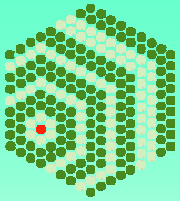
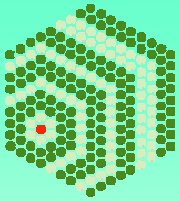


Software Development for Kappa Diffractometers

DNA_dev Meeting
Diamond, UK
March 8-9, 2005

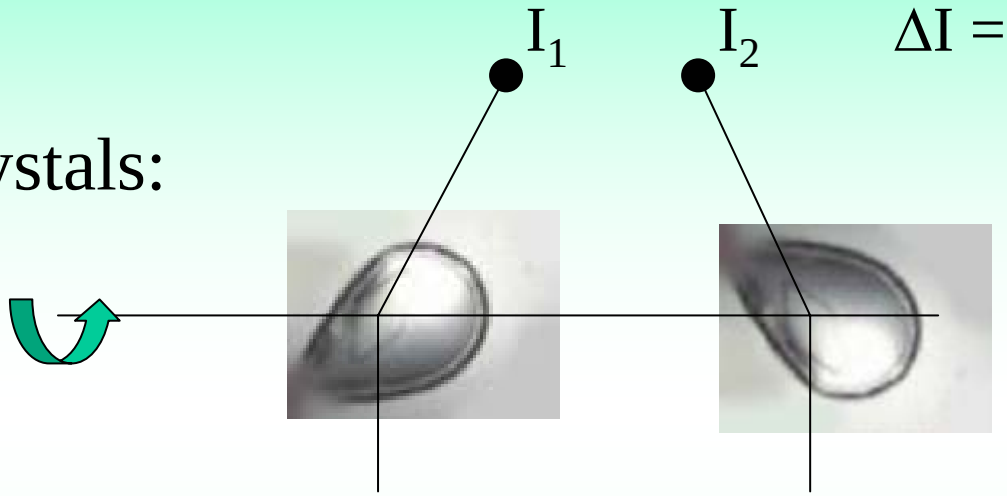


Overview

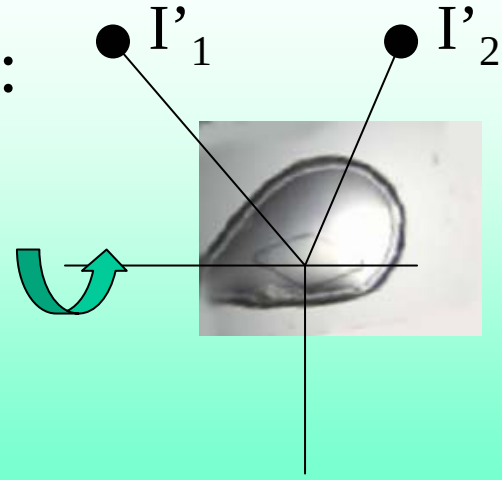
- What and why?
- Current Design
- Status of the Implementation
- DNA Integration Steps

Why a kappa device?

- unaligned crystals:

