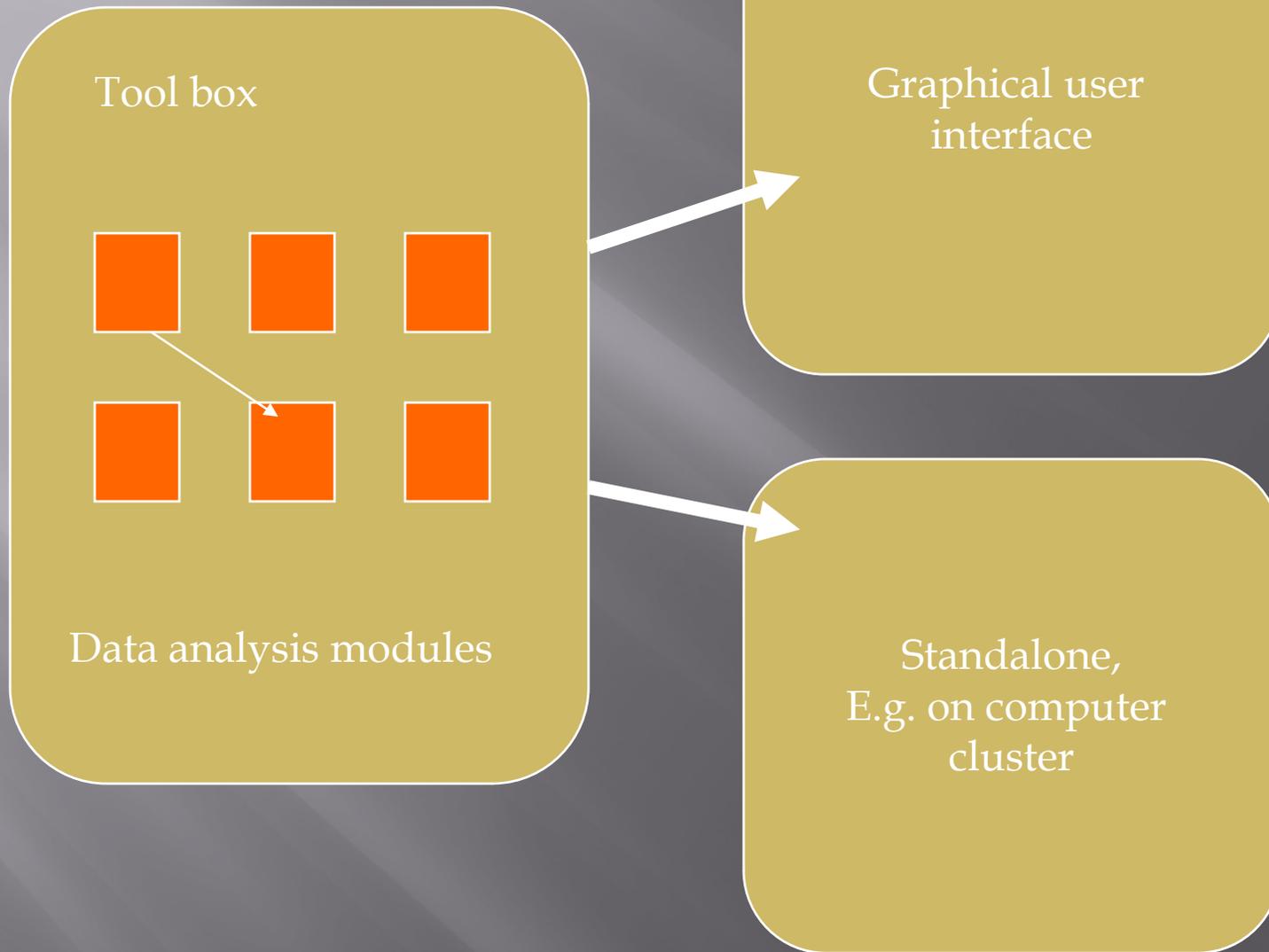
Collaboration initiated between ESRF and Risø DTU in 2003

Later by funded by the EU program: TotalCryst, headed by Risø DTU (M4D).

3DXRD microscopes

ESRF, France  
APS, USA  
PETRA-III, Germany  
SPring-8, Japan





# Fable ImageViewer

File Edit ImageViewer PolyXSim Preprocessor PeakSearch Transformation GrainSpotter Tools Window Help

Transformation (Small Screen) PeakSearch (Small Screen) ImageViewer PolyXSim

Image Navigator Header X\_0\_1.dm3 Relief insulin\_4\_xtal\_1\_001.img

Freeze   Autoscale Minimum 39 Maximum 86

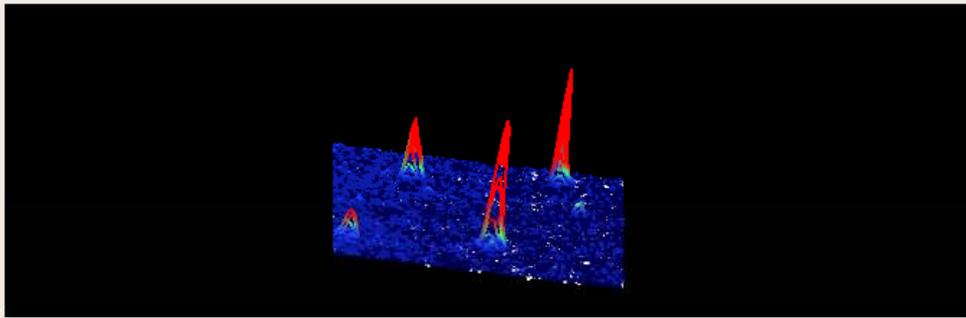
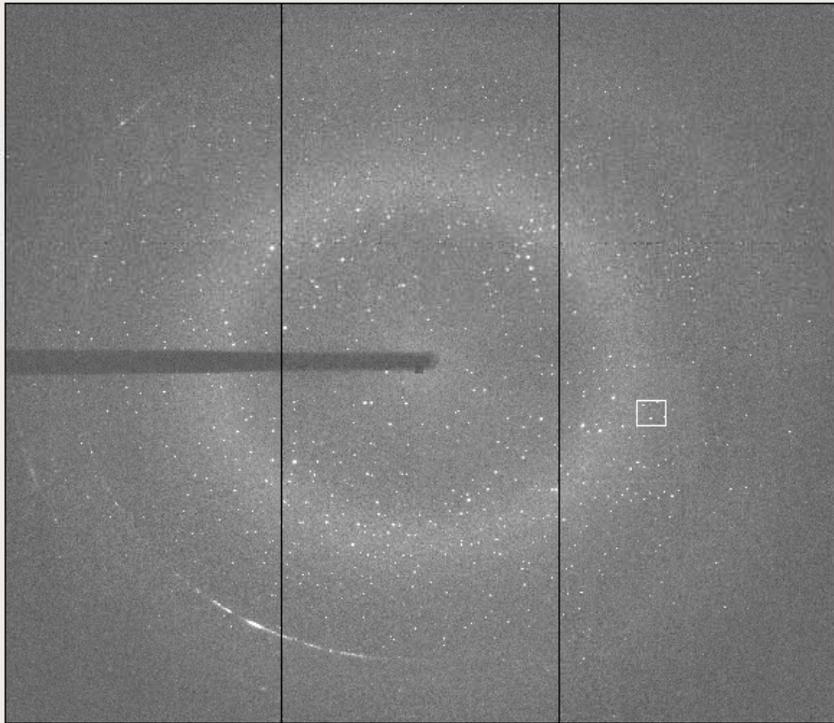


Image insulin\_4\_xtal\_1\_001.img

Original Image (-1 0 0 -1) TL=(0,0) Image Grayscale

Autoscale Intensity Min Intensity: 0.0 Max Intensity: 101.811516

Keep Aspect  Show Peaks Marker Size: 3



x=143 y=1398 value=47

Zoom area insulin\_4\_xtal\_1\_001.img

Original Image (-1 0 0 -1) TL=(0,0) Image Grayscale

Autoscale Intensity Min Intensity: 0.0 Max Intensity: 101.811516

Keep Aspect  Show Peaks Marker Size: 3



# Fable Transformation

File Edit ImageViewer PolyXSim Preprocessor PeakSearch Transformation GrainSpotter Tools Window Help

Transformation (Small Screen) Transformation PeakSearch (Small Screen) ImageViewer PolyXSim

**Parameters**

cell_a	4.1569	<input type="checkbox"/>
cell_b	4.1569	<input type="checkbox"/>
cell_c	4.1569	<input type="checkbox"/>
cell_alpha	90.0	<input type="checkbox"/>
cell_beta	90.0	<input type="checkbox"/>
cell_gamma	90.0	<input type="checkbox"/>
cell_lattice_[P,A,B,C,I,F,R]	P	
chi	0.0	<input type="checkbox"/>
distance	50000.0	<input checked="" type="checkbox"/>
fit_tolerance	0.05	
min_bin_prob	1.0E-5	
no_bins	10000	
o11	1	
o12	0	
o21	0	

**Column File Plot 0** Console

**mypeaks\_esrf\_t200.ftl**

Plot Options:

X	sc
Y	fc
Data	/home/osho/TotalCryst
<input type="checkbox"/> Remove Data	<input type="checkbox"/> Data
<input type="checkbox"/> Switch X Y	<input type="checkbox"/> Update
<input checked="" type="checkbox"/> Clear	

Plot Editor:

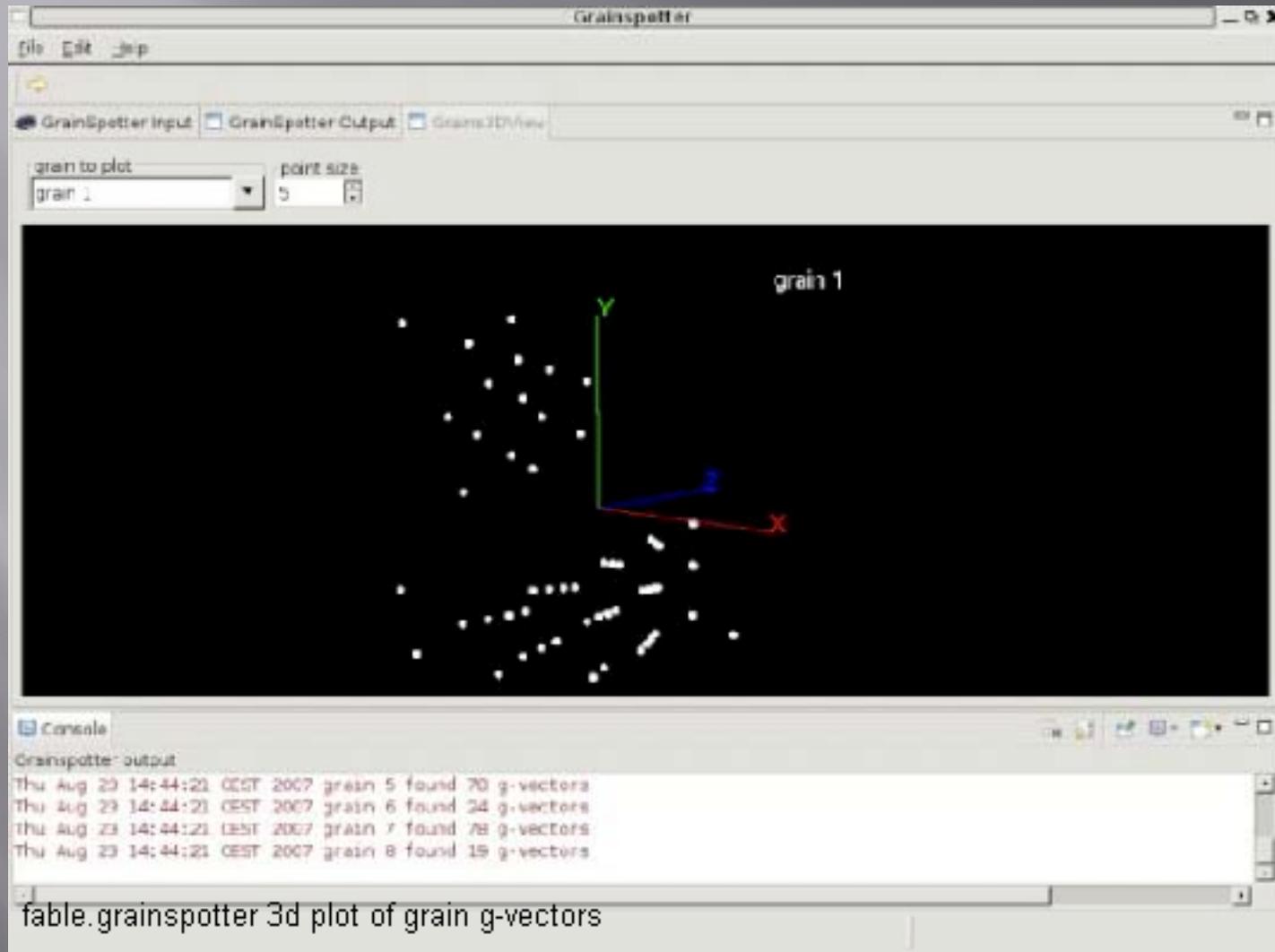
X Min	245.708122
X Max	1666.63580
Y Min	369.366372
Y Max	1725.66625
<input checked="" type="checkbox"/> Keep	<input checked="" type="checkbox"/> Remove

**Transformation Options**

Filtered peaks file: /home/osho/TotalCryst/bbcp\_15mu\_03\_12\_mon\_m\_/mypeaks\_esrf\_t200.ftl

Fit: ...

# Indexing



<http://fable.wiki.sourceforge.net>  
<http://sourceforge.net/apps/trac/fable/wiki>

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## FABLE

Fable is a framework for making [TotalCryst](#) experiments easy and efficient. It has been developed for doing grain mapping experiments in materials science at a synchrotron but could be applied to other types of experiments at synchrotrons or other sources e.g. neutrons. It provides the framework for sequencing the simulation, data taking and analysis online. It uses grid technologies when available for distributing automation tasks. Permanent configuration data are stored in a database (MySQL). Graphical interfaces are developed in Java using Eclipse/RCP and Python/Tk. This [project is hosted at sourceforge](#) and being developed by the staff of [ID11](#) at the [ESRF](#) (France) and [Riso National Laboratory](#), [Technical University of Denmark](#) (Denmark). The project is supported by the [EU Framework 6 NEST Adventure programme](#).

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### Workshop 1-3 April 2009, Grenoble France

We were very happy to welcome users for the first TotalCryst workshop in Grenoble. There were [talks](#) in the morning and demonstration the afternoon. Don't hesitate to have a look at the [talks](#) if you want to use the programs.

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### Users Corner

Fable is being developed for the TotalCryst user community. Users should check out :

- [Getting started with Fable](#)
- [Help desk](#) ;-)>

Please use our mailing list, [fable-talk](#), if you have any questions or see something on this wiki that could be improved.

In TotalCryst it is important to get the geometry right if you want to analyse data from different instruments. Here is a proposal for the TotalCryst geometry:

- [\[file:Geometry\\_version\\_1.0.7.pdf\]](#)

Download page for users

<http://sourceforge.net/projects/fable>

▼  fable	628.4 MB	2009-12-06	411	 
▼  2.0.0.Beta4	149.6 MB	2009-12-06	92	 
 <a href="#">fable_2_0_0_Beta4_win32_x86.zip</a>	82.6 MB	2009-12-06	75	
 <a href="#">fable_2_0_0_Beta4_linux_x86_64.tar.gz</a>	67.0 MB	2009-12-06	17	

## Fable software repository for developers:

**fable**

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**root** Visit:  View revision:

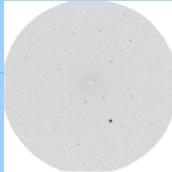
Name ▲	Size	Rev	Age	Last Change
▶ <a href="#">3Dstrain</a>		3793	8 months	h_osholm: moved code into trunk/src
▶ <a href="#">art2d</a>		1361	2 years	eknudsen: bugfix - yy and weight were accidentally declared as ints - they are now ...
▶ <a href="#">branches</a>		619	5 years	anonymous: This commit was manufactured by cvs2svn to create branch 'dev'.
▶ <a href="#">dserver</a>		1333	2 years	andy_gotz: compiled and tested with preprocessor with latest version of spd from ...
▶ <a href="#">fabian</a>		4623	8 weeks	h_osholm: Well does now skip an images if not available for calc of median - there ...
▶ <a href="#">fabio</a>		4734	20 hours	KennethEvans: Fixed bug in next().
▶ <a href="#">fable_python_metapackage</a>		4214	5 months	jpwright: make eggs on lapwright
▶ <a href="#">FableFacility</a>		3337	12 months	gaille_suchet: Correct return value of min and max
▶ <a href="#">fabric</a>		4731	7 days	h_osholm: bugfix: harvest always gave first grain id 0
▶ <a href="#">FitAllB</a>		4647	7 weeks	jetteodder: Bugfix related to options.killfile
▶ <a href="#">GrainMapper2D</a>		3473	10 months	soerenschmidt: GrainMapper?2D, first commit
▶ <a href="#">GrainSpotter</a>		4594	2 months	h_osholm: now GS also writes a .gff file
▶ <a href="#">GrainSweeper</a>		3582	10 months	soerenschmidt: removed system call to 'done reading images'
▶ <a href="#">gui</a>		4736	14 hours	KennethEvans: Corrected comment typo.
▶ <a href="#">id31sum</a>		4622	2 months	jpwright: Fix the ed before or after ef issue. ed now overrides ef
▶ <a href="#">ImageD11</a>		4714	3 weeks	KennethEvans: Removed setting ndigits=0 in PeakSearch? for GE detectors. Causes problems ...

