

The Kappa Workgroup and CCPN

Peter Keller

Global Phasing Ltd.

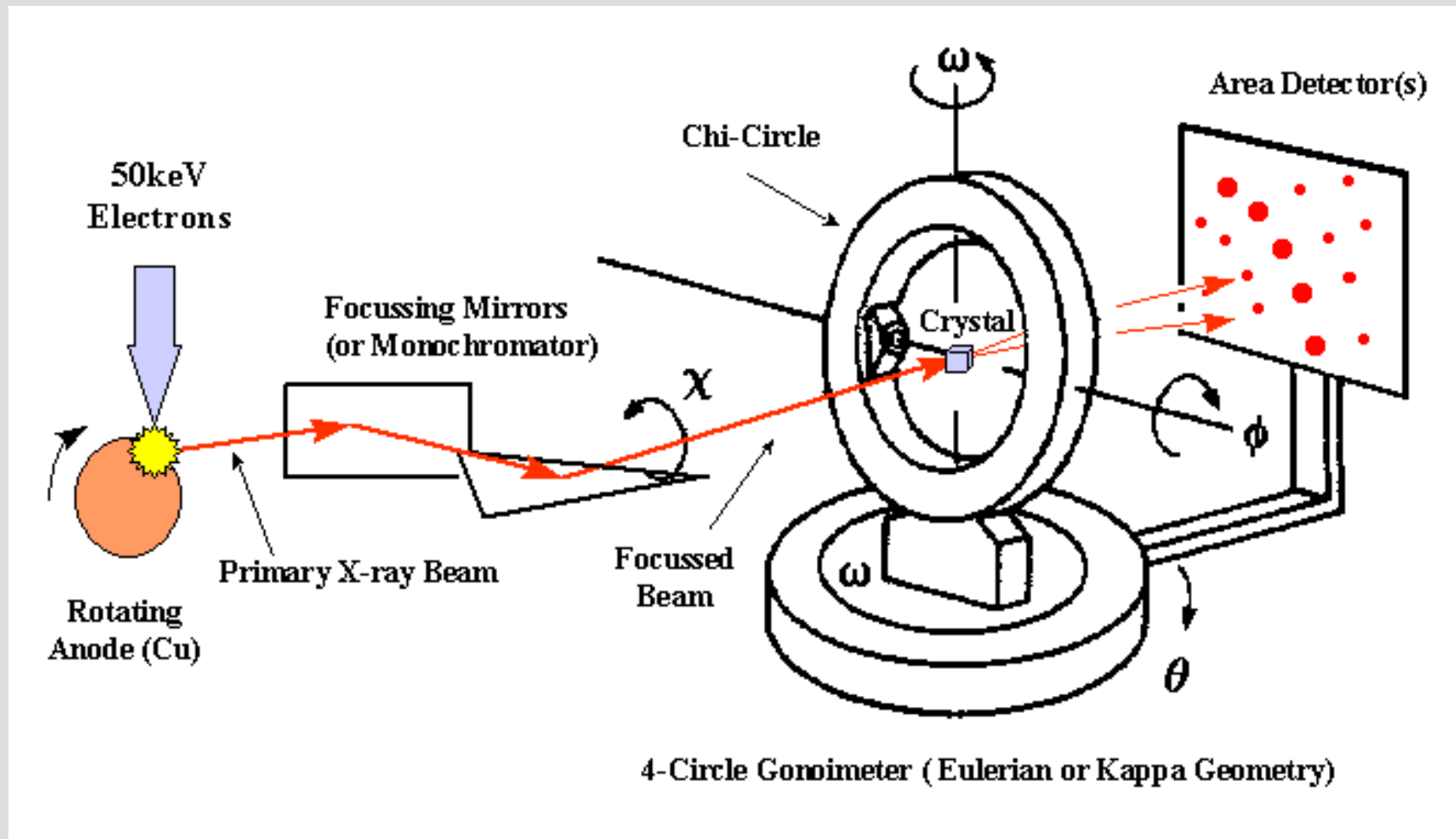
<http://www.globalphasing.com>

<http://www.bioxdm.org>

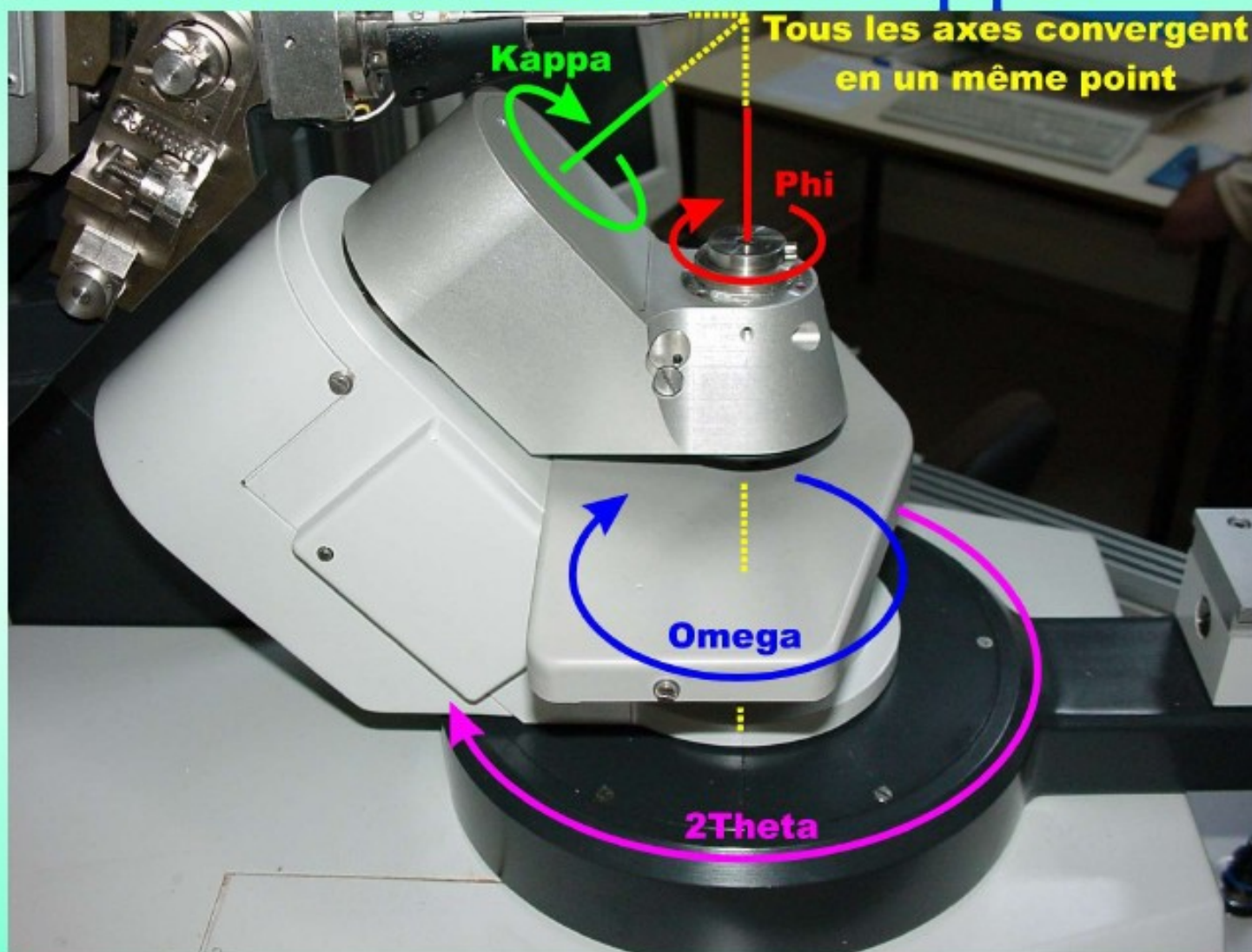
Background to the Kappa workgroup

- Protein crystallography at European synchrotrons
 - part of the EU FP6 BioXHIT project
 - <http://www.bioxhit.org>
 - Currently using CCPN to prototype ideas
 - Decision about whether to use CCPN long-term is some way off.
 - Includes:
 - Sándor Brockhauser (EMBL-Grenoble)
 - Gleb Bourenkov (EMBL-Hamburg)
 - Johan Unge (EMBL-Hamburg)
 - Others ...

