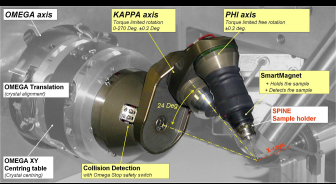


# Automatic Calibration of Multi-Axis Goniometers for Macromolecular Crystallography

Sandor Brockhauser , Bernard Lavault, Doug du Boulay, Peter Turner

NOBUGS 2008 Conference  
Sydney, Australia  
Nov 3-5, 2008



# Crystal Alignment

## Reorientation

problem  
solution

RotCalib

method

xyz ?

TranCalib

method

solution

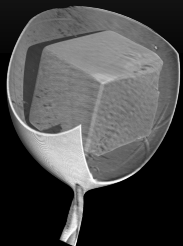
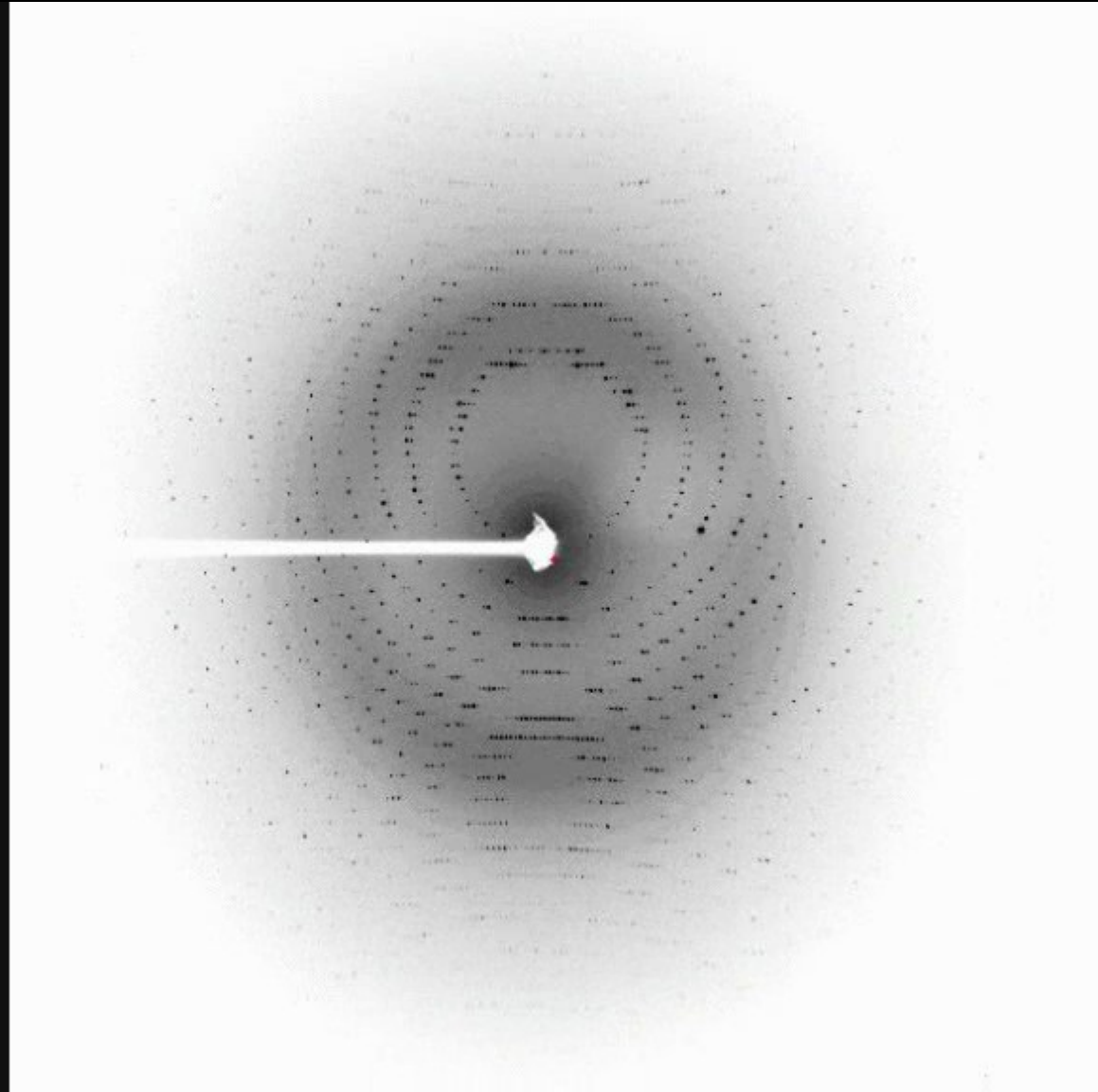
Collision