And more

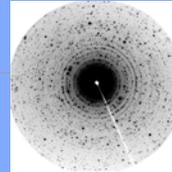
# TotalCryst



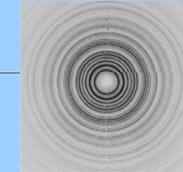
Irradiated crystallites



Single crystal



Polycrystalline compound



Powder

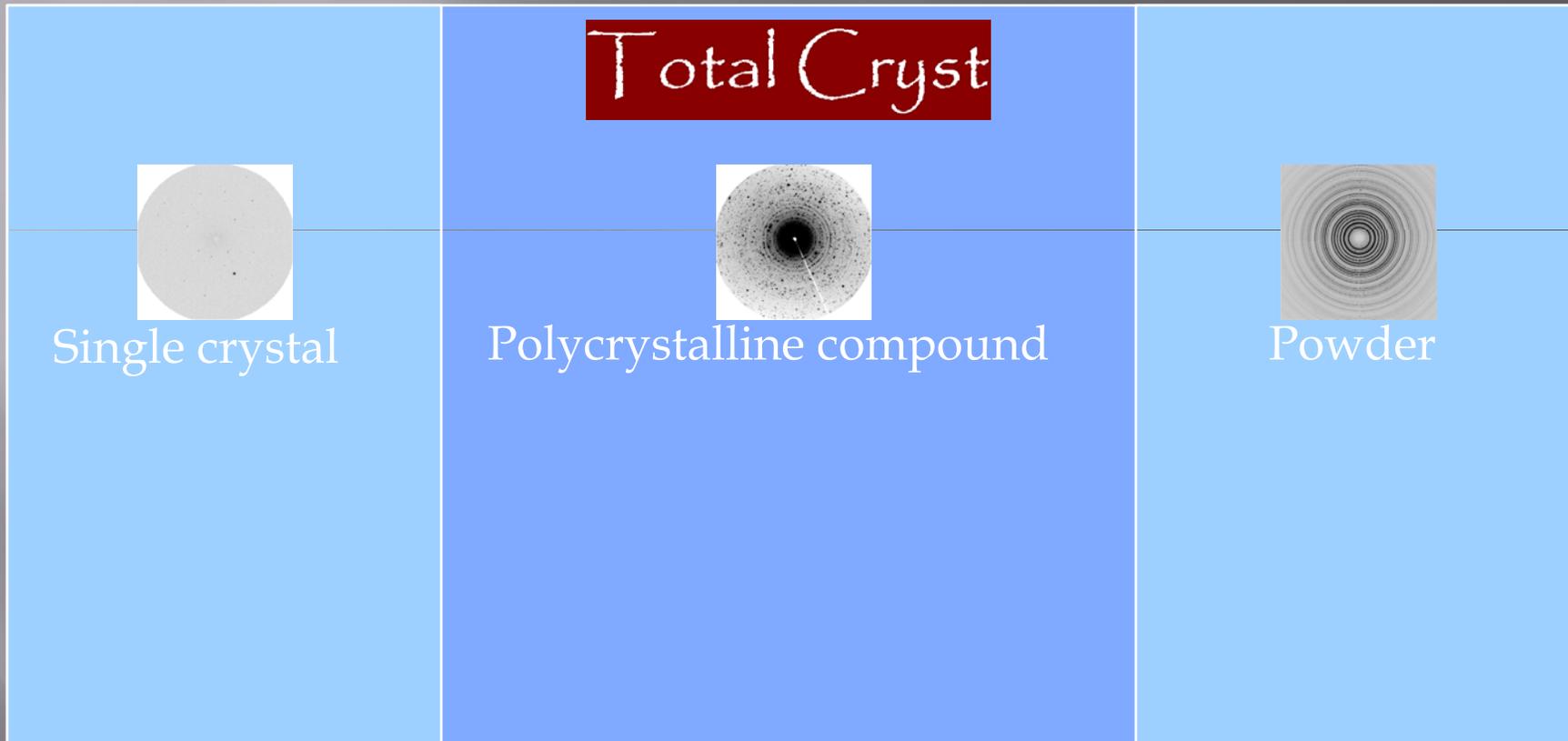


Structural Complexity

# TotalCryst



Irradiated crystallites



Single crystal

Polycrystalline compound

Powder

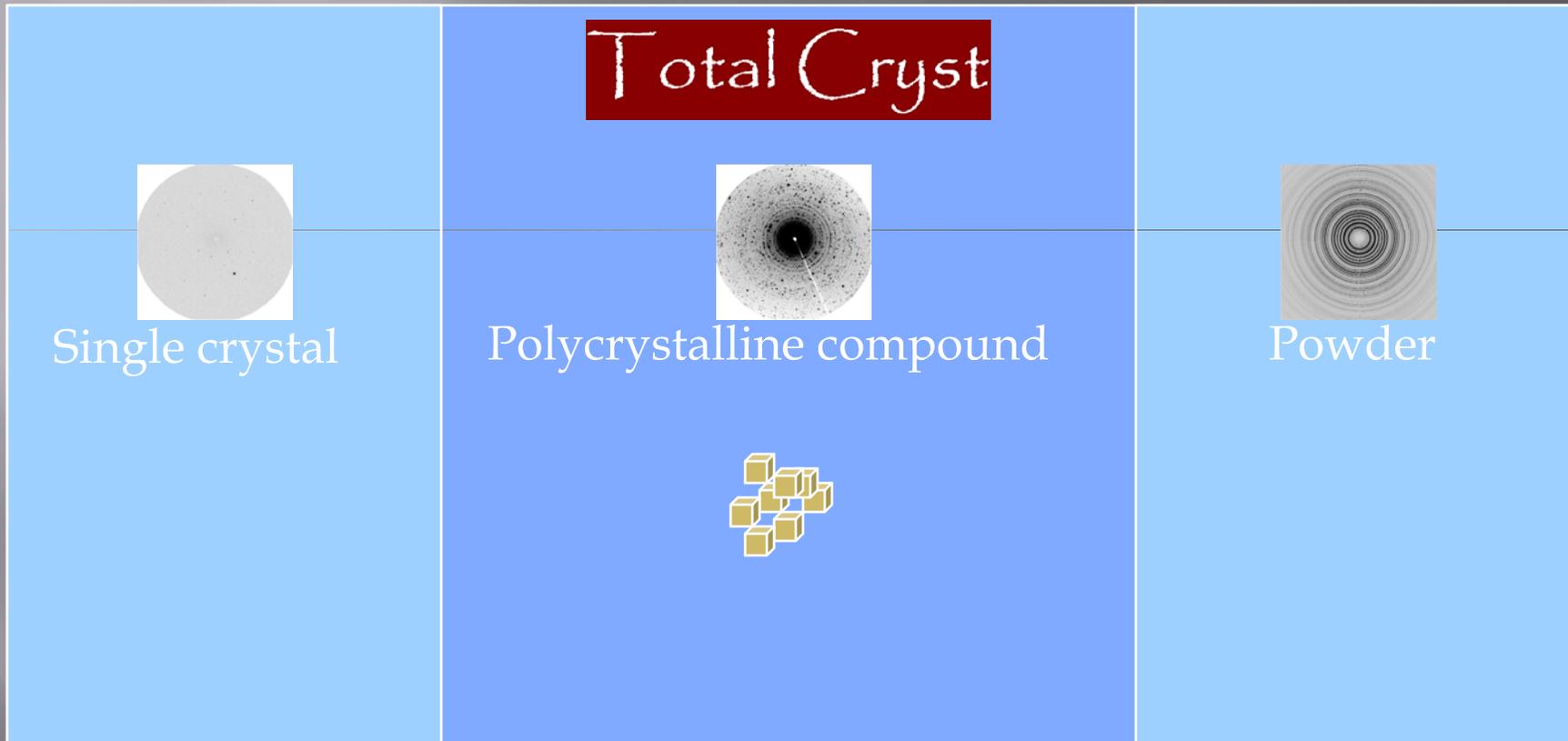


Structural Complexity

# TotalCryst



Irradiated crystallites



Single crystal

Polycrystalline compound

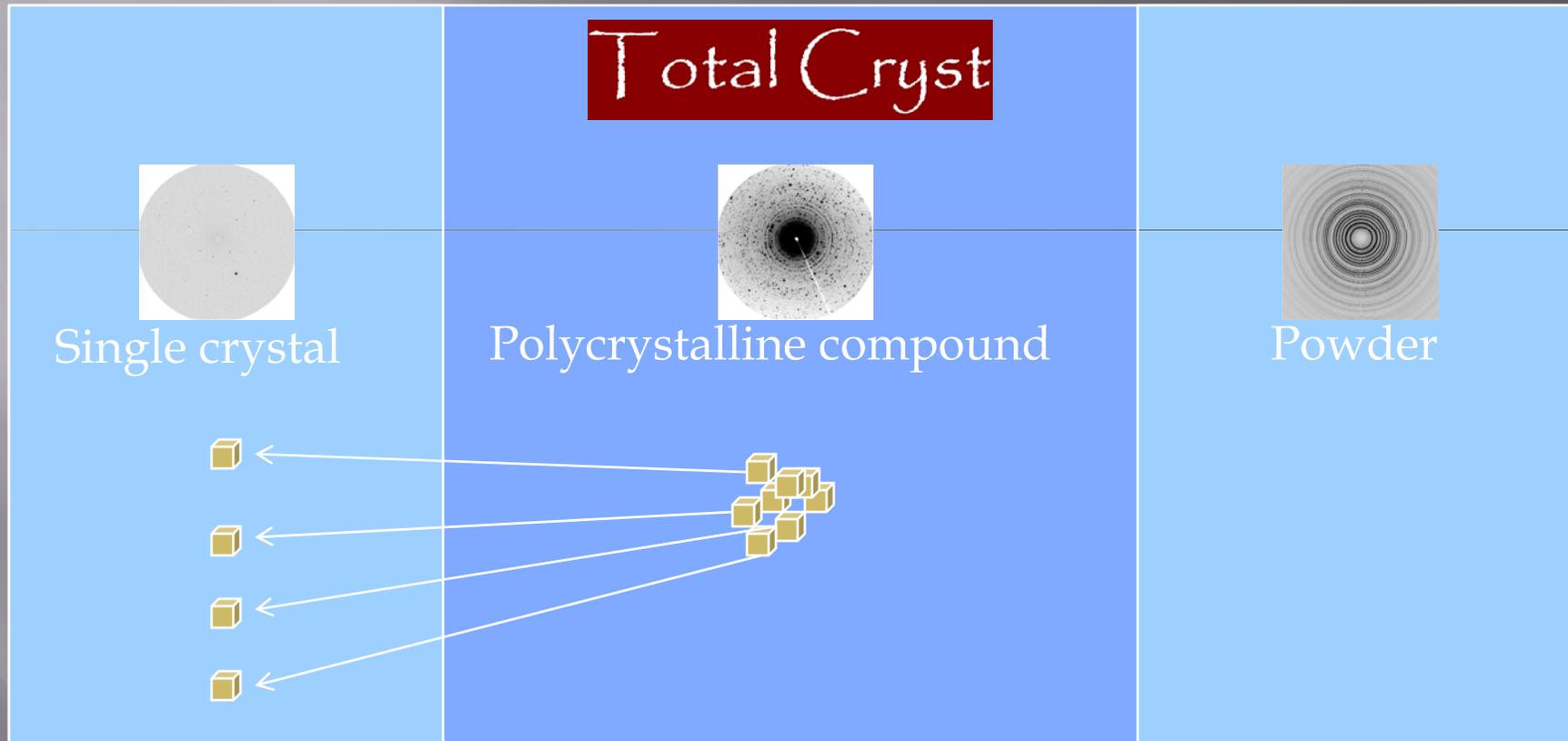
Powder

Structural Complexity

# TotalCryst



Irradiated crystallites



Single crystal

Polycrystalline compound

Powder

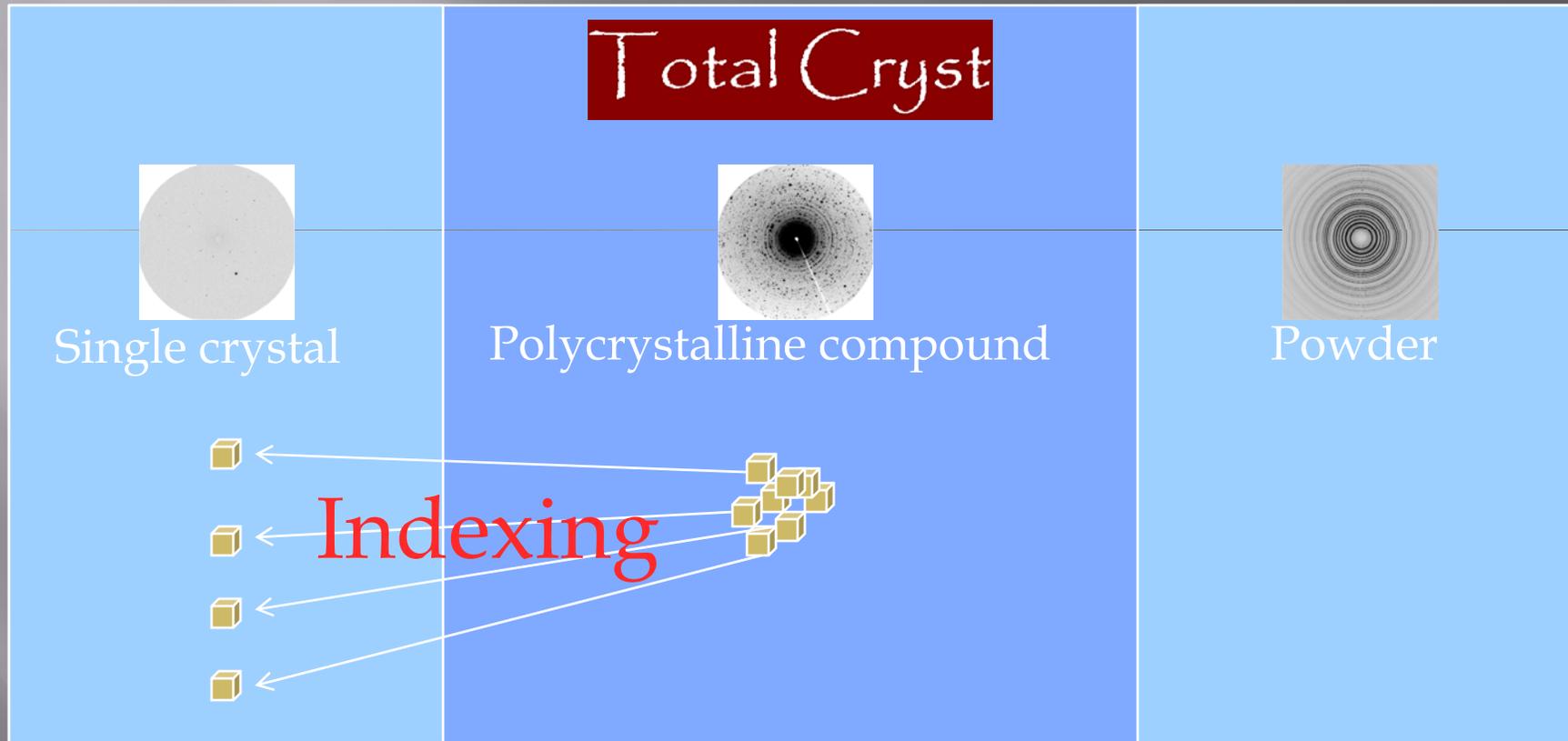


Structural Complexity

# TotalCryst



Irradiated crystallites

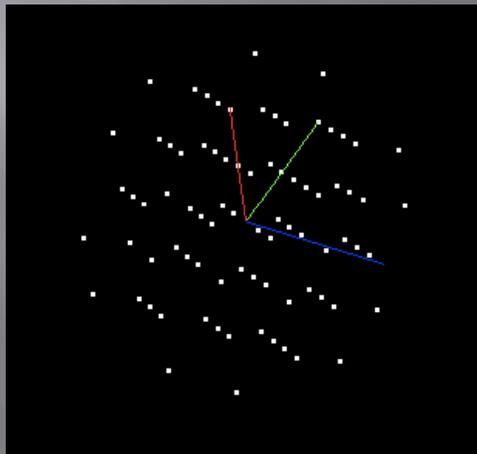


Structural Complexity

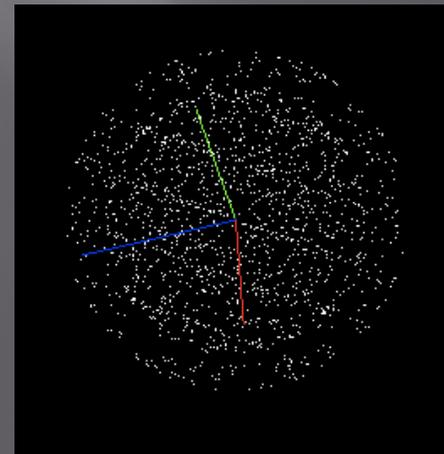
# Indexing polycrystalline compound with known crystallography (extracting orientations)

- Bravais Lattice and Unit cell parameters are known a priori from, typically,
  - Powders, radial spectra (Powder Indexing Programs)
  - Single crystal or few crystallites (single crystal indexing program)

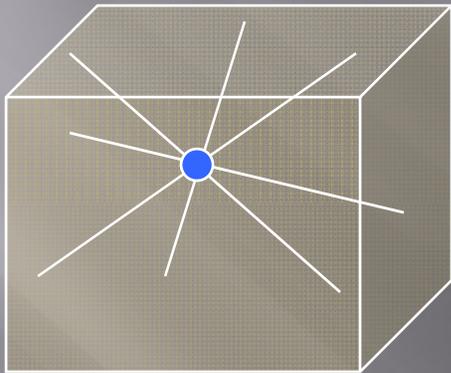
Indexing with known crystallography: Identifying *copies of the set of theoretical reflections* in the polycrystalline dataset.