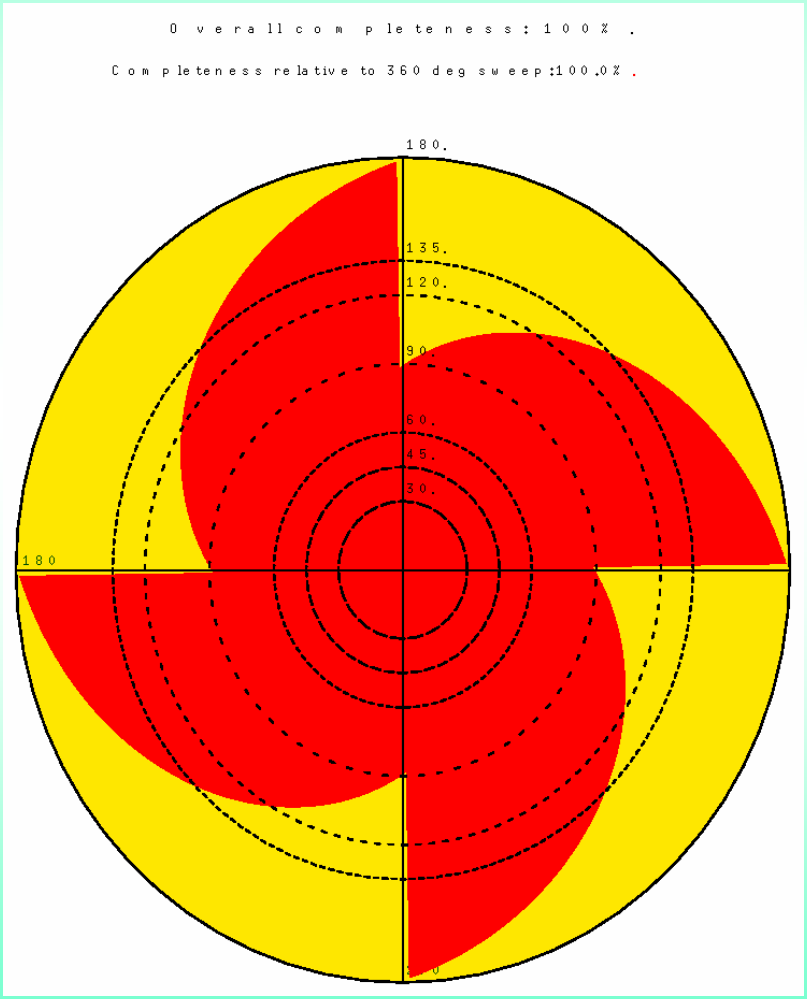


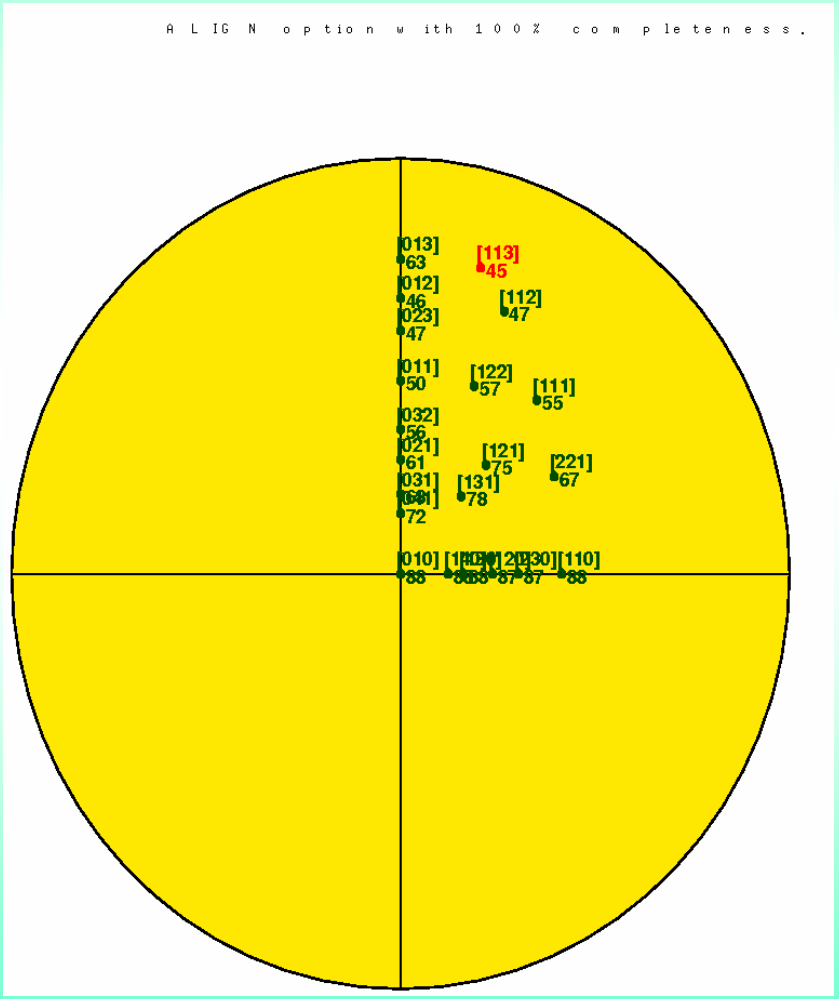
- aligned crystals:

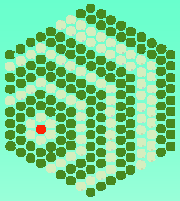


$$\{\varphi_{err}\} > \{\varphi'_{err}\}$$

And why else?


Overall completeness: 100% .
Completeness relative to 360 deg sweep:100.0% .
180.
135.
120.
90.
60.
45.
30.
180


ALIGN option with 100% completeness.
[013] 63
[113] 45
[012] 46
[112] 47
[023] 47
[011] 50
[122] 57
[111] 55
[032] 56
[021] 61
[121] 75
[221] 67
[031]
[131] 78
72
[010] 88
[110] 88