virtual gonio

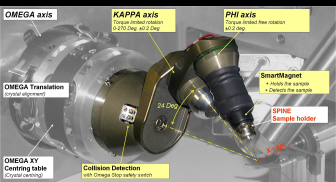
adjustment

collision maps

Summary



# Multi-Axis Goniometers



Reorientation

problem

solution

RotCalib

method

xyz ?

TranCalib

method

solution

Collision

virtual gonio

adjustment

collision maps

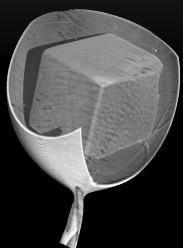
Summary



Newport



Huber

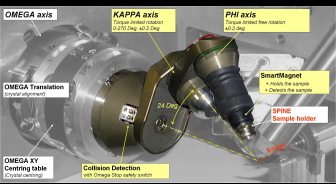


Sandor Brockhauser

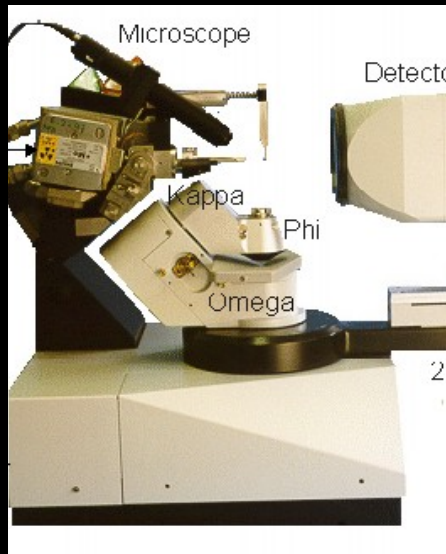


NOBUGS 2008 Conference, Sydney, Nov 3-5, 2008.

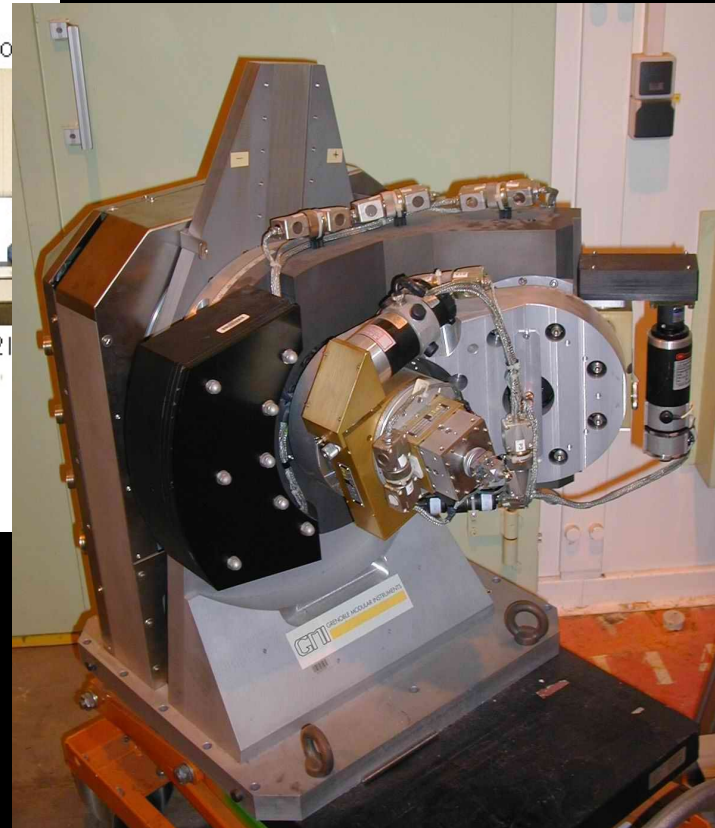
# Multi-Axis Goniometers



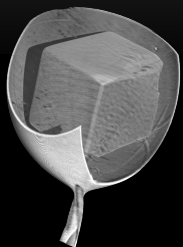
Reorientation  
 problem  
 solution  
 RotCalib  
 method  
 xyz ?  
 TranCalib  
 method  
 solution  
 Collision  
 virtual gonio  
 adjustment  
 collision maps  
 Summary