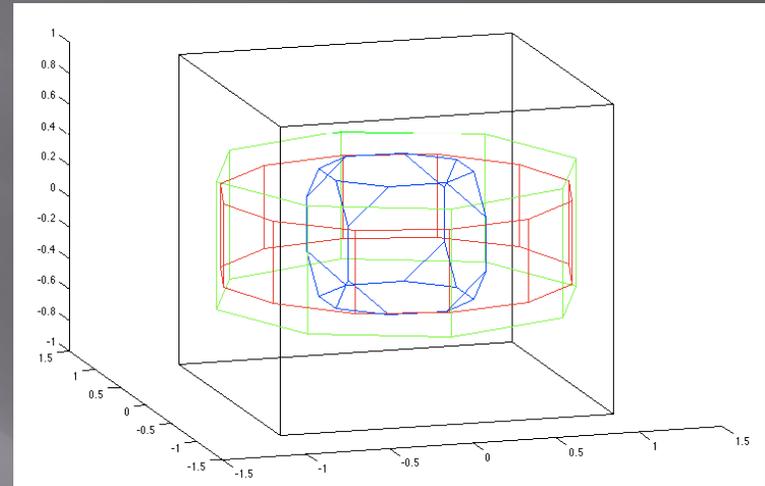
Rotations



# Rodrigues space

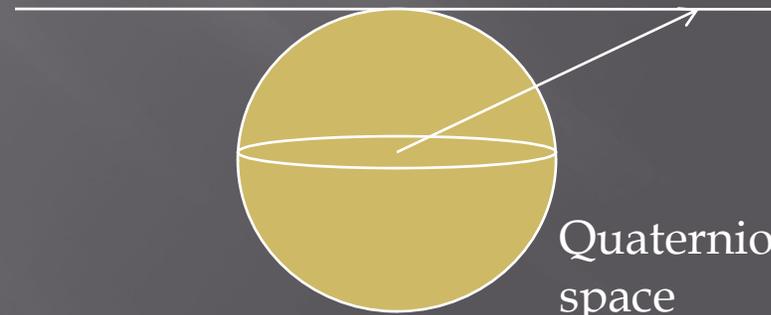


Rodrigues space



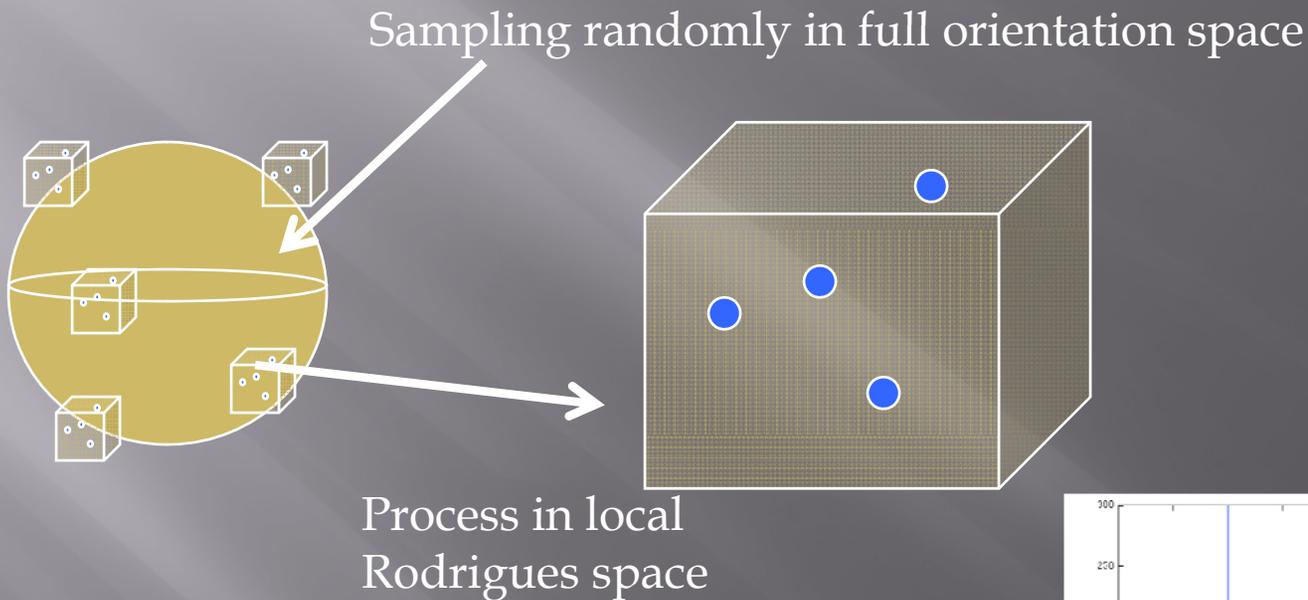
Limitation in orientation:

Rodrigues space

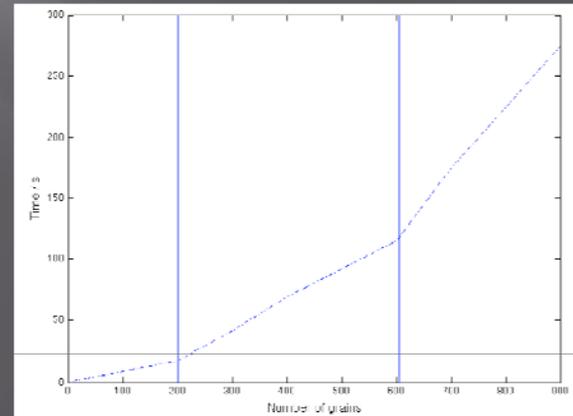


Quaternion space

# Searching for all orientations in the local Rodrigues space

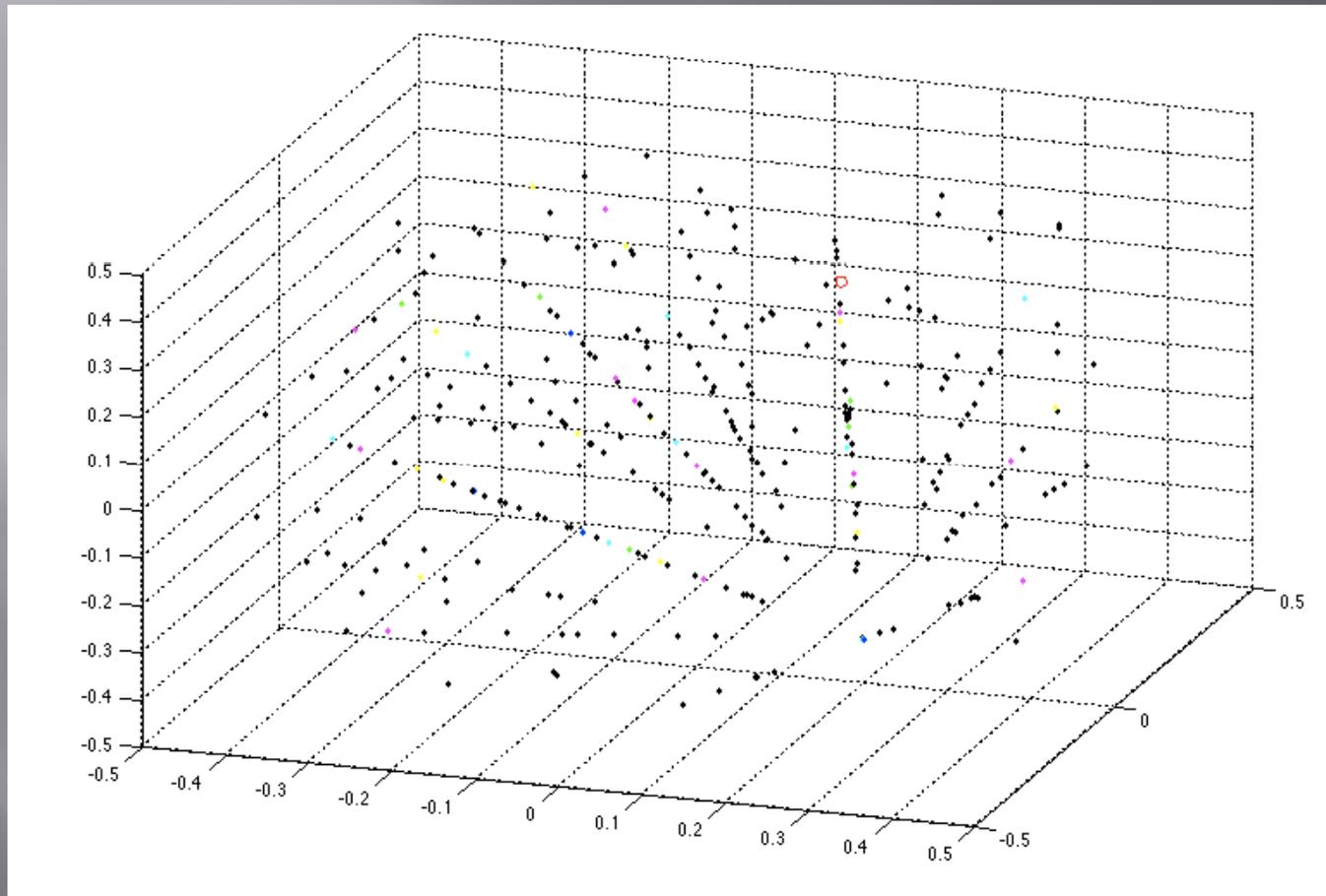


GrainSpotter Algorithm:  
Local maxima can be identified  
in such a way that  $O(N)$  complexity  
is achieved



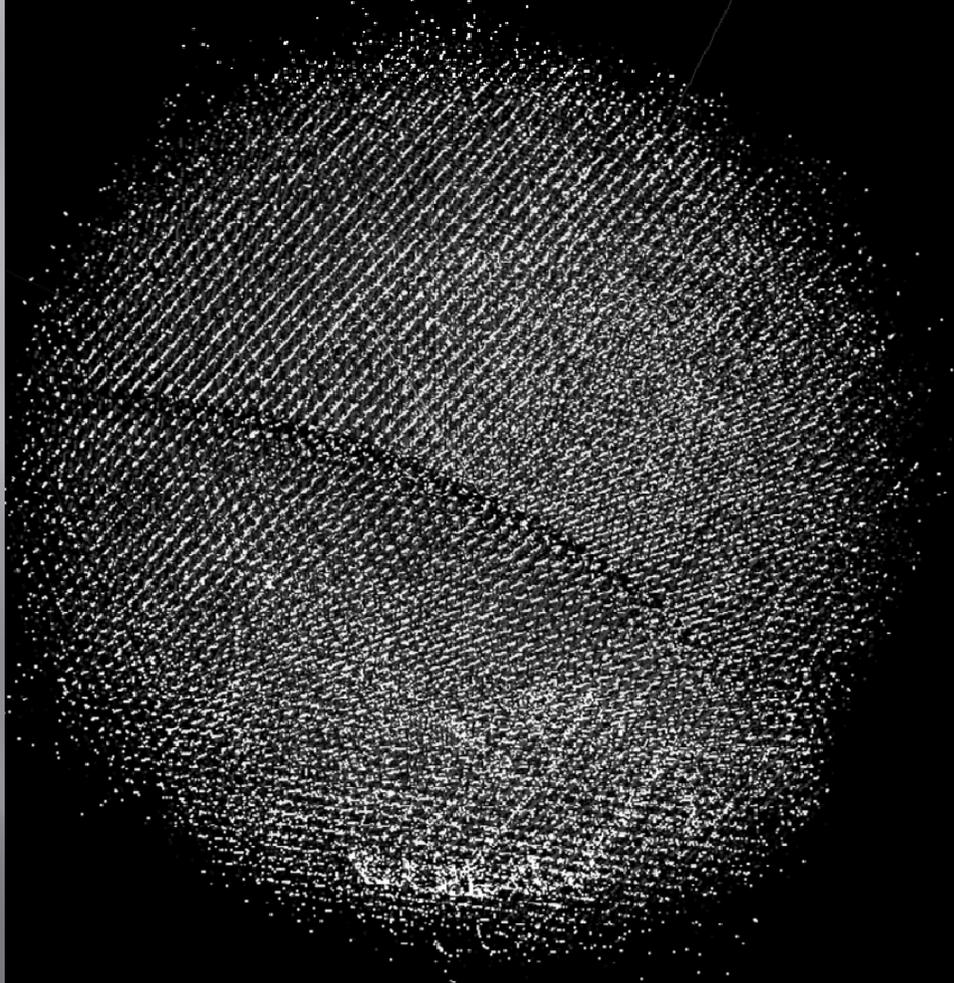
Also the cms position of the grains are fitted.

# Pseudotwins, FCC, example $r \neq 0$



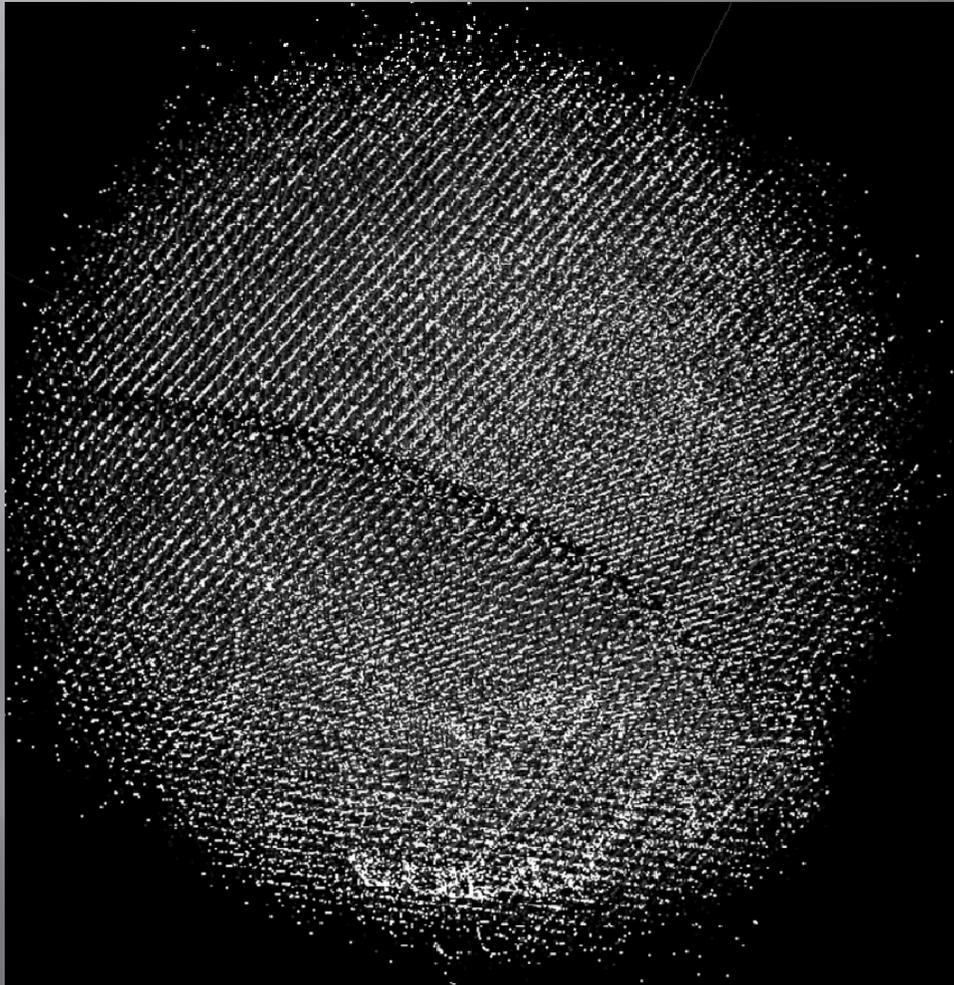
Red: 112, true  
Blue: 34  
Green: 24  
Cyan: 16  
Magenta: 10  
Yellow: 8  
Black: 2, 4 and 6