X-ray diffraction: data collection



Bruker Nonius Kappa



A Kappa goniostat



(Bruker AXS)

GΦL



Cambridge, Jan 2008

Collision map: collimator

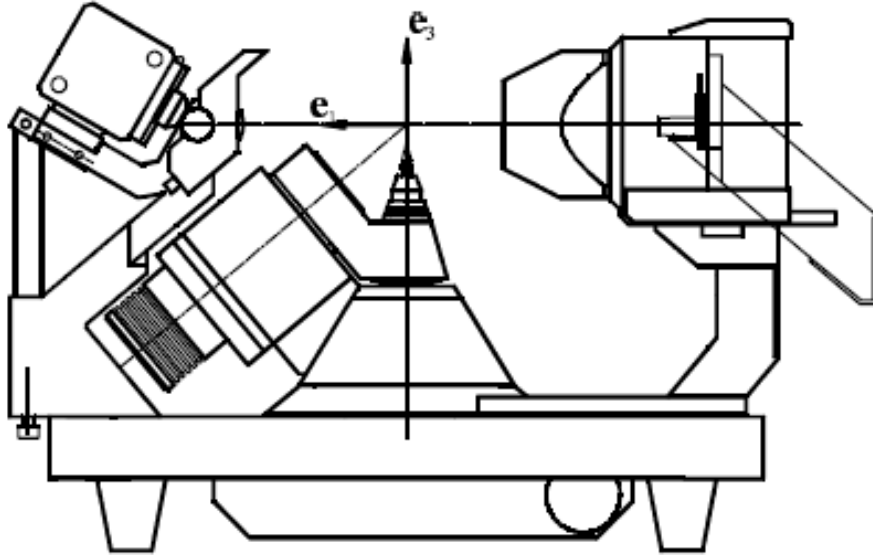


Figure 6.2-1: Side view of experimental setup in the KM4CCD system. The laboratory reference system is shown with bold vectors. The invisible basis vector e_2 points towards the reader. Note the conventional scintillation counter to the side of the CCD detector head.

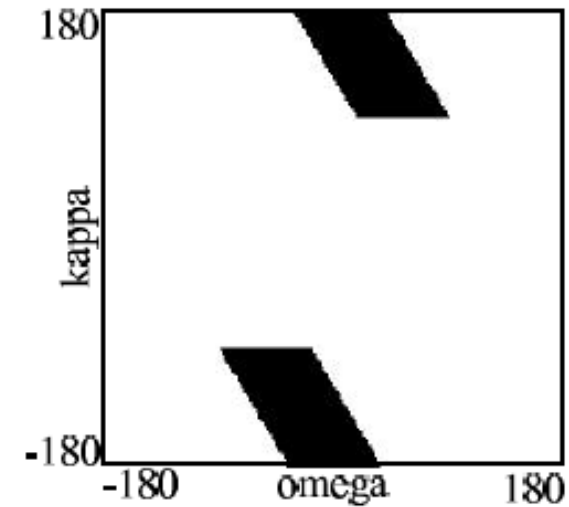


Figure 1.10-1: Collimator - collision map for an - speed ratio of 1.4. The black zones mark the collision areas. Note that this collision component is independent.