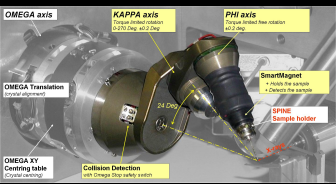
**Bruker-Nonius**



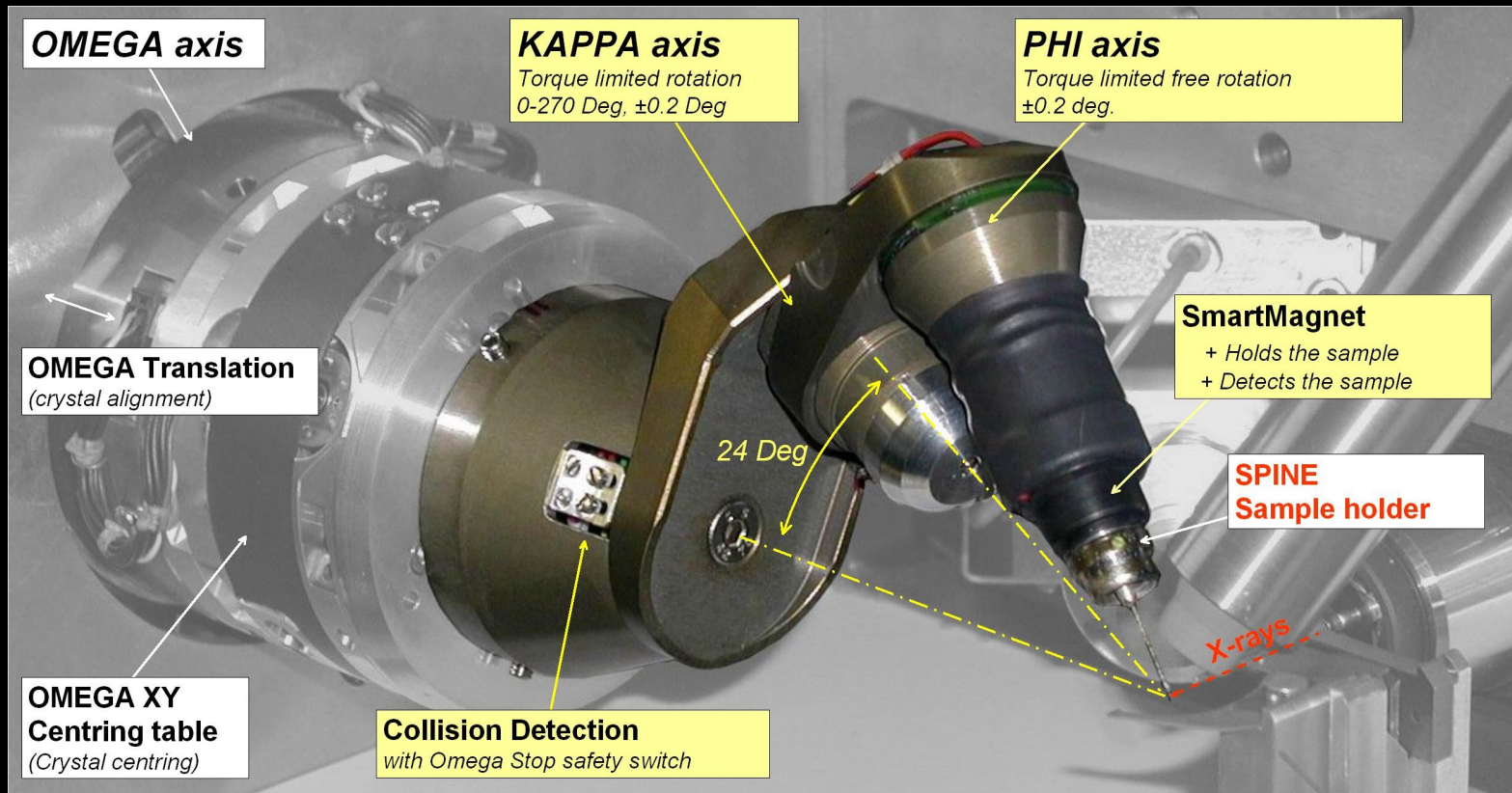
**GMI**



# EMBL/ESRF MiniKappa



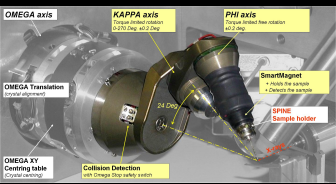
- Reorientation problem
- solution
- RotCalib method
- xyz ?
- TranCalib method
- solution
- Collision
- virtual gonio
- adjustment
- collision maps
- Summary



ESRF: MX (ID14-1,2,4, ID23-1(2), ID29), BM14, BM30  
 APS: 4                      ALS: 1  
 DIAMOND: 1                BESSY: 1                PETRAIII: 1