# Insulin 4X indexed by GrainSpotter



Vectors: 166.845

# Insulin 4X indexed by GrainSpotter



Vectors: 166.845

Grain 1: 36.833

Grain 2: 9.148

Grain 3: 43.227

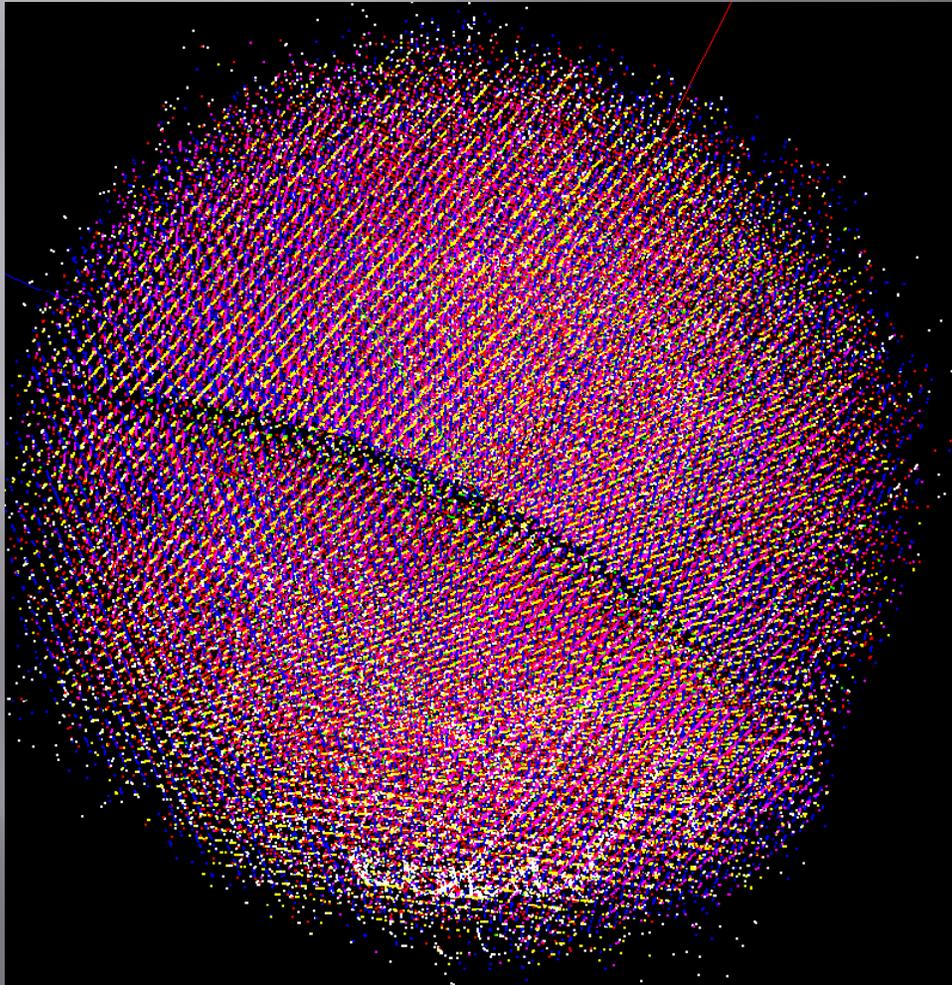
Grain 4: 40.106

Grain 5: 35.949

Total: 165.263

99% matched

# Insulin 4X indexed by GrainSpotter



Vectors: 166.845

Grain 1: 36.833

Grain 2: 9.148

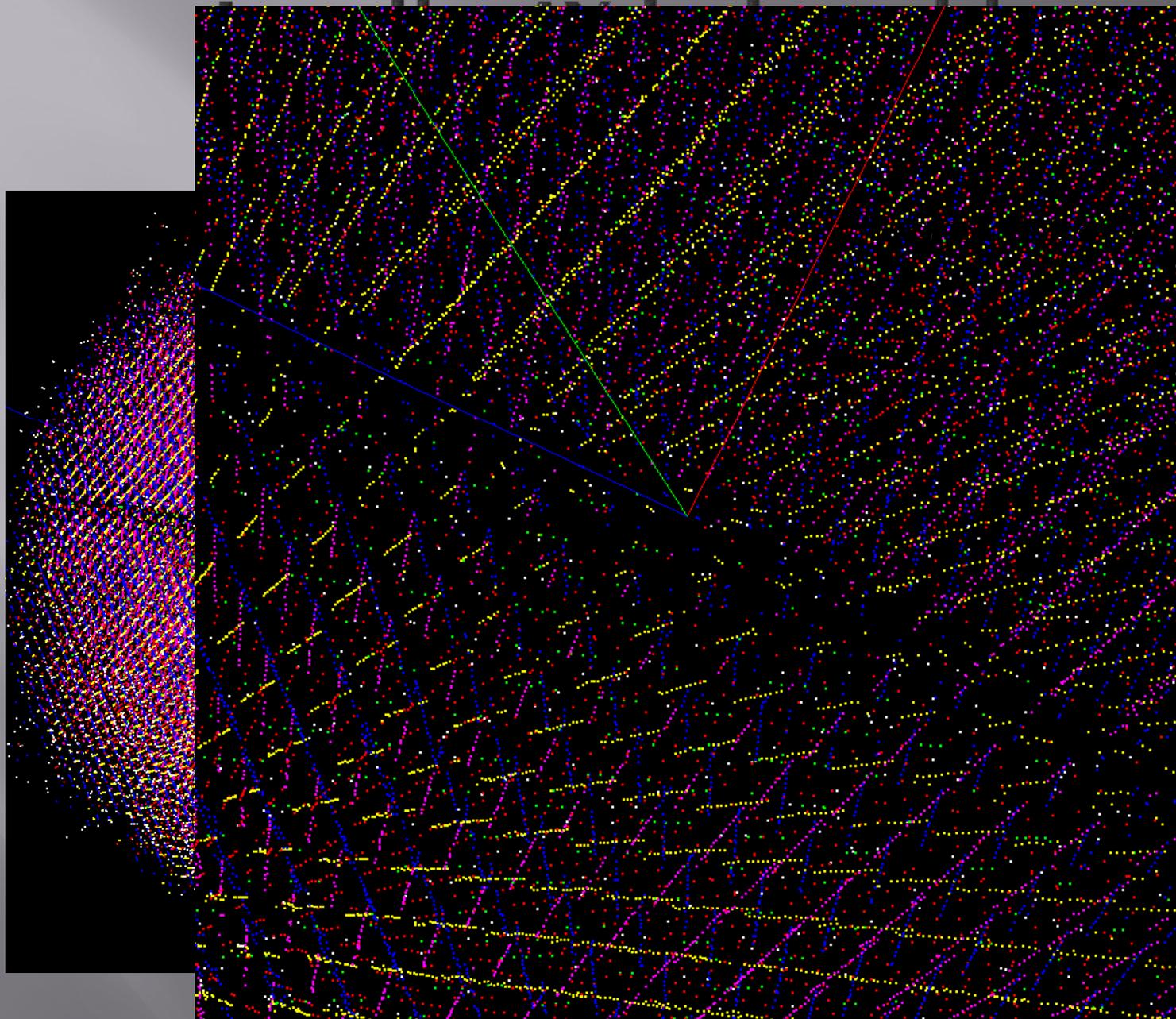
Grain 3: 43.227

Grain 4: 40.106

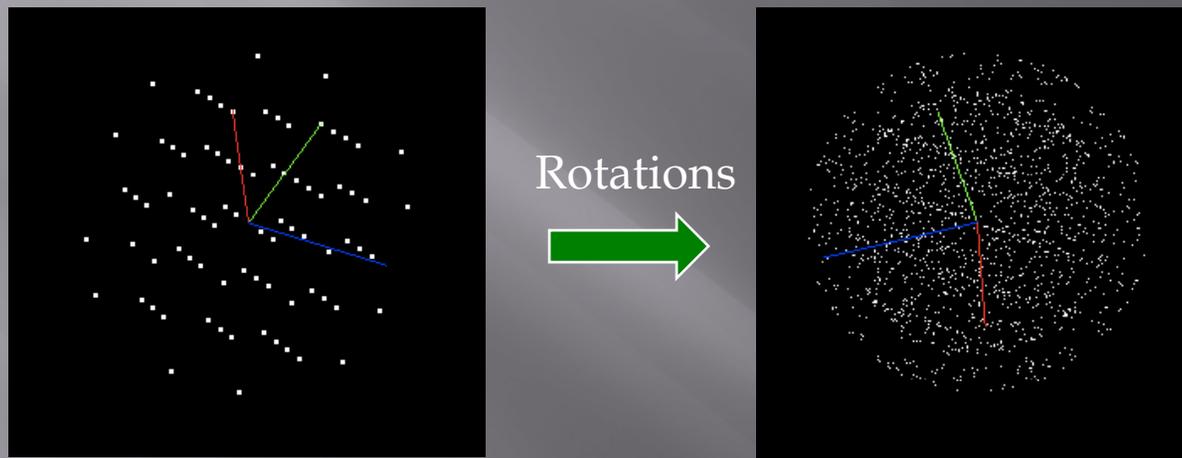
Grain 5: 35.949

Total: 165.263

99% matched

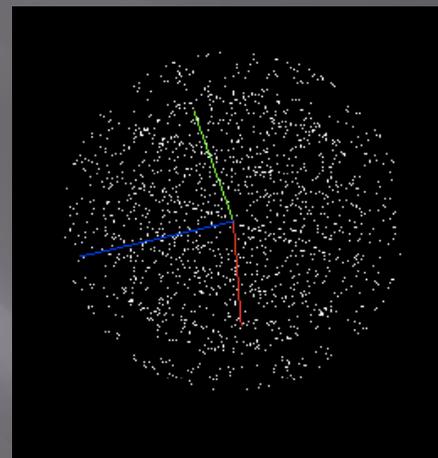


# Indexing compounds with unknown crystallography

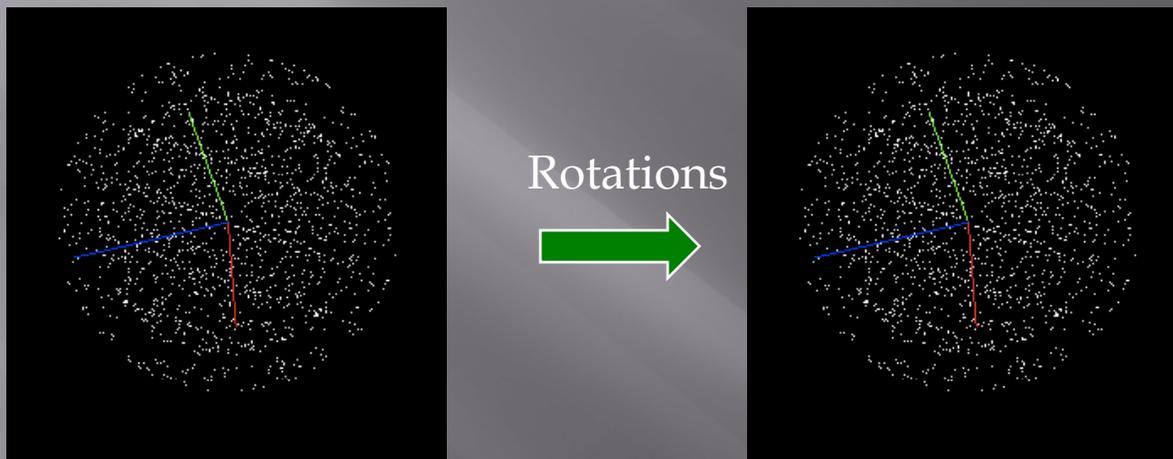


# Indexing compounds with unknown crystallography

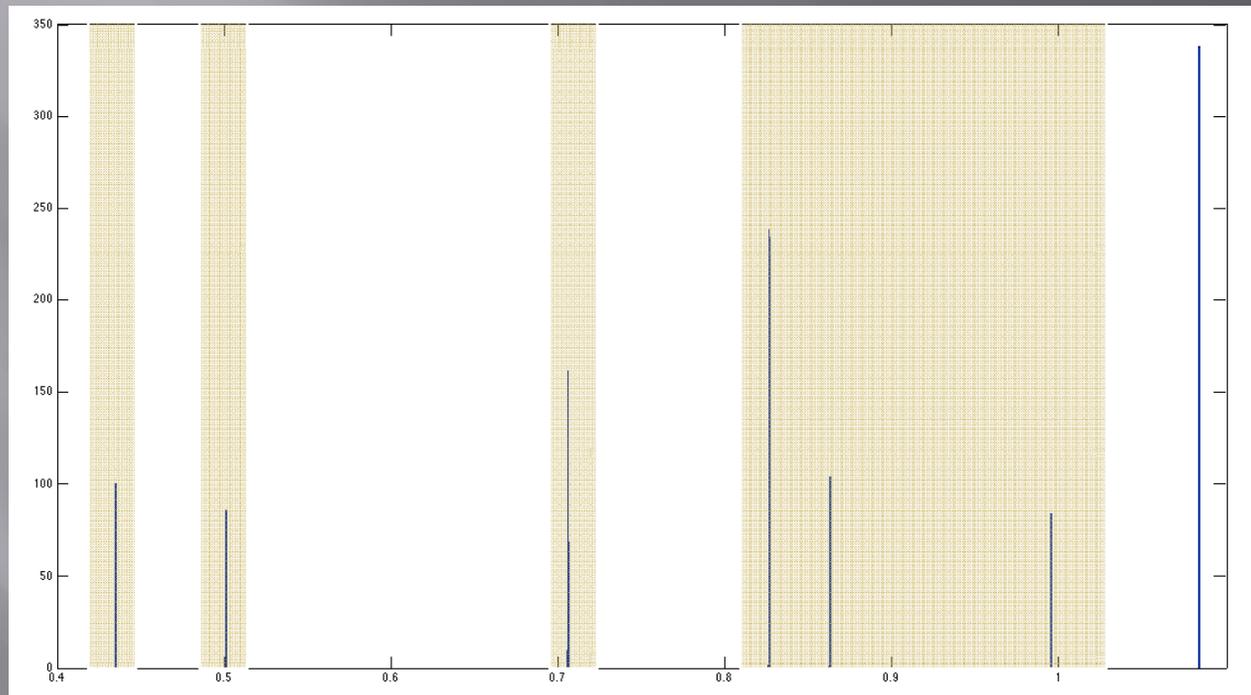
Rotations



# Indexing compounds with unknown crystallography



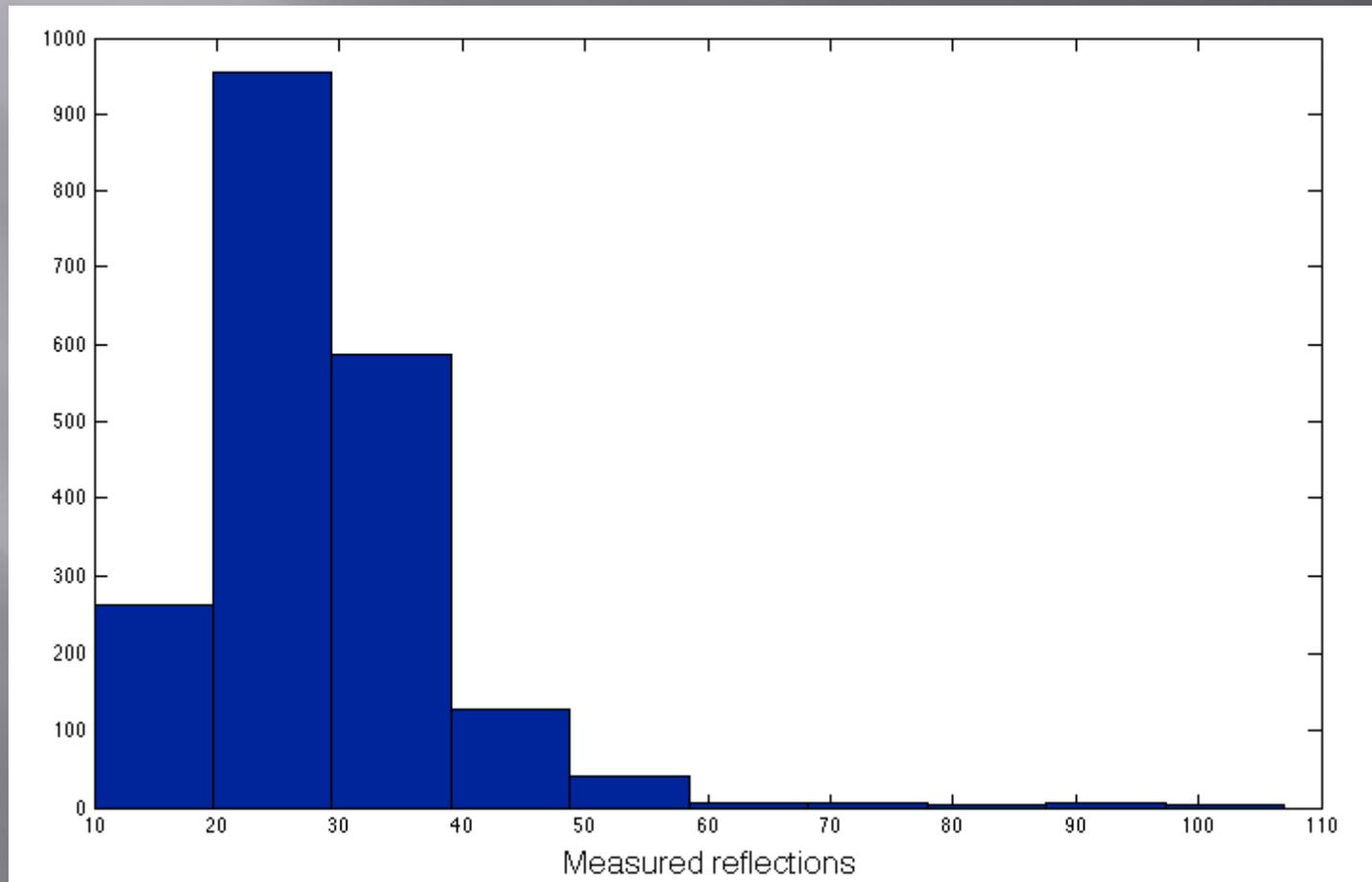
# Indexing unknown, pseudo data

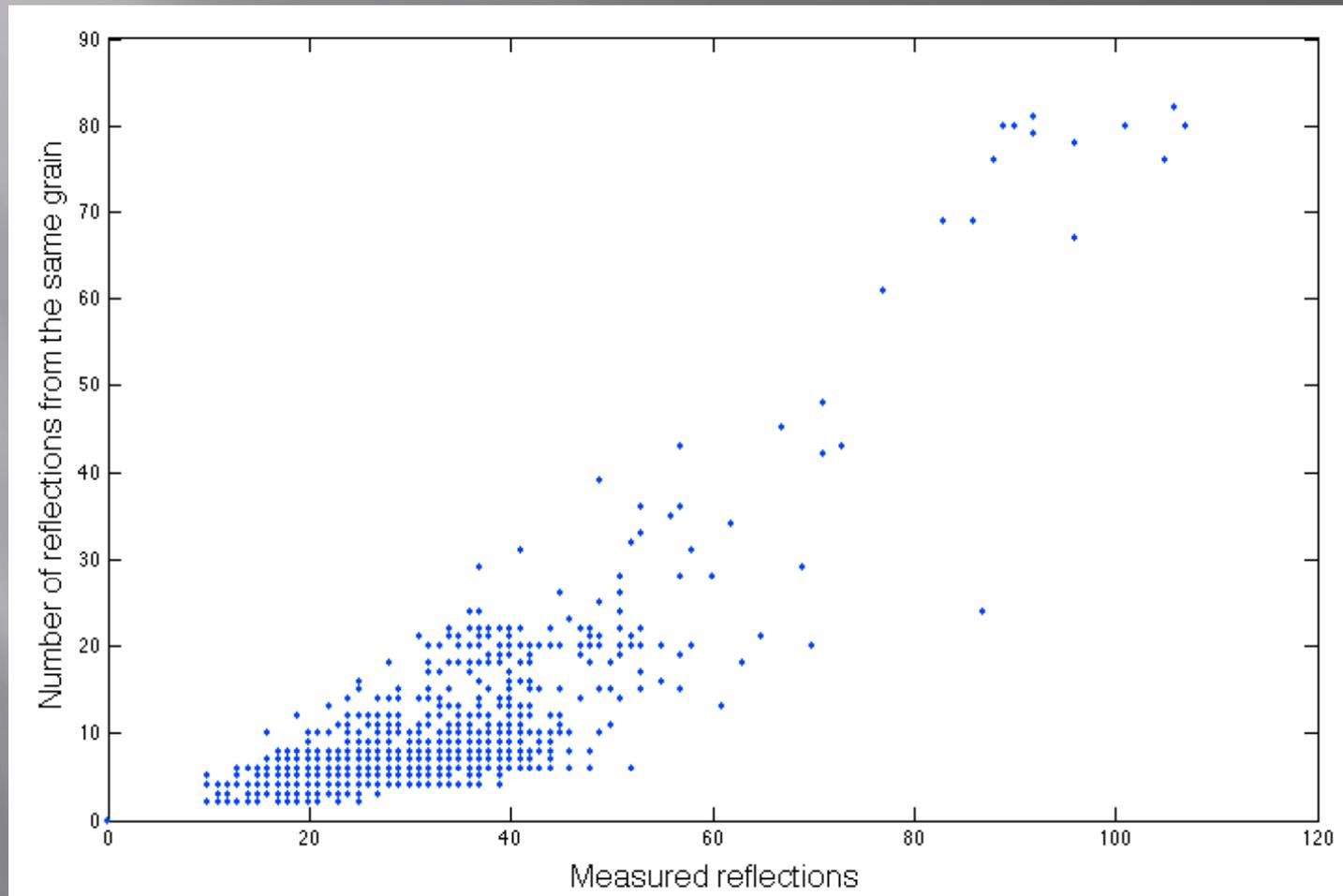


Initial search

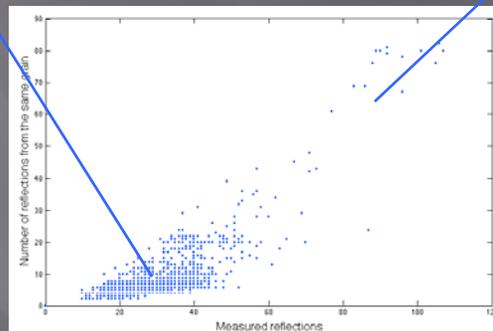