Mathias Meyer's
Ph.D. Thesis
(Lausanne, 1998)

Collision map: collimator + detector

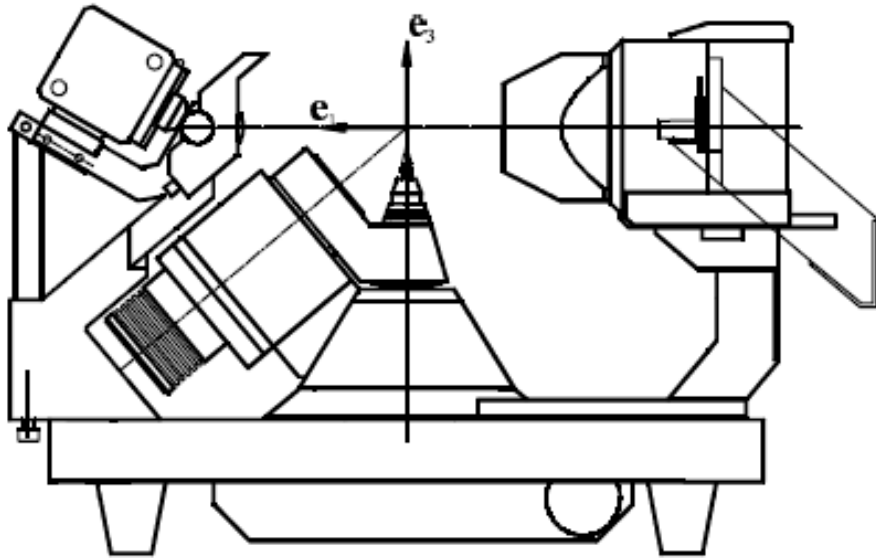


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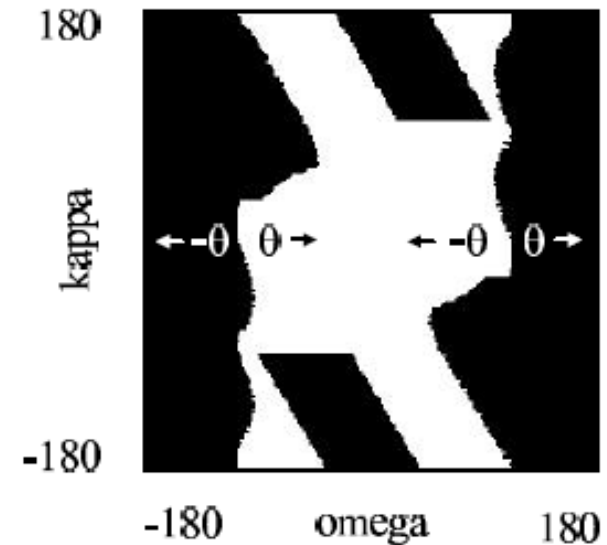