16 units

# Rotation Calibration



Reorientation  
 problem  
 solution  
**RotCalib**  
 method  
 xyz?  
 TranCalib  
 method  
 solution  
 Collision  
 virtual gonio  
 adjustment  
 collision maps  
 Summary

STAC: STrategy for Aligned Crystals

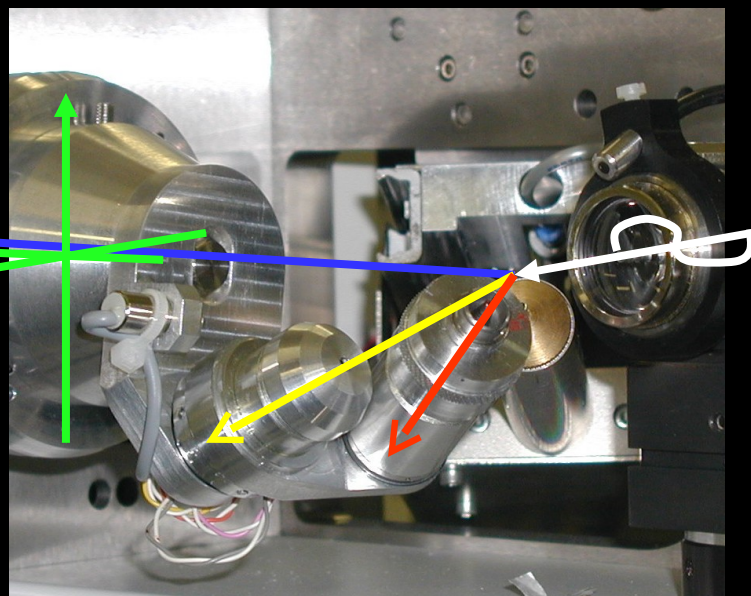
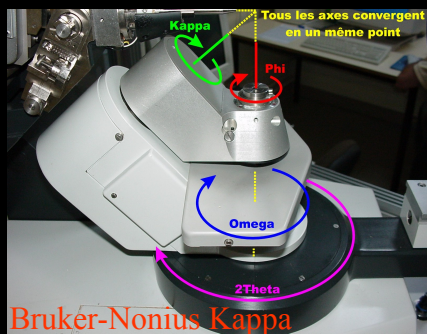
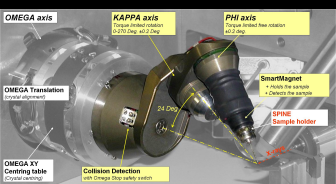
Have you initialized your kappa system?   Translation Corr