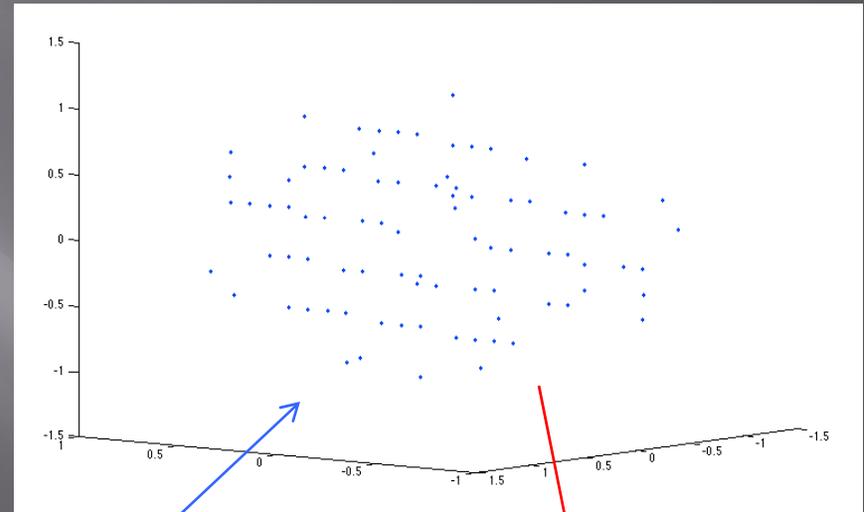
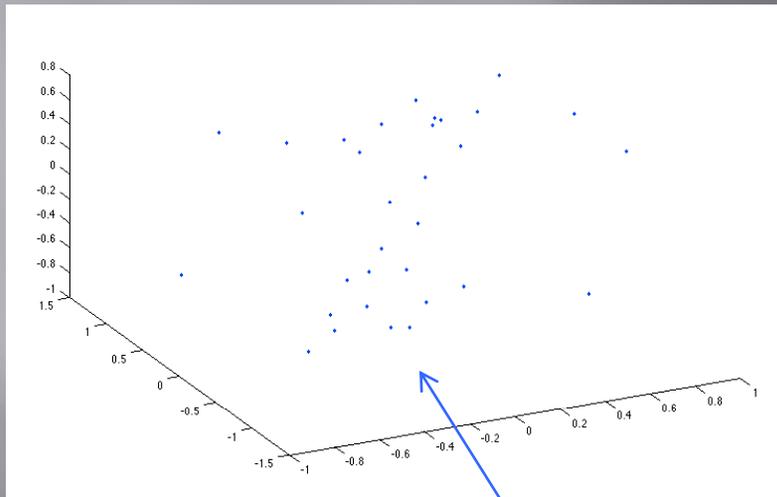
Extended search

# Trying 2000 random (mis)-orientations





# Lattice matches

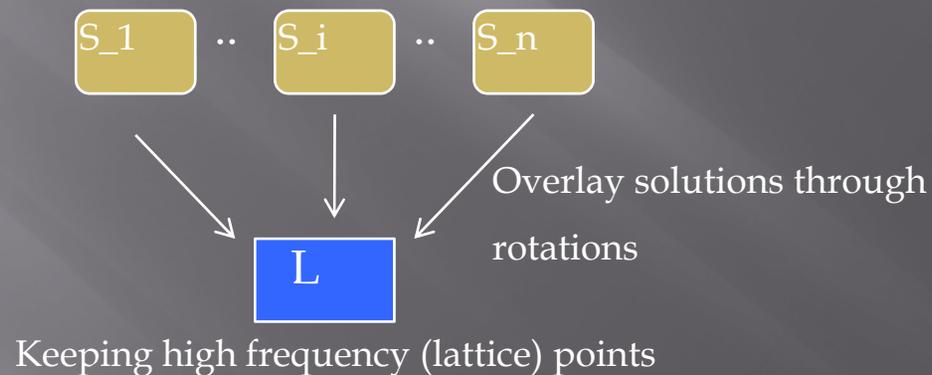


Single crystal indexing  
program

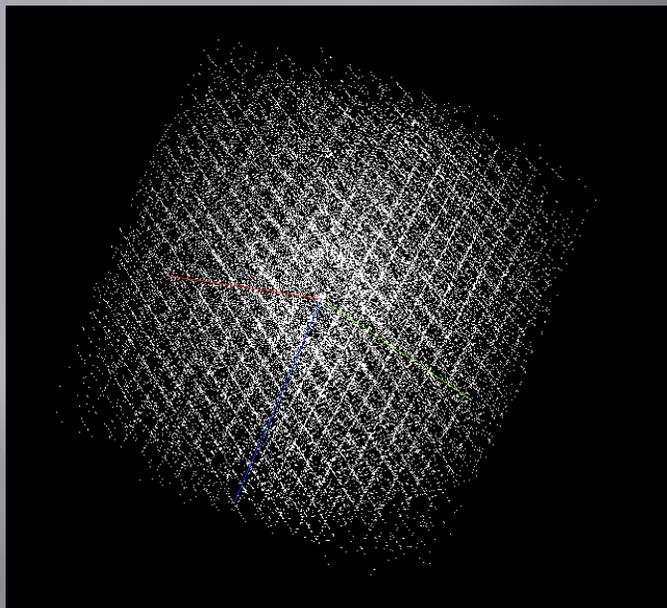
# Additional noise filtering

Keeping the solutions with most points, however still noisy points occur.

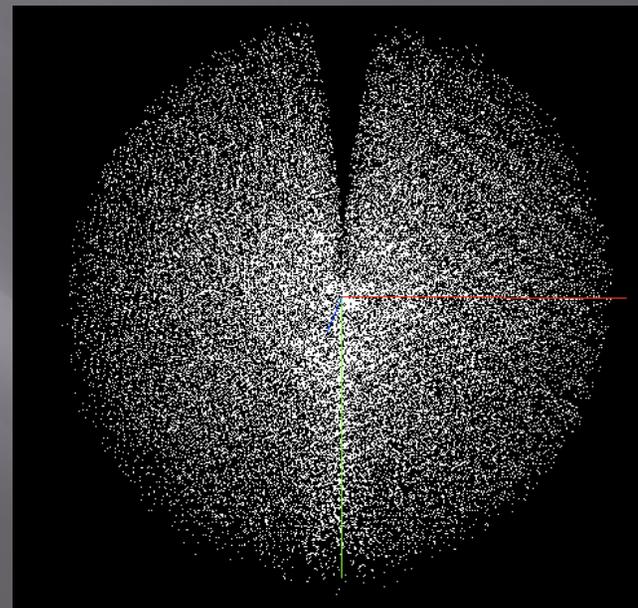
Combine solutions:



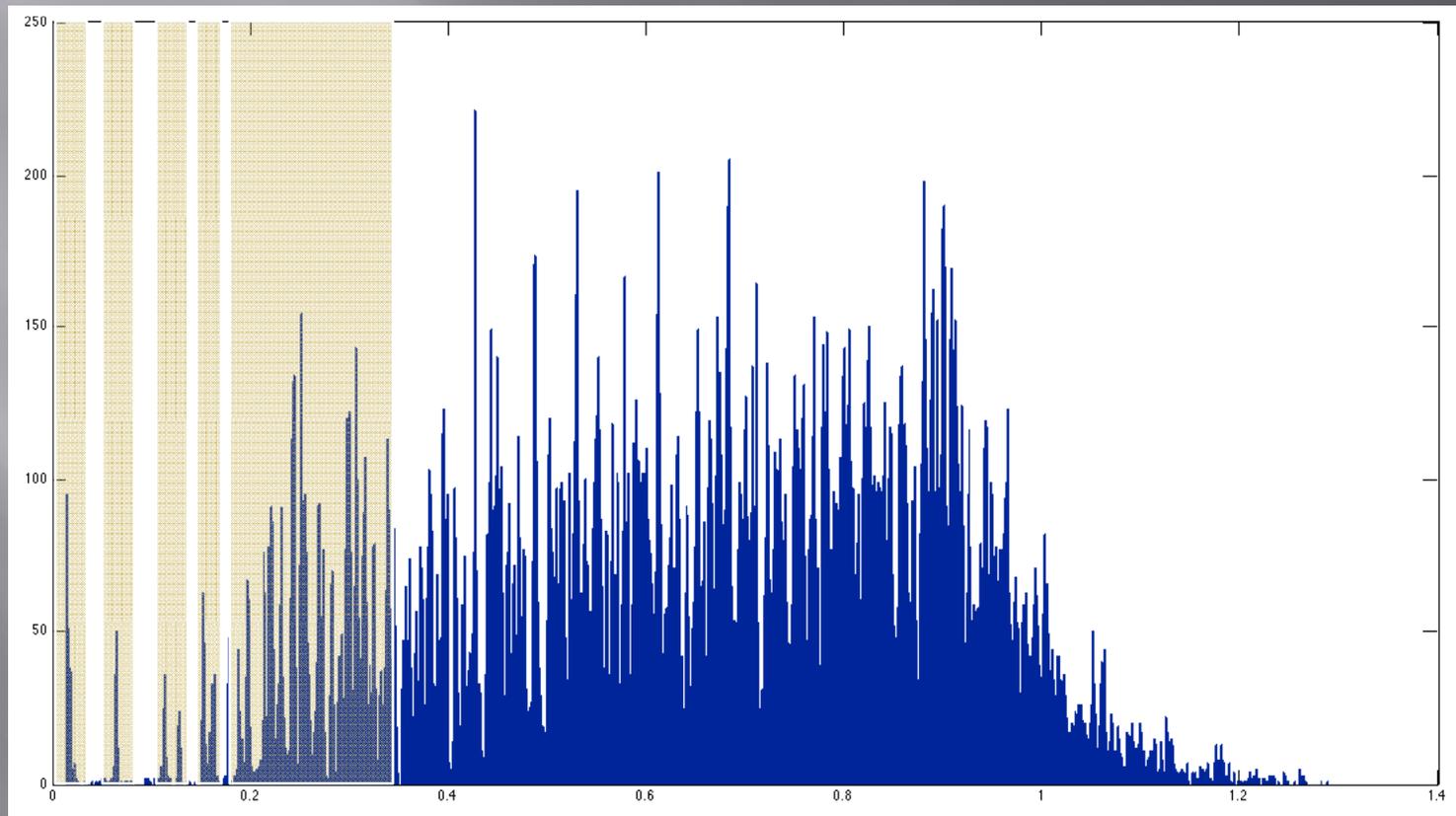
# Example, real data



Few grains



# Distribution of d-spacings

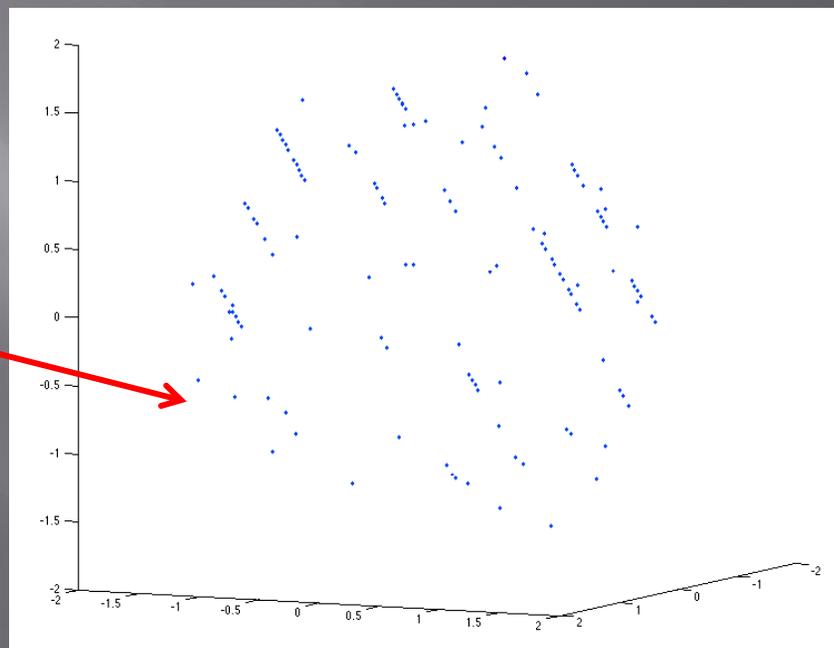


d-spacing ranges used in the search

# Solution with most points

10000 random trials

133, 94, 92, 83, 82,...



Dirax:  $a=8.643$   $b=10.630$   $c=31.378$   $\alpha=90.01$   $\beta=90.24$   $\gamma=90.14$

Duisenberg, A.J.M.(1992). J. Appl. Cryst. 25, 92-96

Compound: (bbcp) 2-benzyl-5-benzylidene-cyclopentanone

Jav Davaasambu et al 2005 J. Phys. D: Appl. Phys. 38 A204-A207.