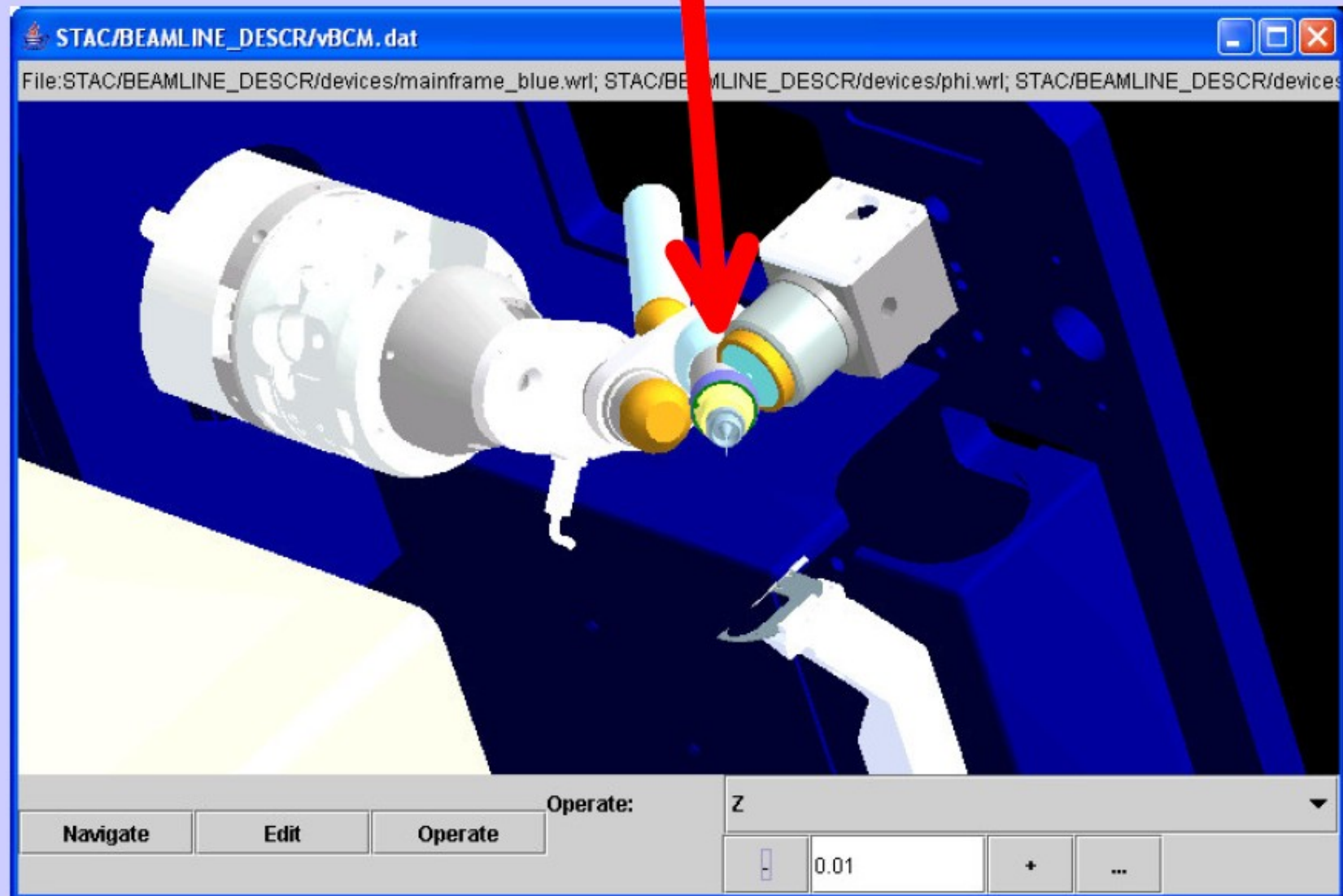
Figure 1.10-2: Detector and collimator collision areas represented in κ - ω space (β -speed ratio 1.4, $\theta = 0^\circ$, sample-to-scintillator distance = 70mm). The black zones mark the collision areas. Note that the seemingly small corridors in the mathematical quadrants I and III still allow the access to the high κ regions. The translation of the detector collision lines with a change of θ is indicated.

Mathias Meyer's
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The Abstract Kappa System

- Part of STAC (STrategy for Aligned Crystals)
 - Sándor Brockhauser
- Full knowledge of instrument characteristics
- Only knowledge of sample is that necessary to calculate collision maps
 - i.e. Physical dimensions.
- External software provides a high-level sample-specific data collection strategy
 - STAC translates this to more specific levels