Mat(-;-):	<input type="radio"/> Mosflm	<input type="radio"/> XDS	<input checked="" type="radio"/> Denzo	ev\STAC\test\kappa_calib\Mat0.x	<input type="button" value="Folder"/>	Calibration (P/K/O):	Mv(0;0;0)
Mat(-;-P):	<input type="radio"/> Mosflm	<input type="radio"/> XDS	<input checked="" type="radio"/> Denzo	ev\STAC\test\kappa_calib\Mat1.x	<input type="button" value="Folder"/>	24	Mv(0;0;P)
Mat(-;K;P):	<input type="radio"/> Mosflm	<input type="radio"/> XDS	<input checked="" type="radio"/> Denzo	ev\STAC\test\kappa_calib\Mat2.x	<input type="button" value="Folder"/>	24	Mv(0;K;P)
Mat(O;K;P):	<input type="radio"/> Mosflm	<input type="radio"/> XDS	<input checked="" type="radio"/> Denzo	ev\STAC\test\kappa_calib\Mat3.x	<input type="button" value="Folder"/>	24	Mv(O;K;P)

Calculated axes:	X	Y	Z	Angle	Diff to current	Diff to Trans
Phi:	0.00673	-0.00958	0.99993	23.984	90.549	0.118
Kappa:	-0.28252	-0.29603	0.91244	23.948	107.219	0.532
Omega:	0.00059	-0.00079	1.00000	23.952	90.045	0.056



# Inverse Kappa System



Beam  
 Omega  
 Translation Table  
 Kappa  
 Phi

Reorientation  
 problem  
 solution

RotCalib

method

xyz ?

TranCalib

method

solution

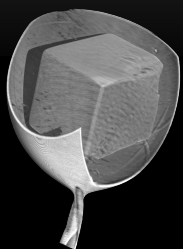
Collision

virtual gonio

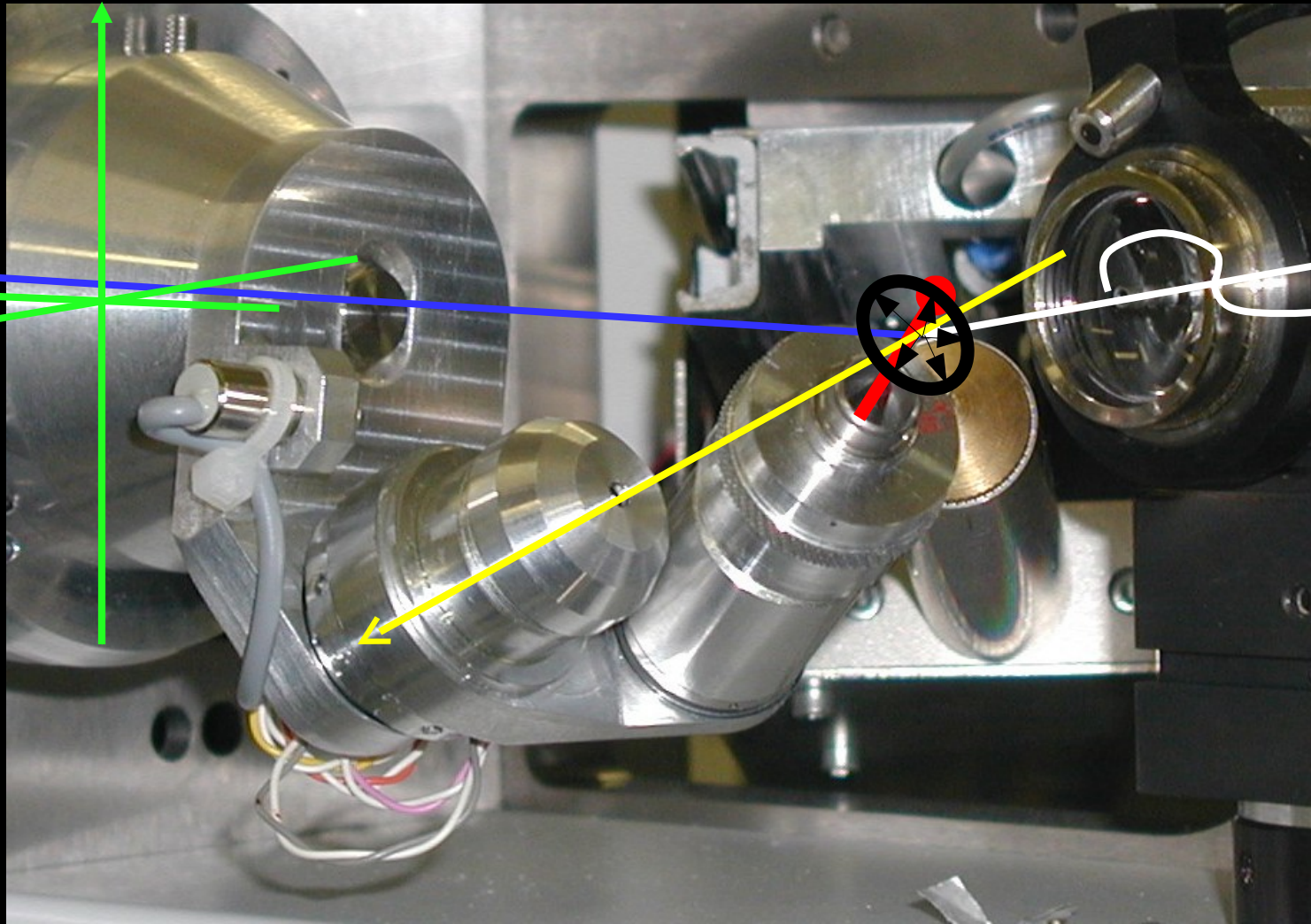
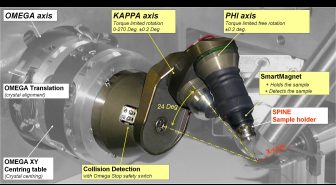
adjustment