Orthorhombic, Pbc<sub>a</sub>, Sp gr. 61

12 grains in data

# Type II stresses

# FitAllB

$$\sum_{i,j(i)} \left( \Gamma_{ij}^{-1} \bar{G}_{ij} - \frac{\lambda}{2\pi} U_i B_i \bar{G}_{hkl,ij} \right)^T V_{ij}^{-1} \left( \Gamma_{ij}^{-1} \bar{G}_{ij} - \frac{\lambda}{2\pi} U_i B_i \bar{G}_{hkl,ij} \right)$$

Observations  
3 per reflection

Global parameters  
10

Grain parameters  
12 per grain

$$\bar{G}_{ij} = \left[ \frac{\bar{d}_{ij}}{|\bar{d}_{ij}|} - \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \right]$$

$$\bar{d}_{ij} = R \begin{pmatrix} 0 \\ (y_{det,ij} - y_{det,0}) p_y \\ (z_{det,ij} - z_{det,0}) p_z \end{pmatrix} + \begin{pmatrix} D \\ 0 \\ 0 \end{pmatrix} - \Gamma_{ij} \begin{pmatrix} x_{0,i} \\ y_{0,i} \\ z_{0,i} \end{pmatrix}$$

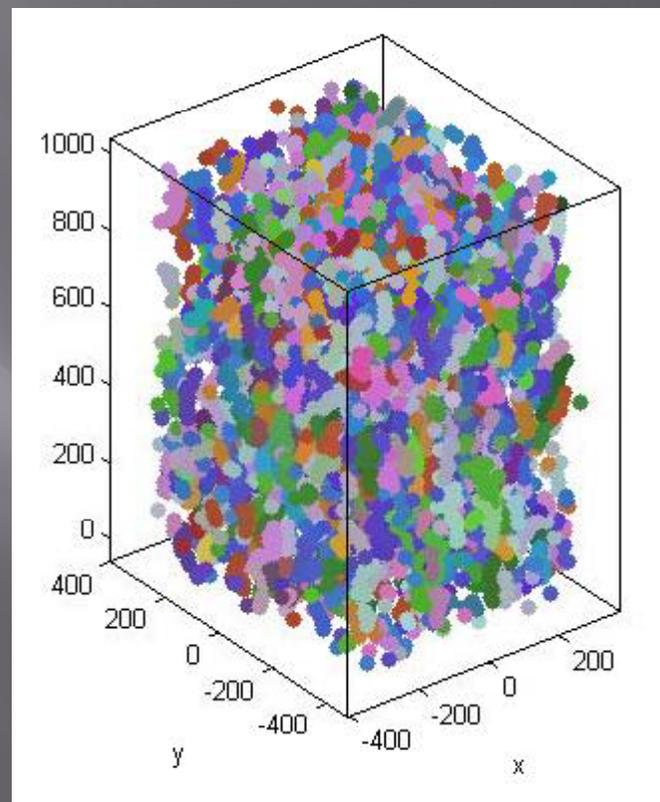
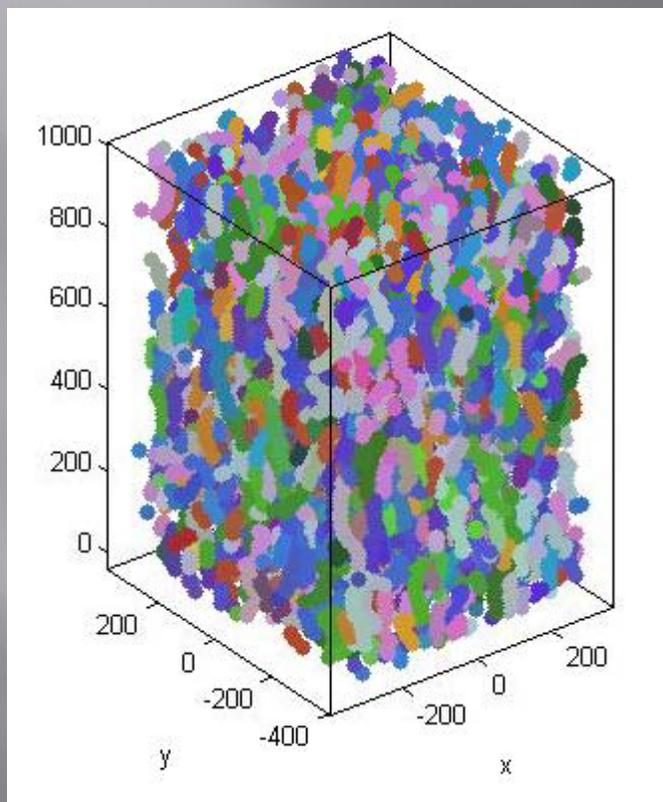
Jette Oddershede, Søren Schmidt, Henning Friis Poulsen, Henning Osholm  
Sørensen, Jonathan Wright and Walter Reimer, in print.

38

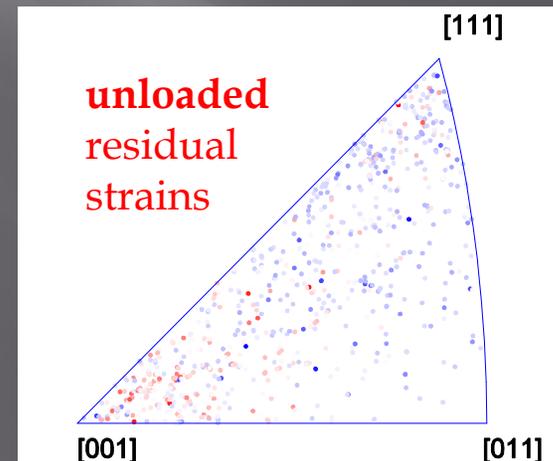
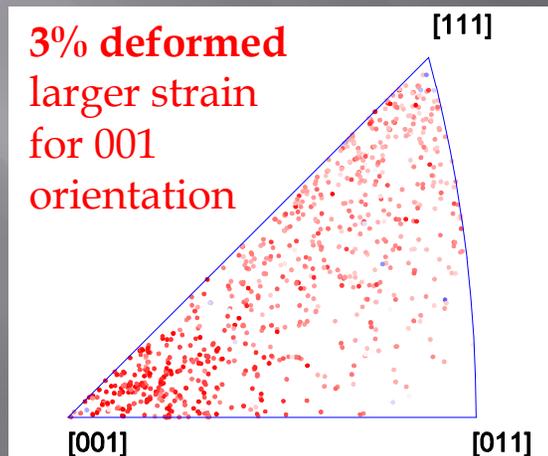
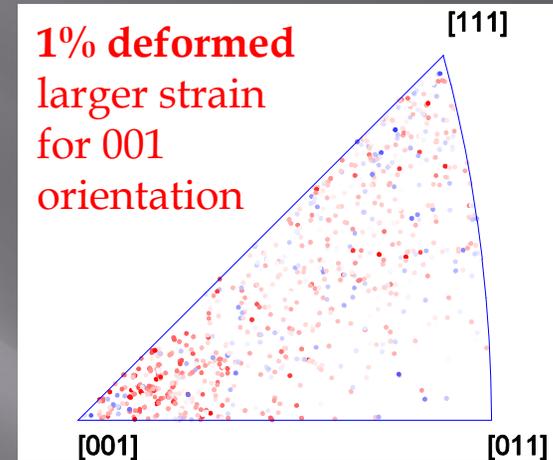
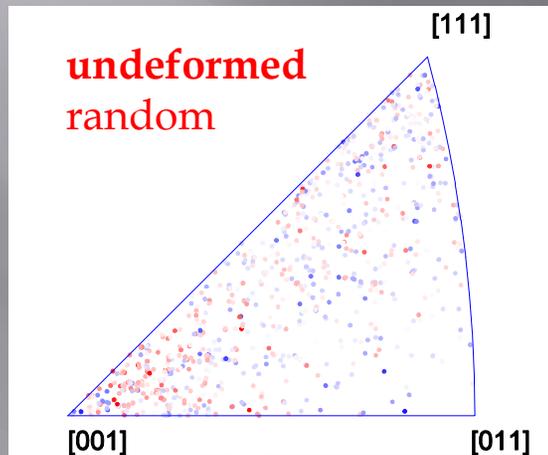
# Experimental data

## Centre of mass position and orientations

### IF steel, ex situ deformed

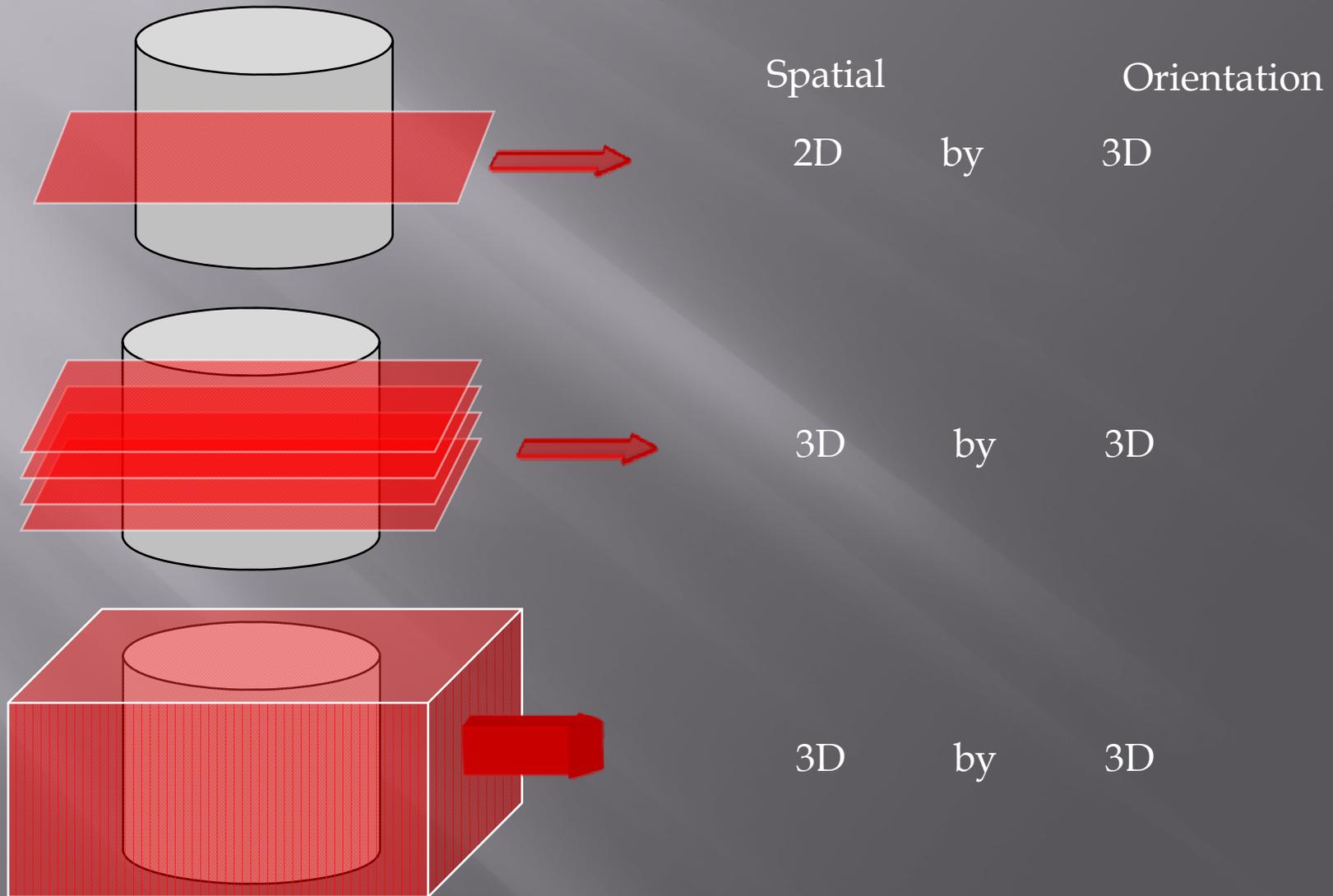


# Experimental data, Correlating strain and orientation Cu, deformed tensionally in situ

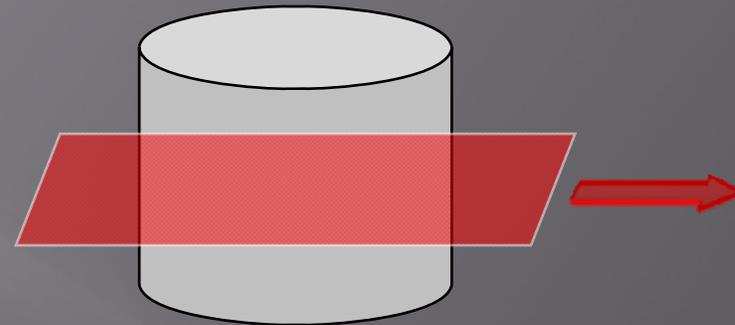


# Mapping

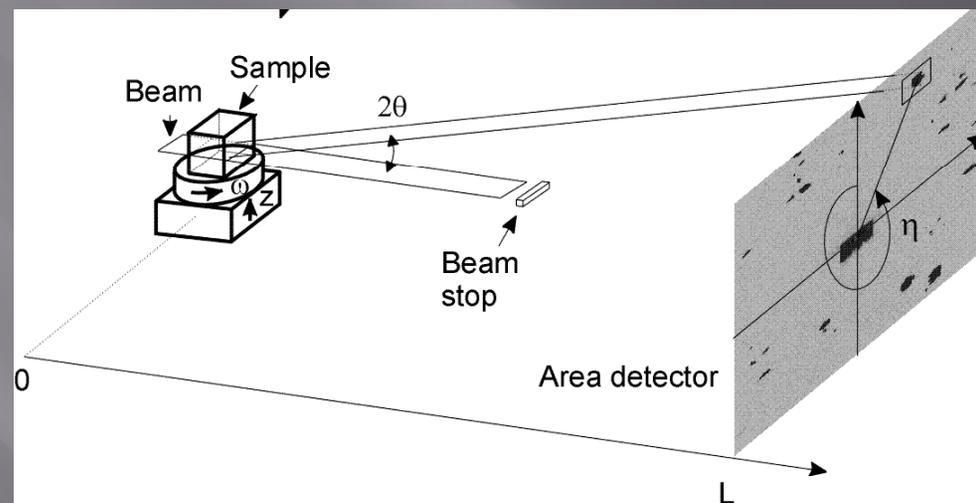
Data collection schemes



# GrainSweeper

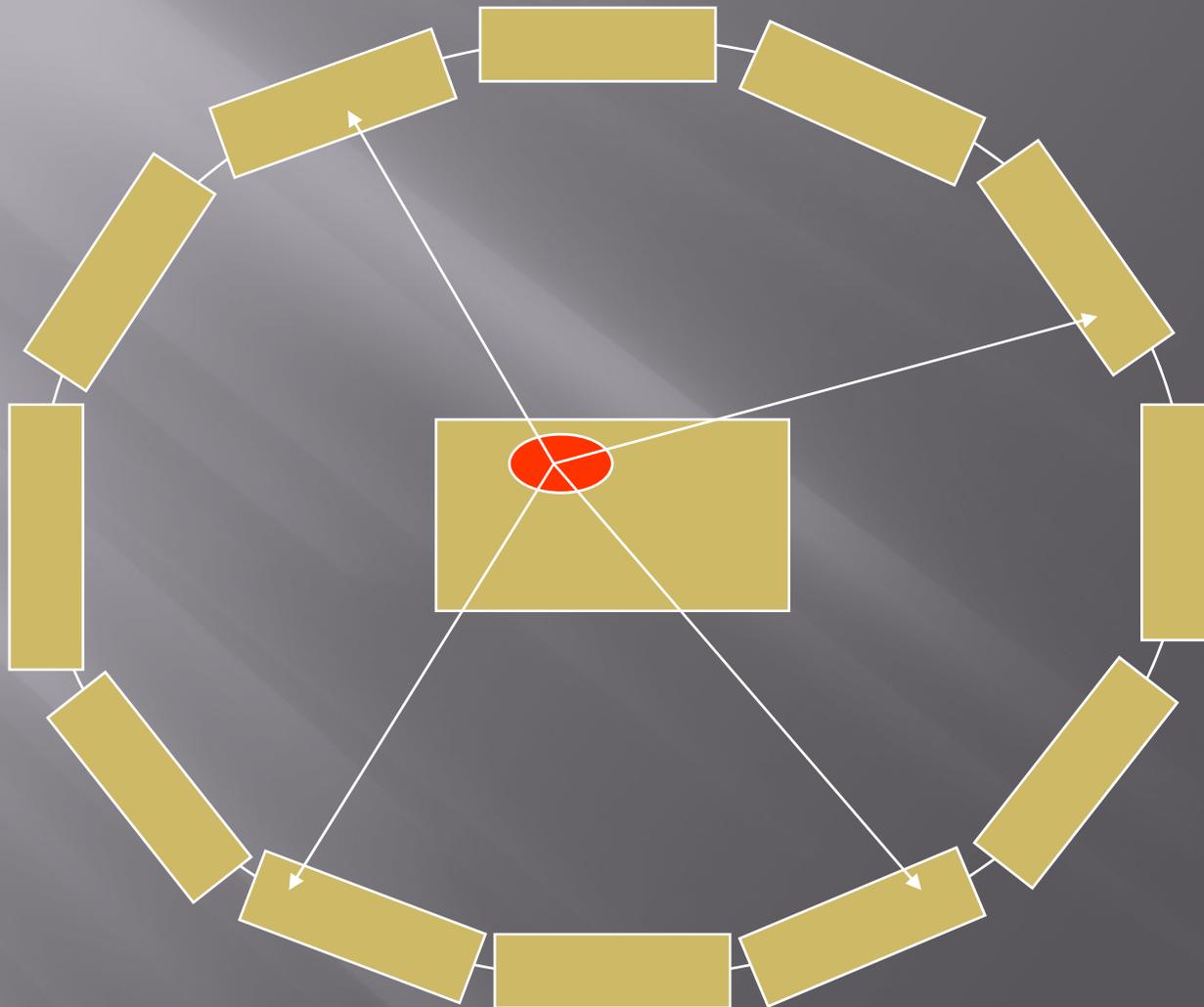


- (Semi-) forward reconstruction algorithm (indexing+grain shape reconstruction)
- Only one detector distance is needed but several can be used