MiniKappa in Action



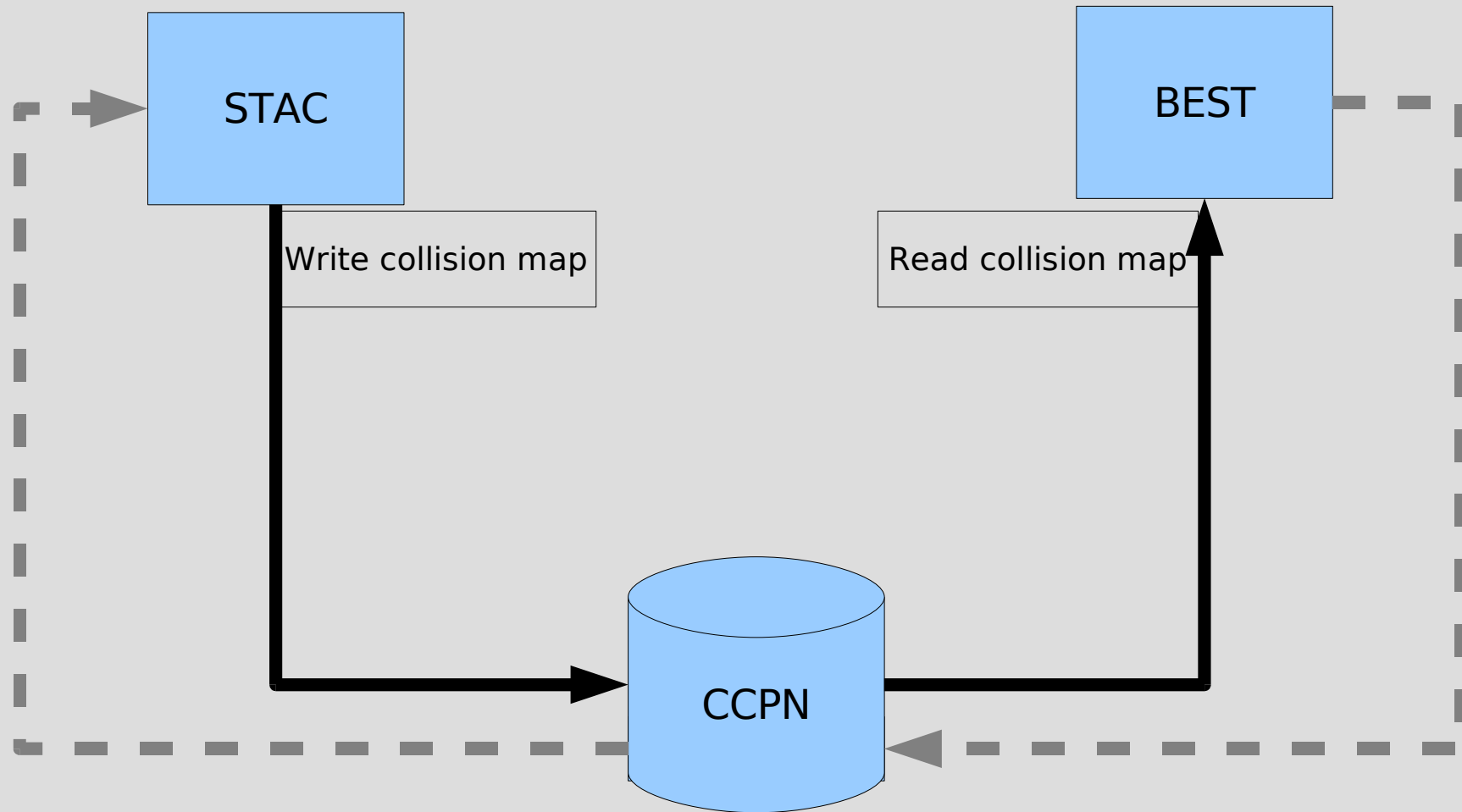
BEST

- Application to calculate a data collection strategy
 - Gleb Bourenkov and Sasha Popov (ESRF, Grenoble)
 - <http://www.embl-hamburg.de/BEST/>
- Allows for sample decay in X-ray beam
- Limited knowledge of goniostat
- Currently cannot cater for Kappa goniostats
 - Johan Unge working on adding this facility.

BEST + Kappa (1)

- BEST knows about:
 - Sample orientation
 - Requirements for successful data collection
 - Sensitivity of sample to X-rays
 - X-ray beam and detector characteristics
- BEST needs access to the collision map and associated data
 - No point calculating a strategy that cannot be collected because of physical restrictions on the goniostat!