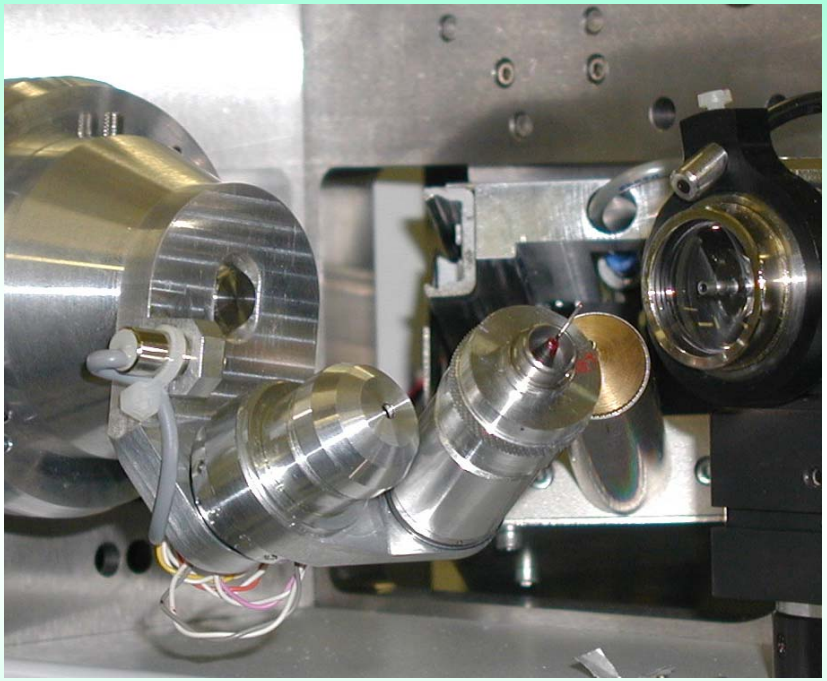
Aims

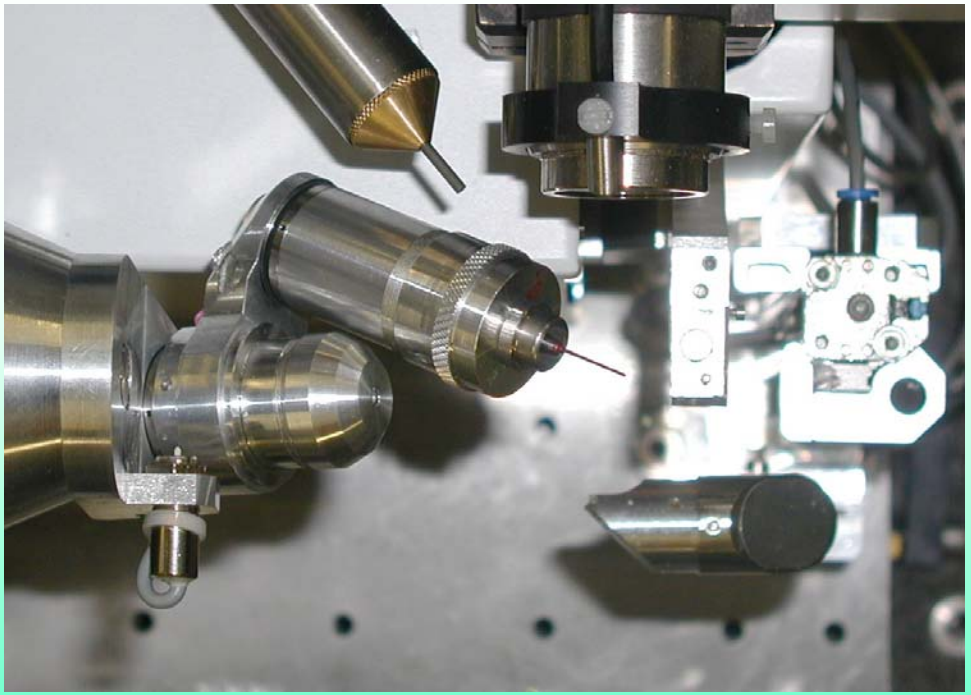
- Aligning crystals along a special axis
- Smart data collection strategies
- Get equivalent images from different crystals by reorienting them
- Sample ranking based on images with the same alignment
- Alignment to get better images for point group determination