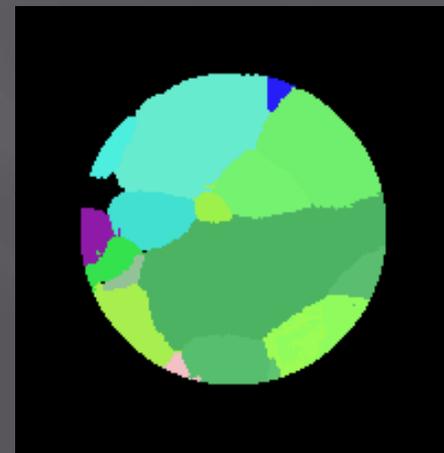
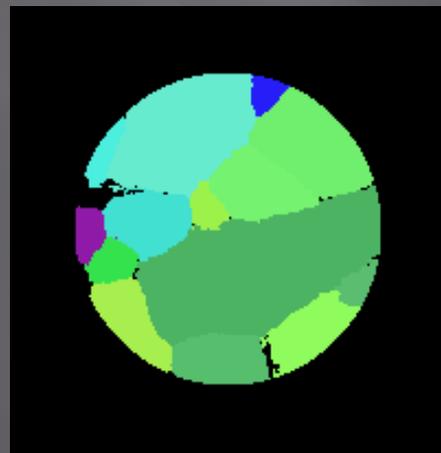
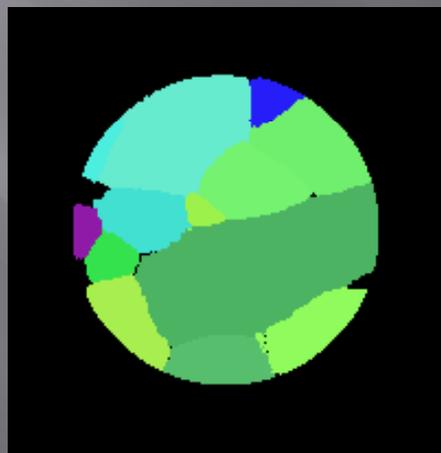
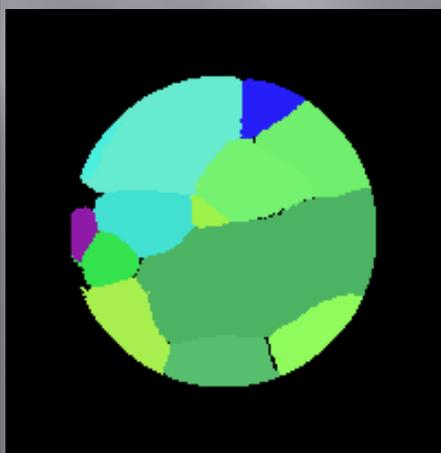
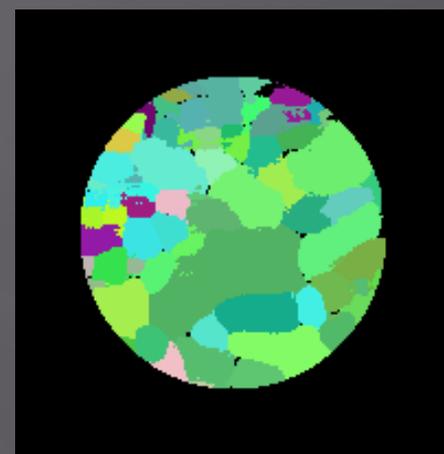
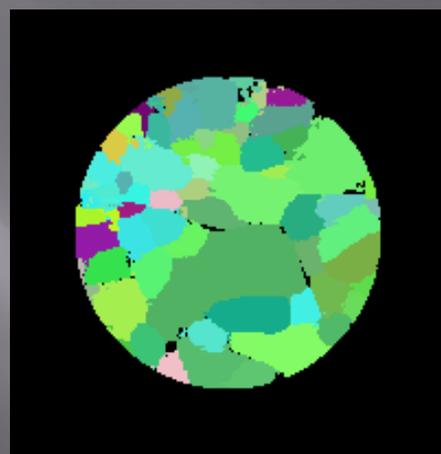
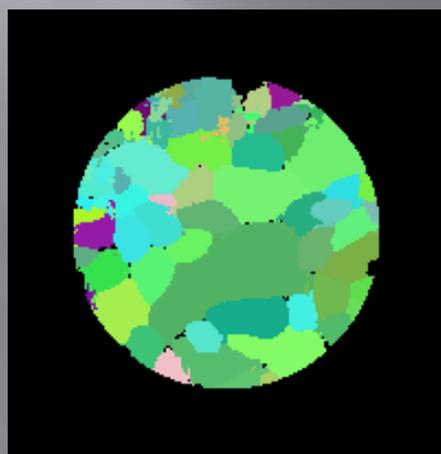
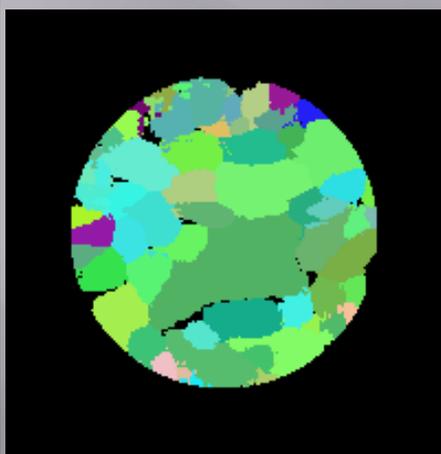
- Output 2D voxel grids -> 3D grain volumes by stacking

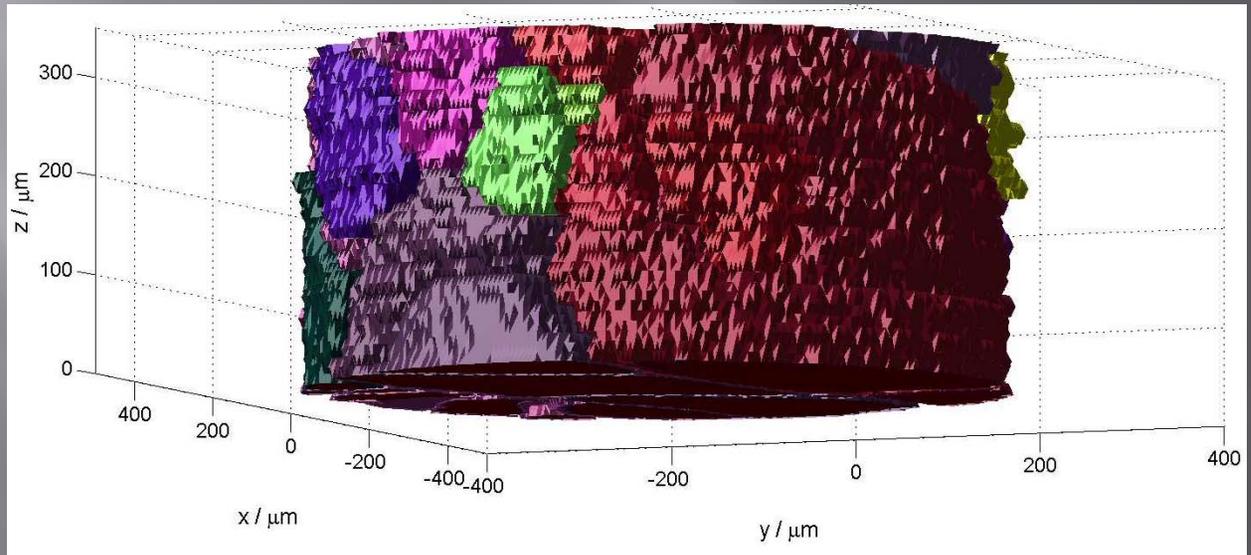
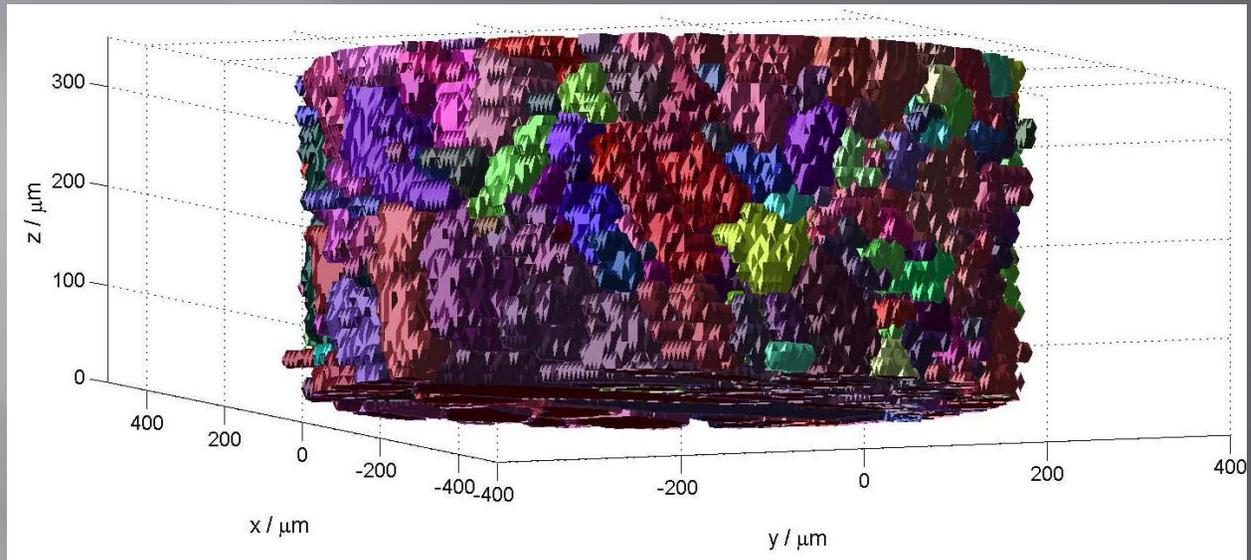
# Forward projections



AlMn sample

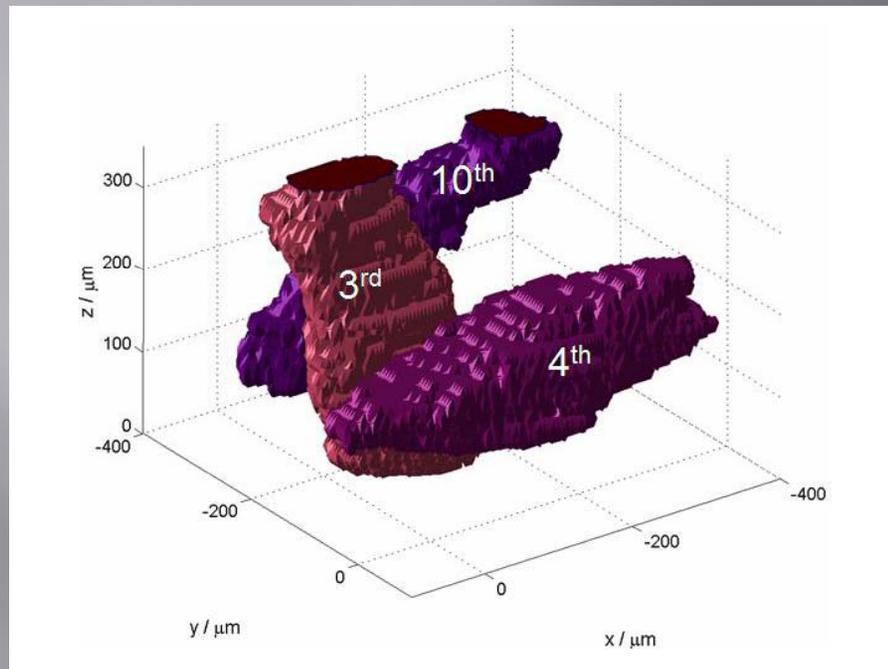
Top: 15 min at 400 °C  
Bottom: 45min at 400 °C  
+ 919 min at 450 °C



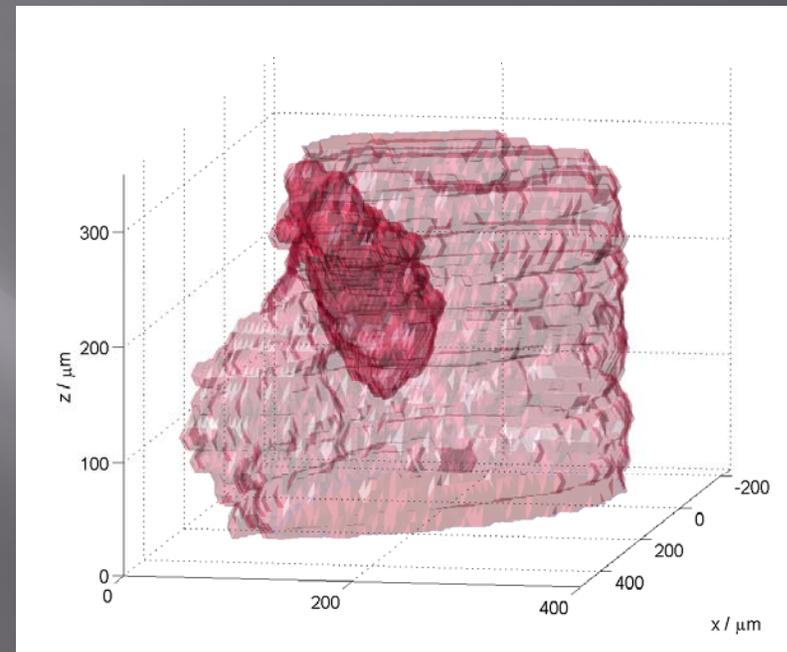


S. Schmidt, U.L. Olsen, H.F. Poulsen, H.O. Sørensen, E.M. Lauridsen, L. Margulies, C. Maurice, D. Juul Jensen,, *Scripta Mater.*, 59 (2008), 491-494

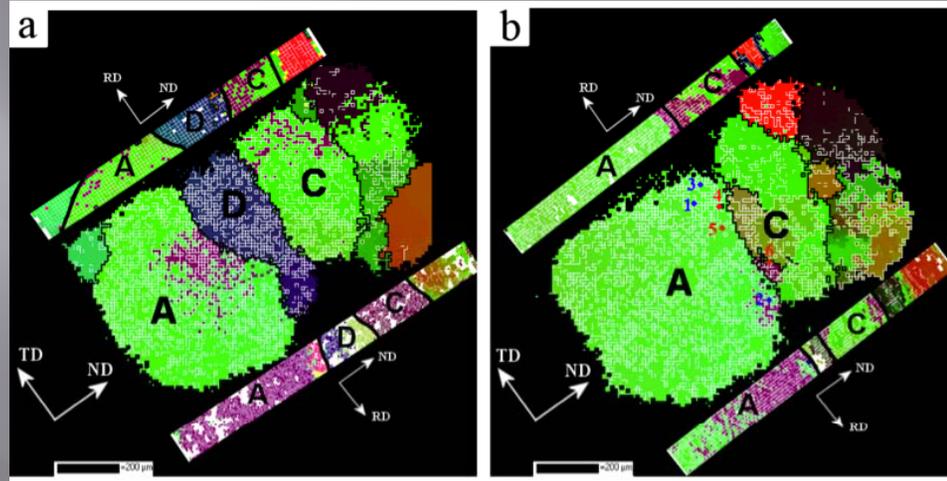
## Individual grains



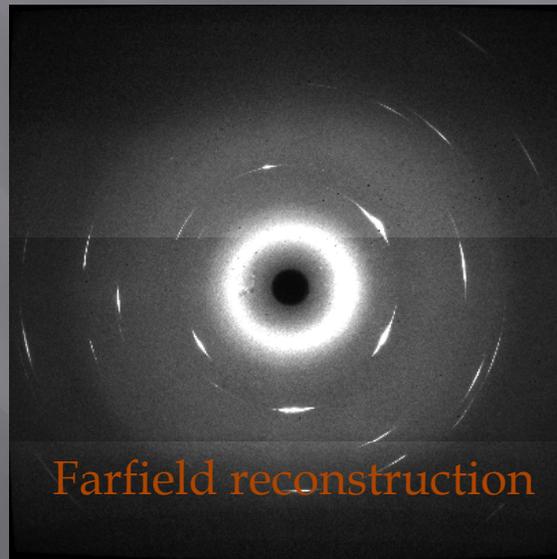
## Growth



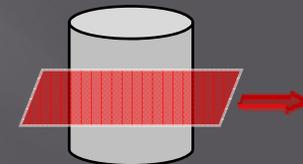
# Nucleation study



GrainSpotter,  
New nuclei:



Grain map of 30% deformed Aluminum on Farfield detector.