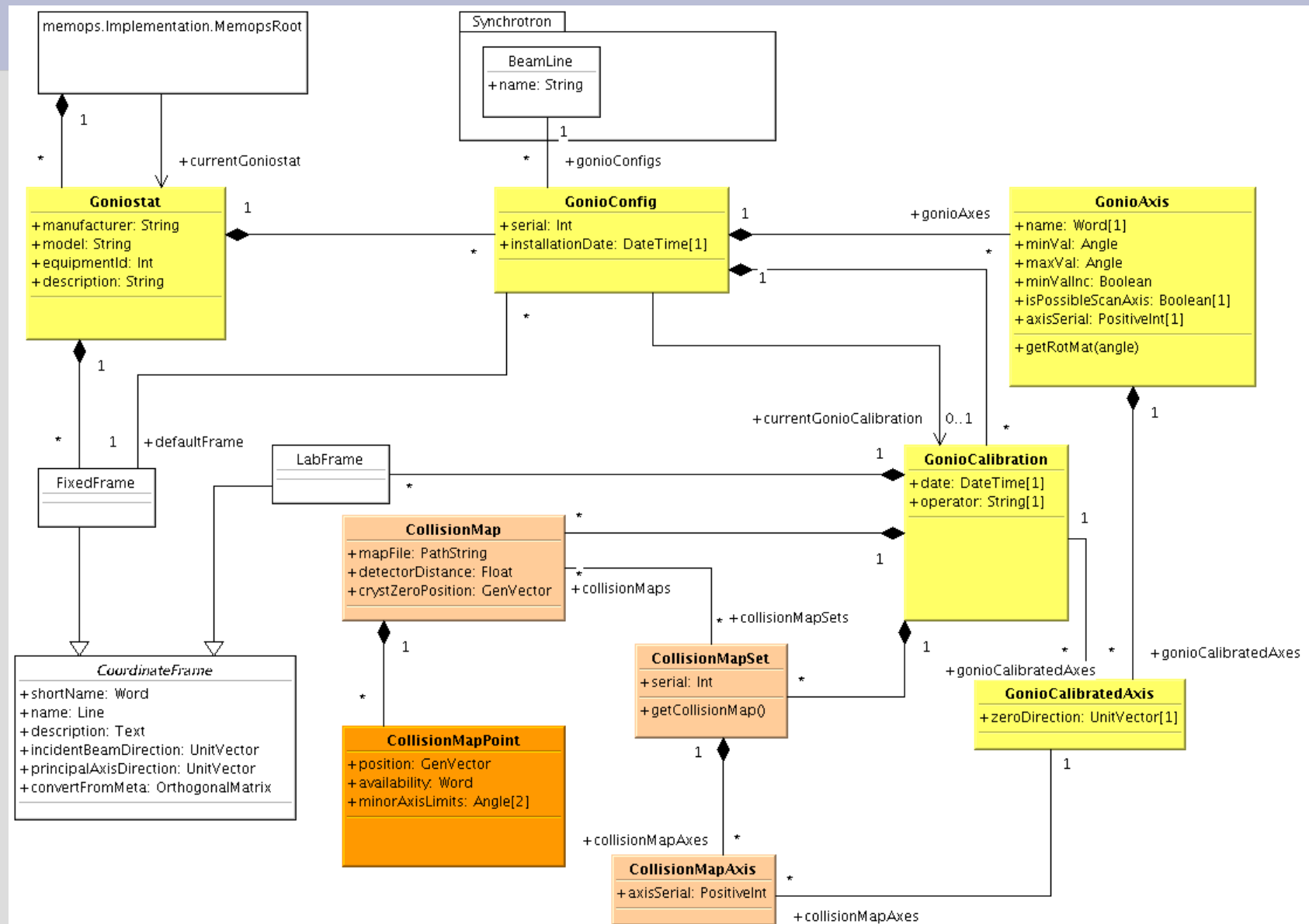
BEST + Kappa (2)