collision maps

Summary



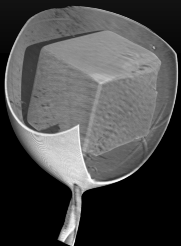
# Centering

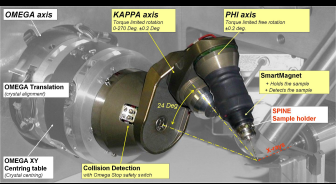


Reorientation  
problem  
solution  
RotCalib  
method  
xyz ?

TranCalib  
method

solution  
Collision  
virtual gonio  
adjustment  
collision maps  
Summary



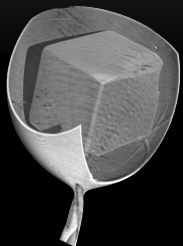


# Automatic Centering by C3D

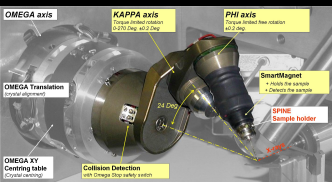
Reorientation  
problem  
solution  
RotCalib  
method  
xyz ?

TranCalib  
method

solution  
Collision  
virtual gonio  
adjustment  
collision maps  
Summary



# Translation Calibration



Reorientation  
problem  
solution  
RotCalib  
method  
xyz ?

TranCalib  
method  
solution

Collision  
virtual gonio  
adjustment  
collision maps  
Summary



STAC: Strategy for Aligned Crystals

Have you initialized your kappa translation?