- Find the orientation giving the best spot shapes (eg.: in case of bent crystals)

Software Requirements

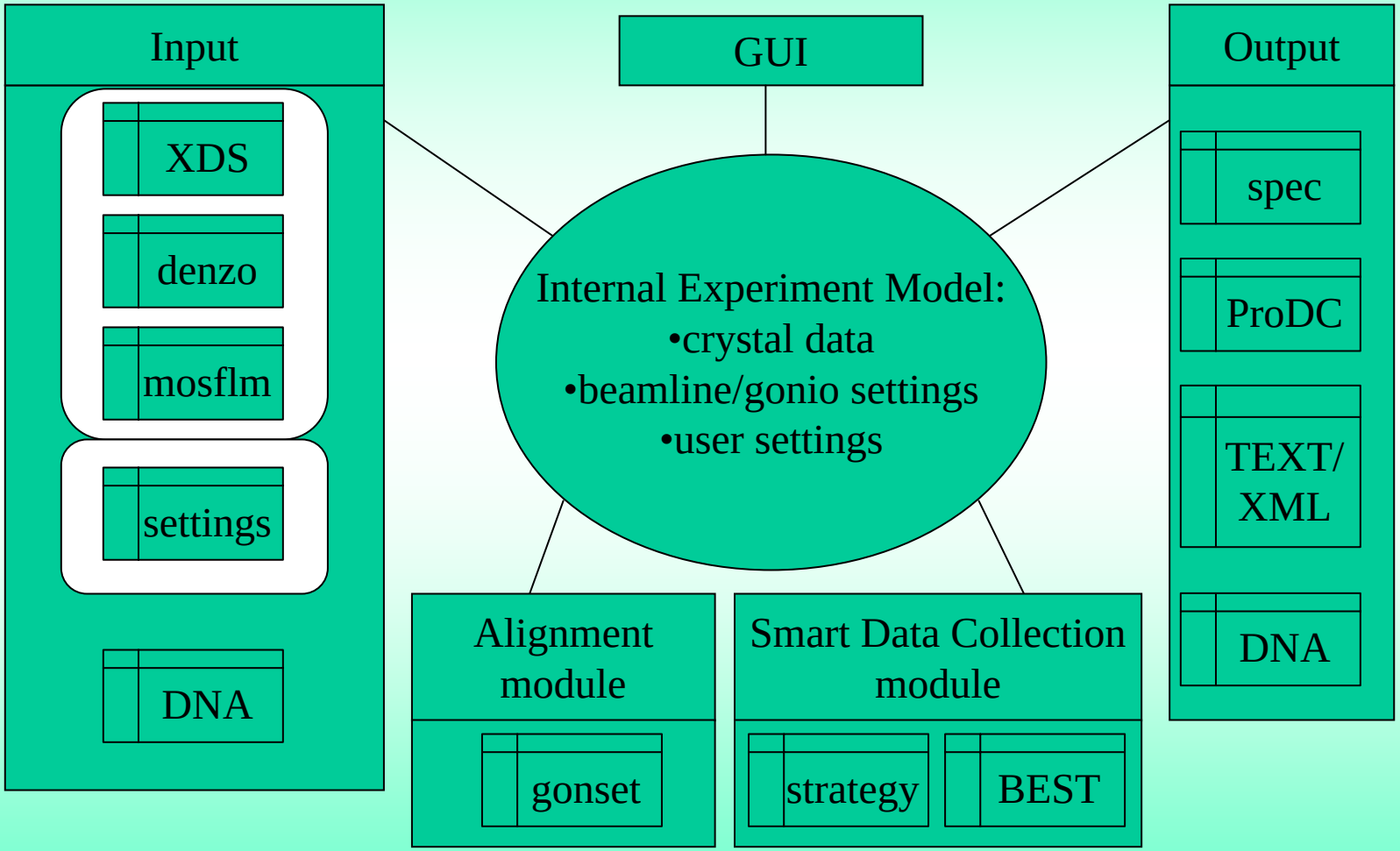
- Clear and easy to use GUI
- Combining existing tools:
  - Cell alignment calculation (gonset)
  - Two-sweep data collection strategies (strategy)
- Platform independent solution
- General solution for all possible kappa goniometers