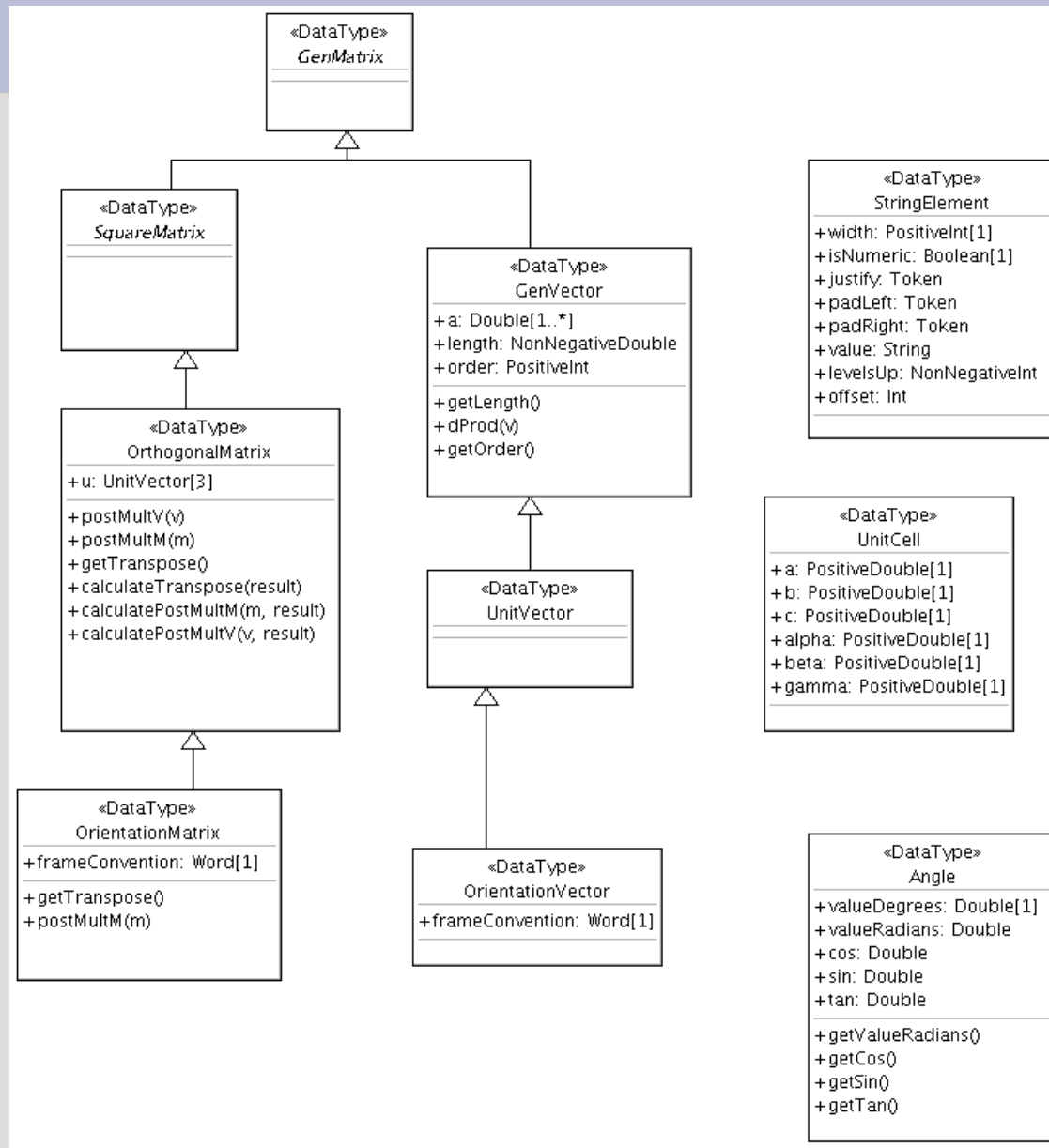
Characteristics and status

- Java API
- XML backend
- Complex datatypes
- Initial model
- API generated and tested
- Work on adding CCPN API to applications about to start
 - STAC: Java
 - BEST: Fortran90

BioXDM style data model (1)



BioXDM style data model (2)



Collision map data

- Currently handled as an external binary file: the model contains the filename
- Should the map be handled directly by the CCPN-generated API?
 - Binary object?
 - XML document?
 - Model map contents?

Concurrent access

- Concurrent access will be required
 - Parallelisation of computations
 - Central maintenance of configuration data
 - This probably implies that the ACID* criteria will need to be satisfied
 - RDBMS the “traditional” way of doing this
 - There are others, e.g. Oracle DbXML (formerly Sleepycat), available under the GPL.
- Python API probably not required for the immediate future.

* Atomicity, Consistency, Isolation, Durability

Support

- Global Phasing consortium
- BIOXHIT (EU 6th Framework Programme)

GΦL



SIXTH FRAMEWORK
PROGRAMME