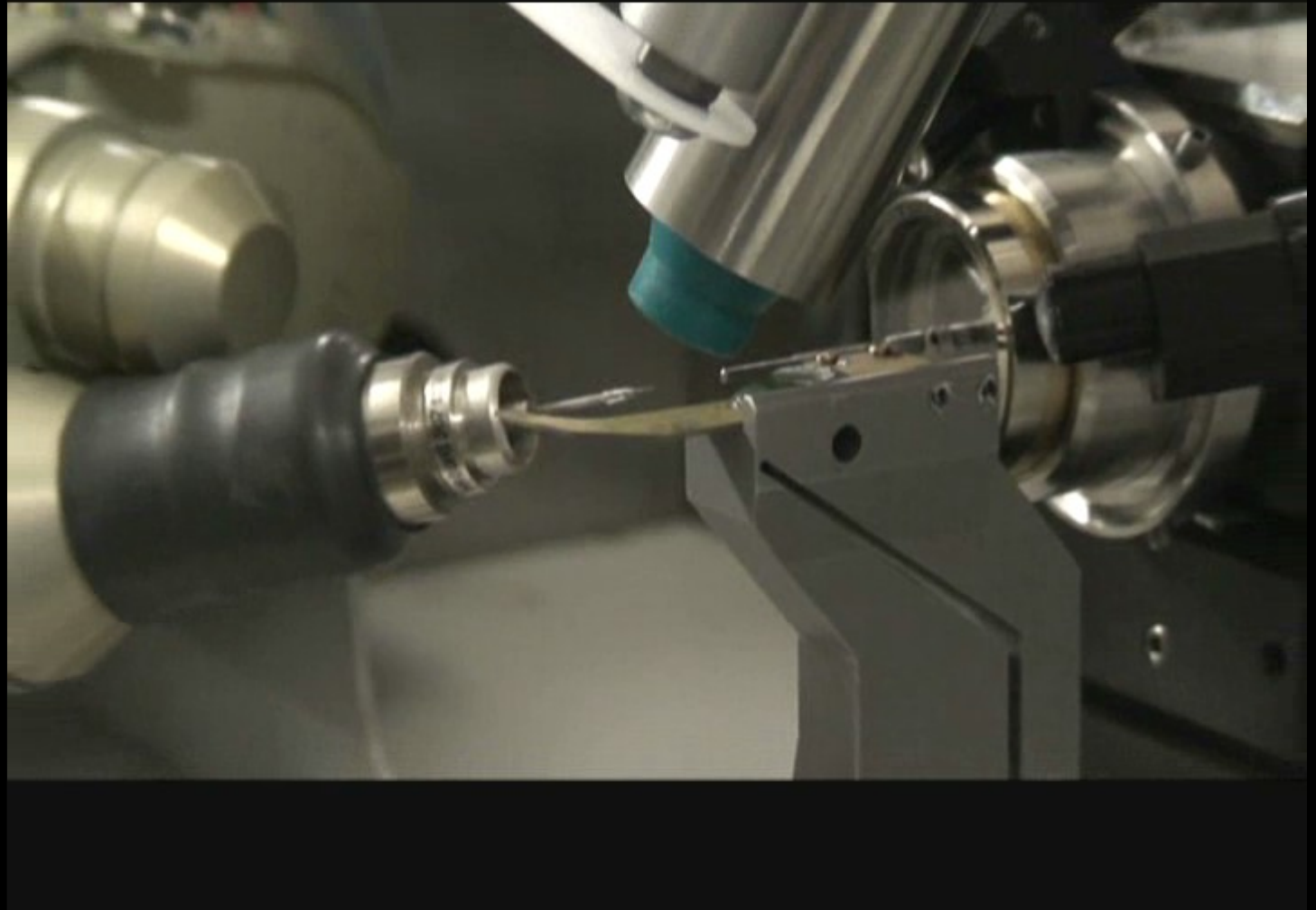
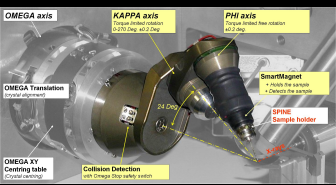
Angle	X	Y	Z
Phi translation (datum = only ...)	180.0	Mv Phi	
90.0014	-0.1598	0.3095	0.0022
180.0028	-0.4360	0.1640	0.0029
270.0042	-0.3053	-0.1296	0.0002

Angle	X	Y	Z
Kappa translation (datum = o...)	180.0	Mv Kappa	
79.9979	0.0451	0.3493	0.1249
159.9958	-0.2903	0.4623	0.0578
240.0025	-0.4405	0.1856	-0.0837

Calculated axes:	X	Y	Z	Diff to current	Diff to RotCalib
Phi:	0.00434	-0.00599	0.99997	0.336	1.877
Kappa:	-0.29172	-0.29570	0.90965	34.157	48.382

Pts on axes:	X	Y	Z	Axis dist	Reconstr.Error
Phi axis:	0.21699	-0.08480	-0.00128	0.364	0.02867
Kappa axis:	0.17545	-0.21360	-0.01185	0.927	0.01991