EMBL/ESRF Mini-Kappa

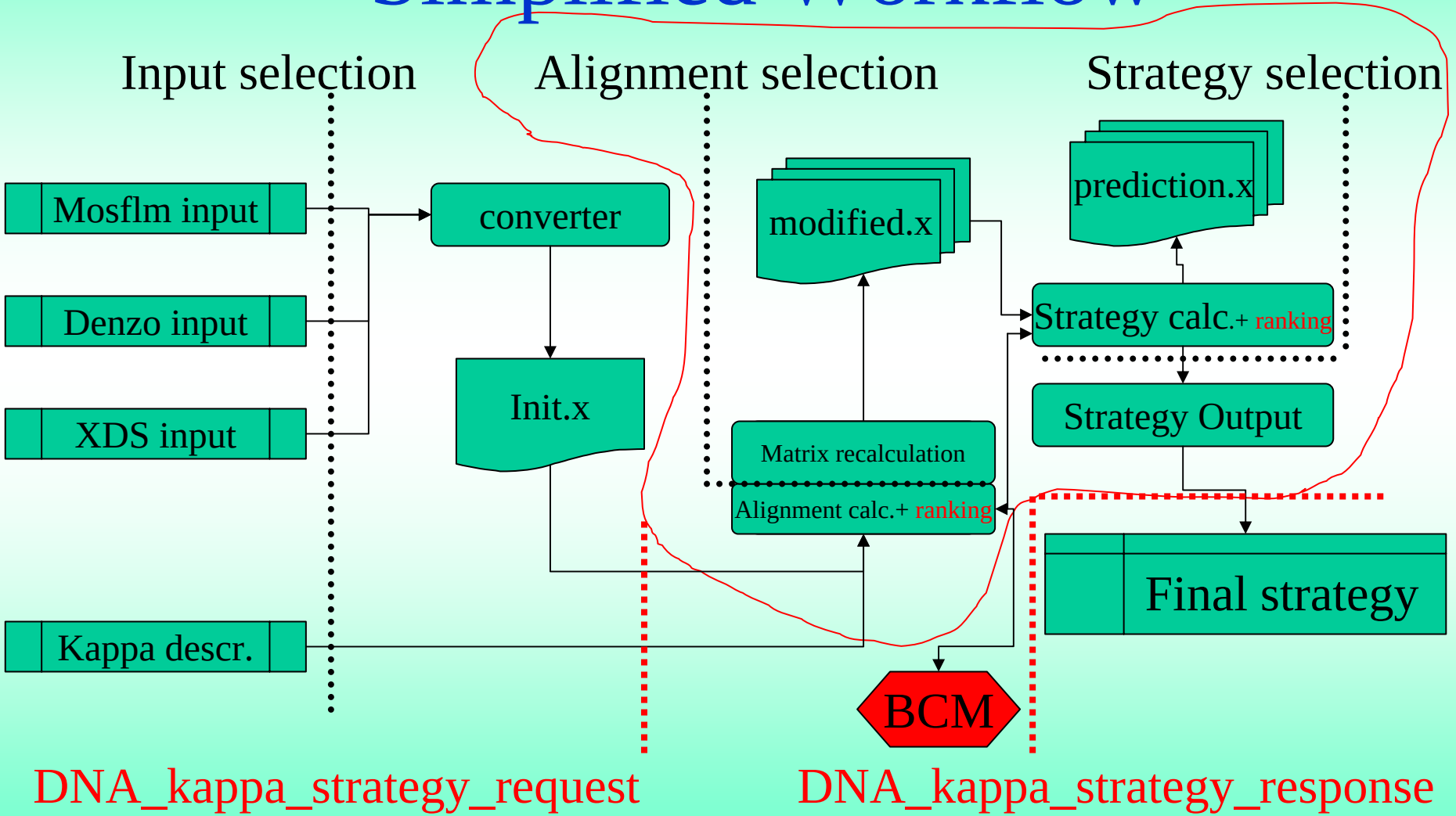


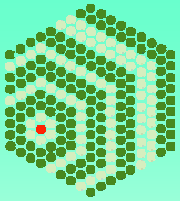


Software Structure



Simplified Workflow



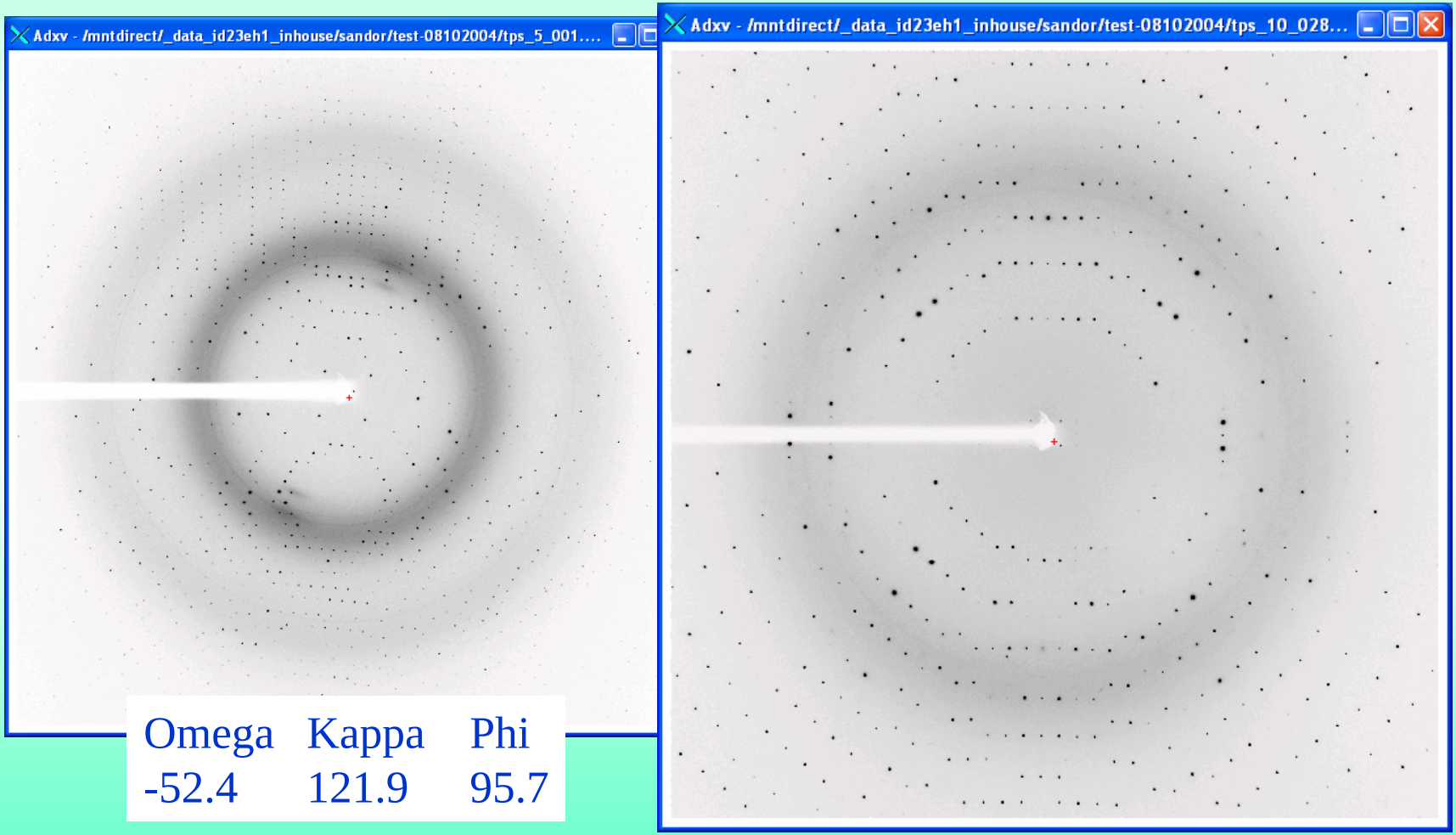


Development Stage

- Initial Revision (Java/Fortran/Python)
- Basic functionalities for experimental verification
- Direct access to motors via internal BCM
- Structural implementation of BCM with two plugins:
    - Spec for ESRF minidiffs
    - Tango for Microdif (MD2)