*S.S. West, S. Schmidt, H.O. Sørensen, G. Winther, H.F. Poulsen, L. Margulies, C. Gundlach, D. Juul Jensen, Scripta Mater. (2009) 61, 875-878*

# McXtrace – an X-ray Monte Carlo ray-tracing software package

Building on the McStas (since 1998): Neutron simulation program

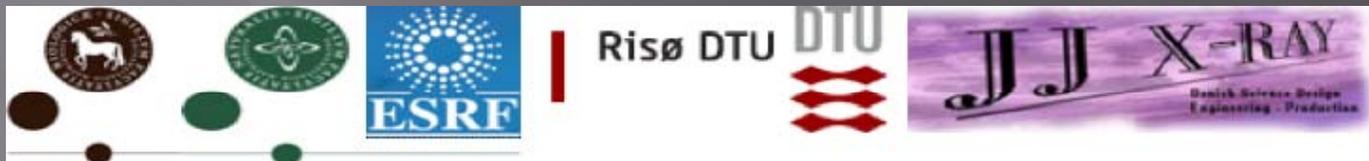


<http://www.mcxtrace.org>

Estimated first release: Fall 2010

Erik Knudsen, Peter Willendrup, Søren Schmidt  
*Risø-DTU*

Kim Lefmann, Andrea Prodi, Jana Baltser, Søren Kynde  
*University of Copenhagen*



... and some ideas on how to  
“remove all possible causes why  
the user shouldn’t publish data  
collected at a synchrotron”

- ▣ ... in order to optimize the scientific output.

Scientific and  
Technical goals

Users

Synchrotron

High Impact,  
Legacy

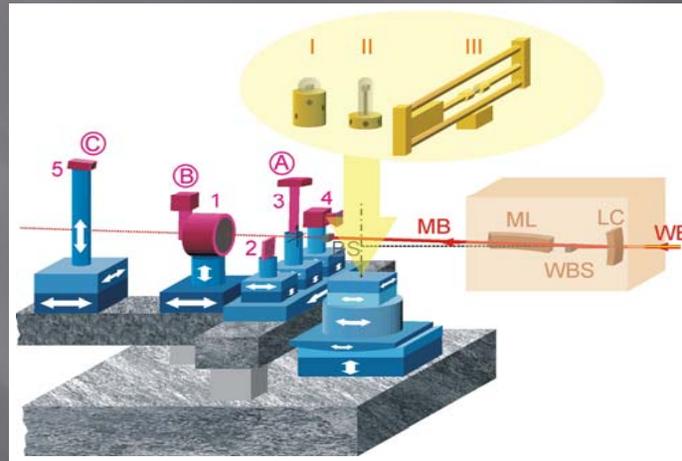
# A beamline is not a stationary entity

New Idea

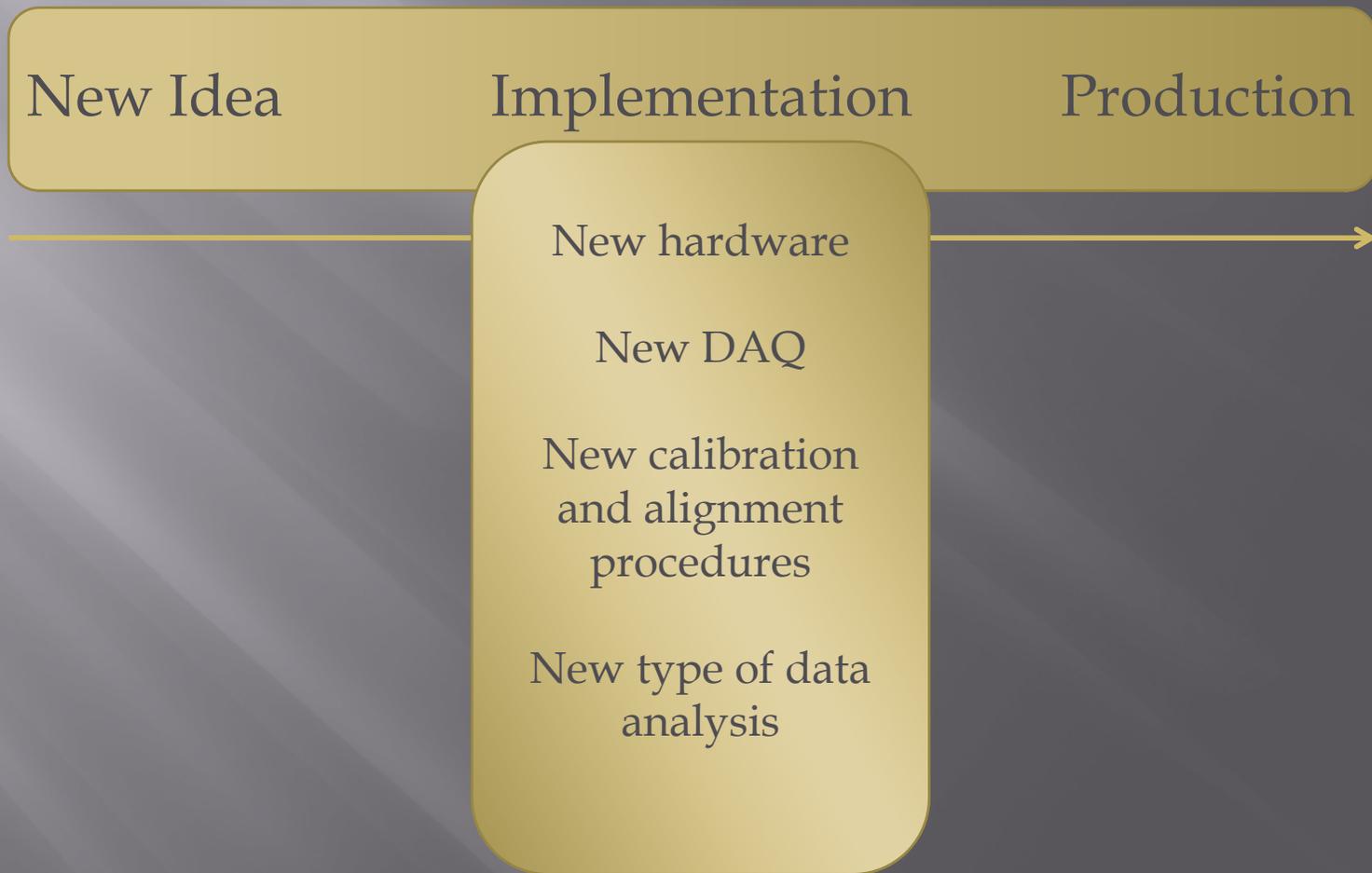
Implementation

Production

Constant flow



# A beamline is not a stationary entity



# A beamline is not a stationary entity

New Idea

Implementation

Production

New hardware

New DAQ

New calibration  
and alignment  
procedures

New type of data  
analysis

Routine operation

Instant evaluation  
of data quality,  
diagnostics,  
data analysis  
(perhaps data  
reduction)

# A beamline is not a stationary entity

New Idea

Implementation

Production

New hardware

New DAQ

Routine operation

Instant evaluation  
of data quality,

diagnostics,

analysis

(helps data

collection)

Challenges:

Easy transition between production modes  
and co-existence of new implementations  
and production modes

# A beamline is not a stationary entity

New Idea

Implementation

Production

New hardware

New DAQ

Routine operation

Further optimization

Instant evaluation  
of data quality,

diagnostics,

analysis

(helps data

collection)

Challenges:

Easy transition between production modes  
and co-existence of new implementations  
and production modes

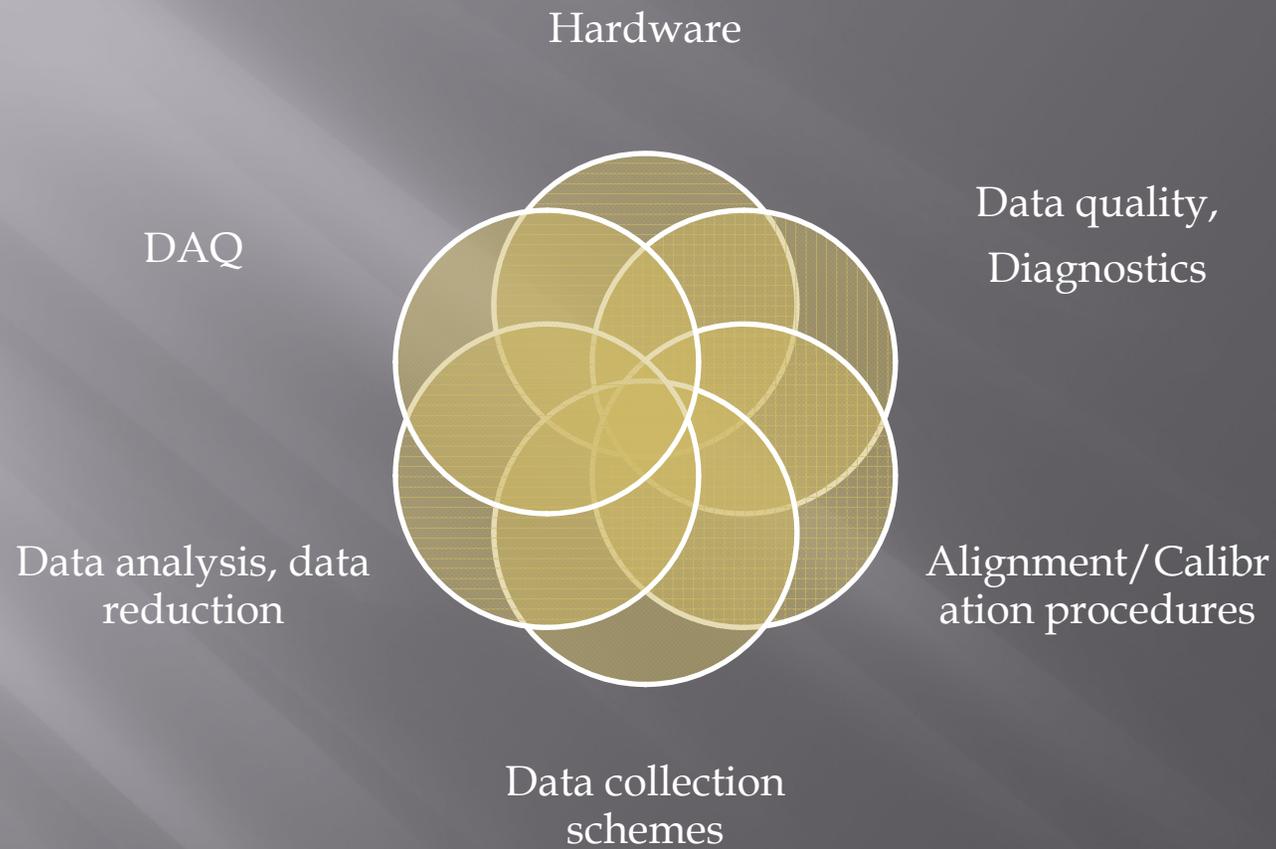
# Users

## Deliverables to the users

First Principle	Analysis platform	Finalized analysis
Starting from scratch, new type of analysis.	Existing analysis procedure, but refined analysis needed.	Existing analysis procedure.
Raw data. Brave users.	Raw (or pre-processed) data + platform. Experienced users.	Data analyzed. All users.

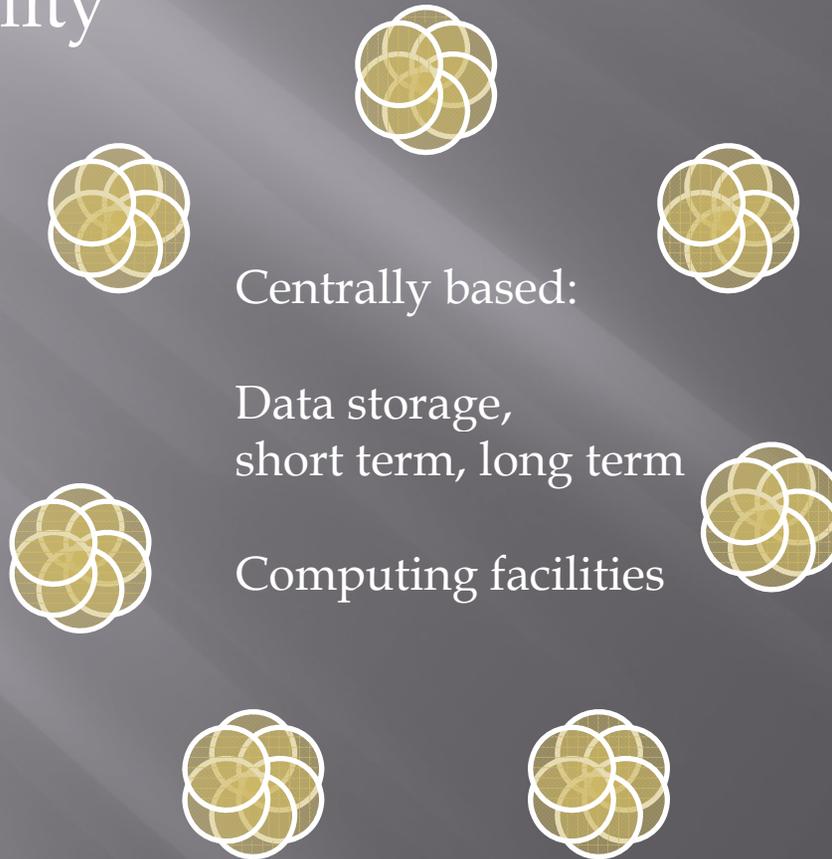
Beamline's experience with this specific type of experiment

In the proposal for the experiment: ballpark estimation of complexities and requirements evaluated through simulations.



# N beamlines, especially for $N > 1$

## ▣ Scalability



# DAQ and analysis platform

- ▣ Not to reinvent the wheel, but to modify the wheel according to your needs
- ▣ Find an existing platform “above the critical mass”
  - Development of core activities are guaranteed for years to come.
  - New modules for DAQ and analysis can easily be added.
  - Accommodating both GUI- and prompt- people
    - ▣ SPEC interpreter (many SPEC macros around).
- ▣ Analysis procedure is automatically stored in a database such that the analysis can be repeated at a later stage.

# Platforms

- ▣ On-site analysis, using centralized computing facilities, interfaced
  - GUI or Scripts
    - Can also be accessed off-site through e.g. NoMachine software
  - Web interface
  
- ▣ Well structured data storage facility
  - Data is there when needed
  - Export to external users.
  
- ▣ Off-site analysis, platform users can bring home to their own computers

# Computing facility

- ▣ Different types of analyses have different needs in terms of hardware architecture
  - A computing cluster optimized for, e.g. atomistic simulations may not be optimized for high throughput data analysis
- ▣ Heterogeneous hardware architecture may be desirable
  - Well-masked network connections for high throughput data analysis

# Current and future computing hardware

- ▣ Multi-core CPU : MPI or openMP
- ▣ GPU: (e.g. CUDA for NVIDIA), but not suitable to all types of analyses
- ▣ future CPU-GPU shared memory
  
- ▣ openCL to all of the above

# Most importantly

- ▣ Coordination and Communication
  - Locally on site – challenging
  - Off site - “Off shore programming” – very challenging
  - Especially user interfaces need to be evaluated constantly, documentation, examples of analysis

# In the real world, when pressure is building up, deadlines etc.

- ❑ Easy to implement local solutions, but rarely ensures scalability
- ❑ Scientists come up with great algorithms – implemented in their preferred programming language, leading to a variety of languages
  - Rewrite? (takes time, scientist may not be able to support new version) or include “as is”? (likely to break interface rules)
- ❑ People tend to focus on their own speciality, but it is equally important to keep track of activities in adjacent areas

# FABLE, what's next?

- ▣ Matt Gerring starting at ESRF in June – “Graphical workbench for online data analyses”
- ▣ Making FABLE as an eclipse plugin (Ken Evans, APS), e.g. for use in GDA
- ▣ HDF5 – hyper spectral – new file format
- ▣ Further algorithm developments

# Projects you could look into, among others:

- ▣ GDA, see next talk
- ▣ EDNA, MX, batching (scripting work flow),  
<http://www.edna-site.org/>
- ▣ KINME biophysics – graphical workflow editor  
(eclipse) <http://www.knime.org/>
- ▣ ICAT: Centralized database, from proposal to  
publication, <http://code.google.com/p/icatproject/>
- ▣ PANDATA – EU project – network of institutes  
using ICAT, [http://pandata.nd.rl.ac.uk/Main\\_Page](http://pandata.nd.rl.ac.uk/Main_Page)

# FABLE/TotalCryst gang

Current and Former

Andy Goetz, Gavin Vaughan, Jon Wright, Henning Osholm Sørensen, Ken Evans, Andreas Alpers, Jette Oddershede, Ulrik Lund Olsen, Henning Friis Poulsen, Gaelle Suchet, Simone Techert, Jav Davaasambuu, Carsten Gundlach, Larry Margulies, Anders Svensson, Elspeth F. Garman, Karthik Paithankar, Gabor T. Herman, Vaclav Petrick, Michal Dusek, Søren Schmidt

**Thank You!**