Trypsin - orthorhombic

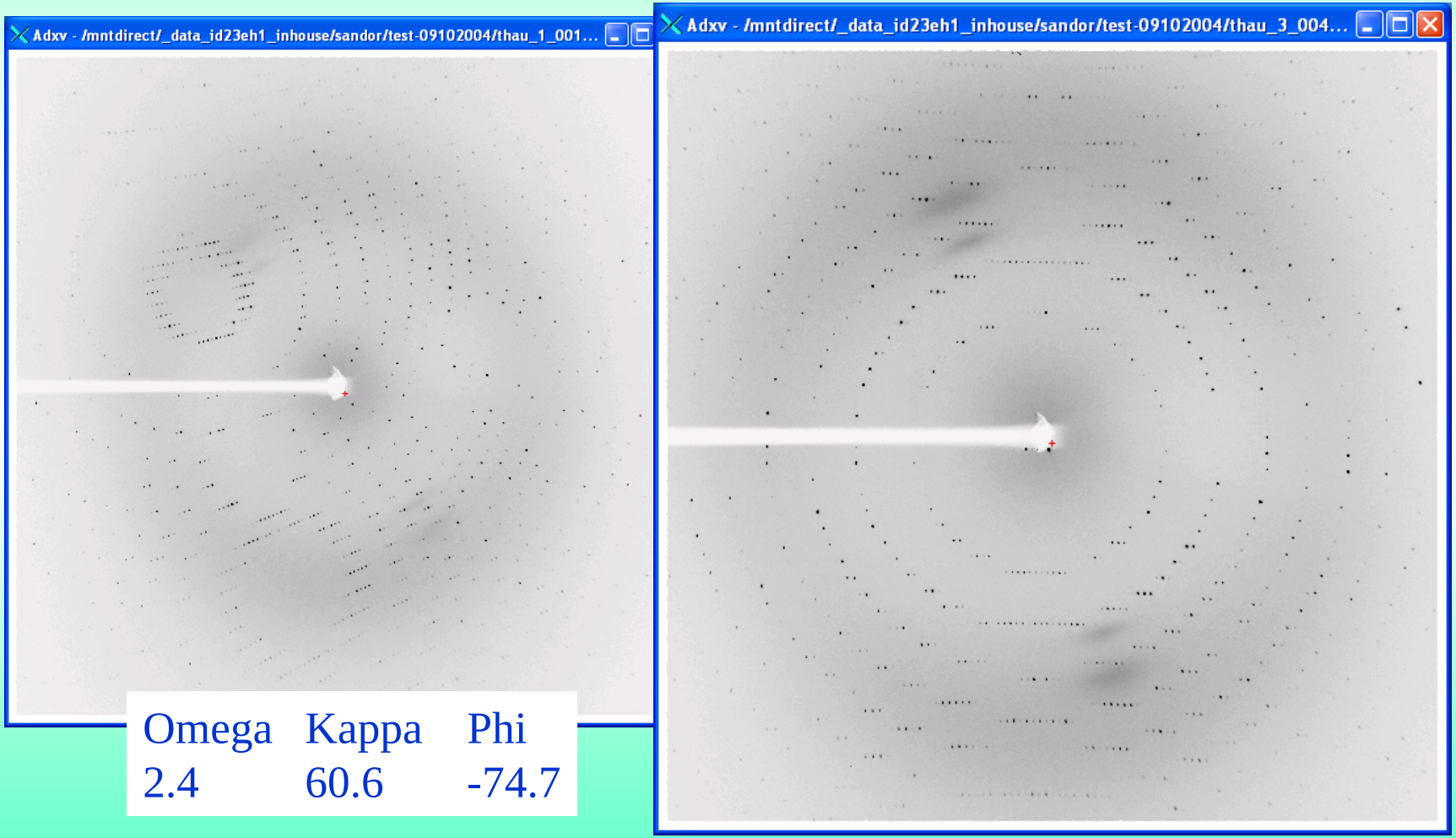
(ESRF-ID23 Test)



Omega	Kappa	Phi
-52.4	121.9	95.7

Thaumatin - tetragonal

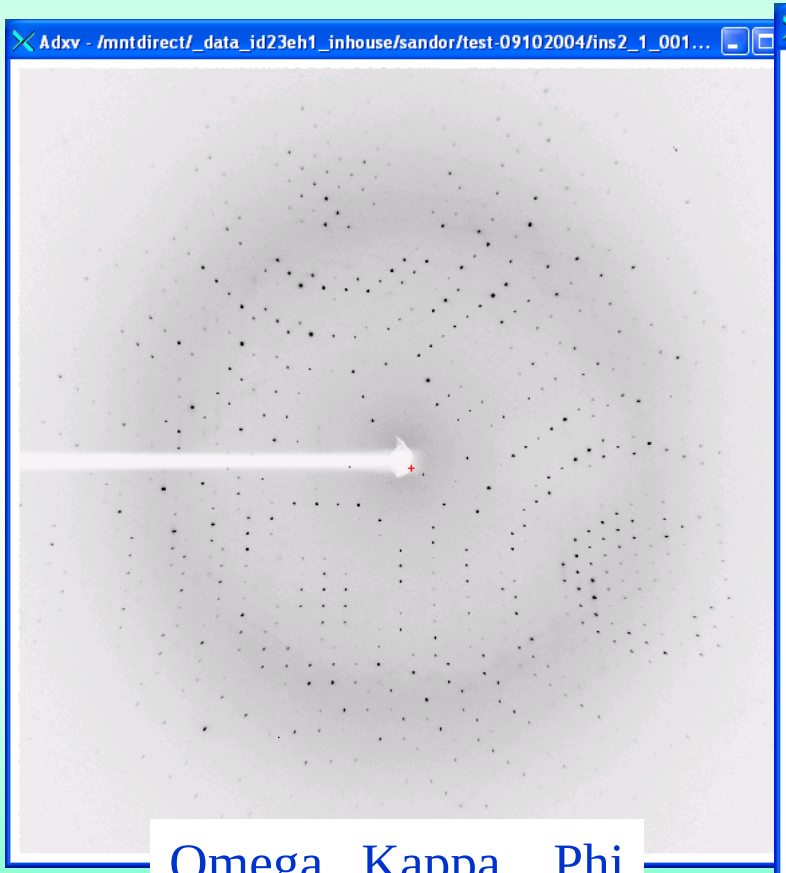
(ESRF-ID23 Test)

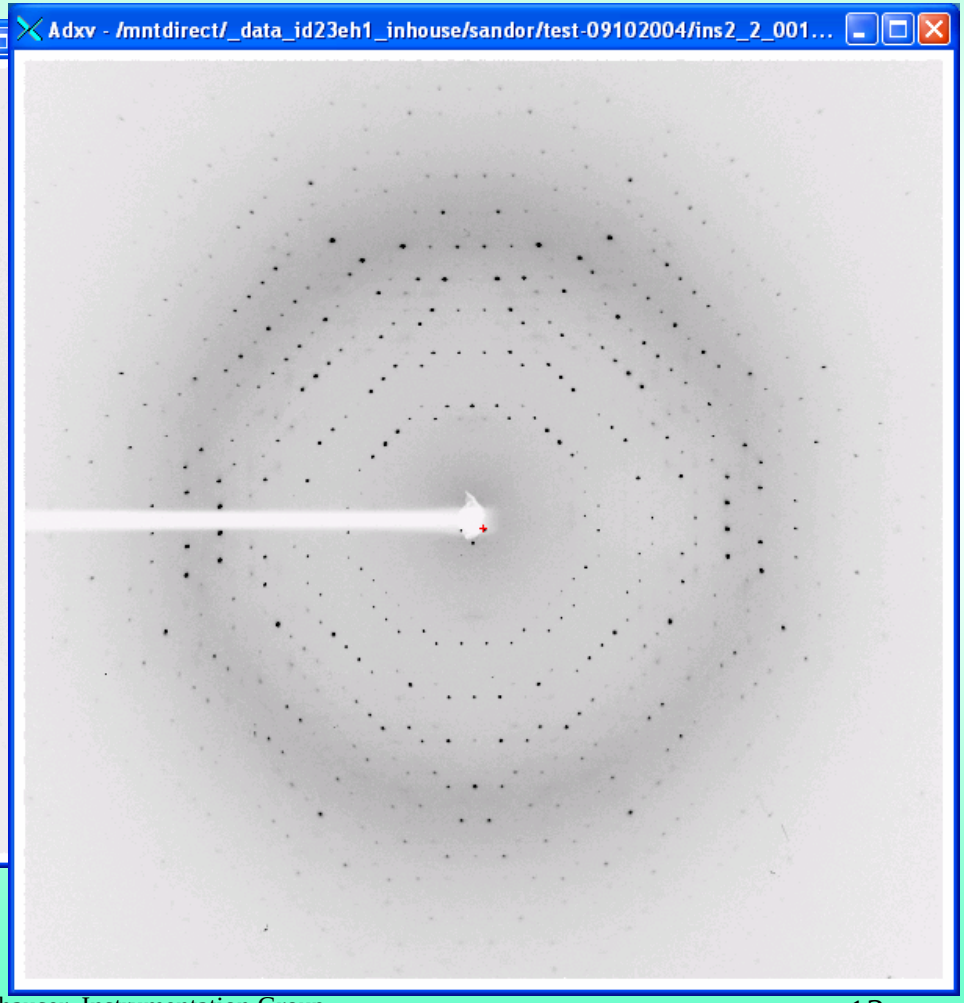


Omega	Kappa	Phi
2.4	60.6	-74.7

Insulin - cubic

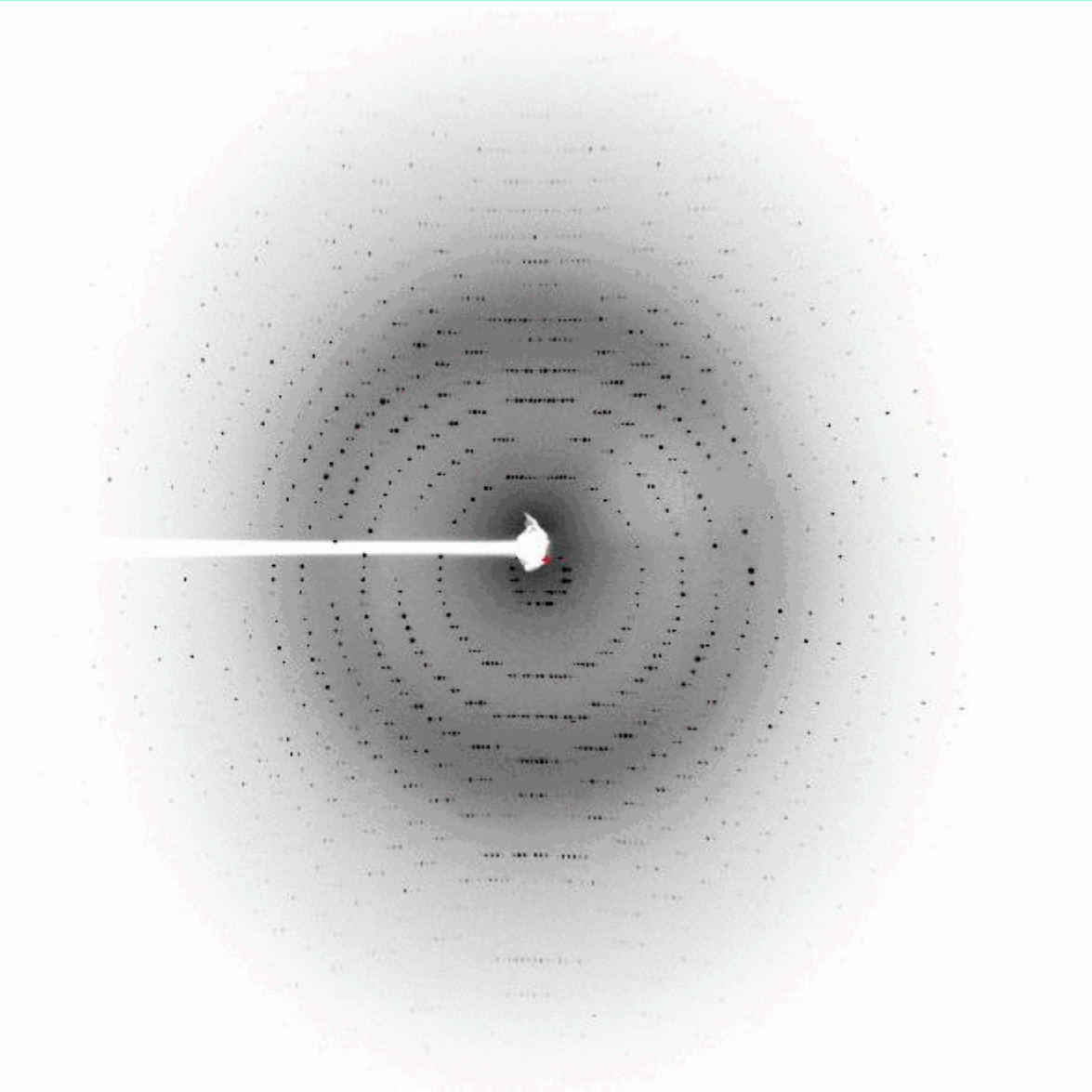
(ESRF-ID23 Test)

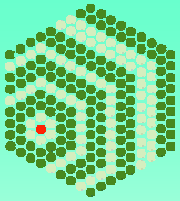




Omega	Kappa	Phi
-53.8	22.2	3.2

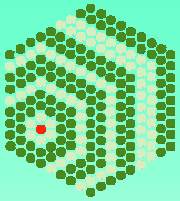
STAC- Data Collection





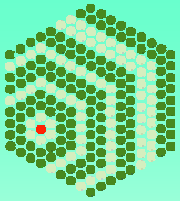
Improvement Plans

- Automatic Gonio Calibration
- Collision prediction
- Self-shadow prediction
- Flexible multi-pass strategy to fill in blind/inaccessible zones
- Offer closest possible solution if exact reorientation is not possible



DNA Integration: why?

- Make these options available for beamline users on an easy and integrated way
- Offer better calculation techniques made available by kappa gonios



DNA Integration

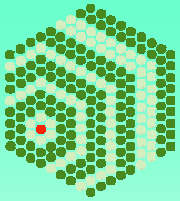
- 1st milestone (Dec 2005): geometric strategy for requested alignments
  - Kappa strategy Request/Response
  - Canvas to handle user interactions
  - Multiple pass strategies in DNA
- Later:
  - Integrating BEST strategies for kappa devices
  - Library offered for general crystal reorientation problems

Acknowledgements

- ESRF MX Group
  Sean McSweeney, Didier Nurizzo, Martin Walsh
- EMBL-Grenoble
  Florent Cipriani, Raimond Ravelli
- Kappa Workgroup
  Gerard Bricogne, Pierre LeGrand, Takashi Tomizaki
- DNA Collaboration
  all of us

Movies

- Crystal movement without Translation Correction
- Movement with automatically calculated translation correction
- Go even closer
- See the EMBL/ESRF Mini-kappa in action



Thank you for your attention!

My Questions

- What would you expect from using kappa gonios in general
- How would you rank the possible strategies
- How can a unit of DNA get information on beamline-specific static/dynamic settings (eg.: rotation axis of kappa and used motor positions taking an image)
- Can a unit directly send requests/queries to any other units (Database/BCM/…)