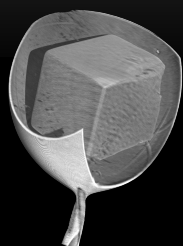
# Virtual Beamline Simulator



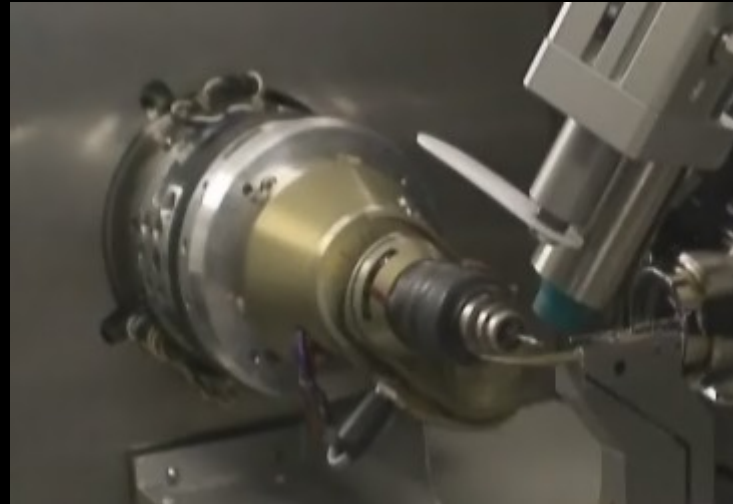
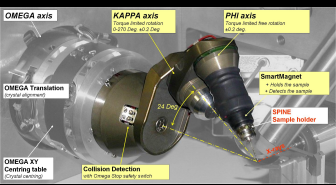
Reorientation  
problem  
solution  
RotCalib  
method  
xyz ?  
TranCalib  
method  
solution

## Collision

virtual gonio  
adjustment  
collision maps  
Summary



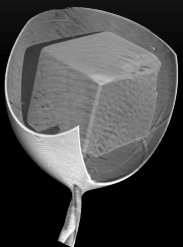
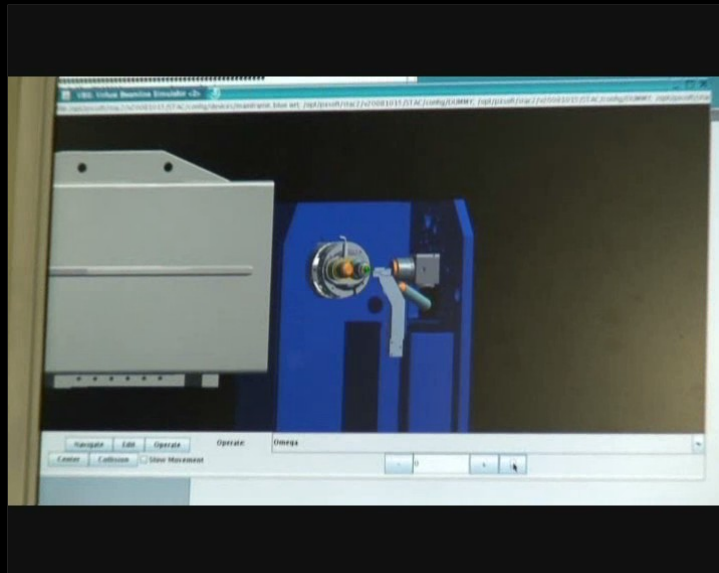
# Virtual Beamline Simulator



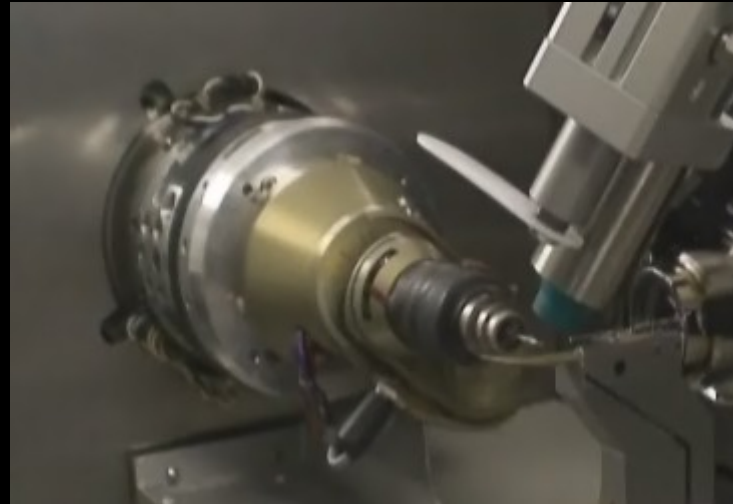
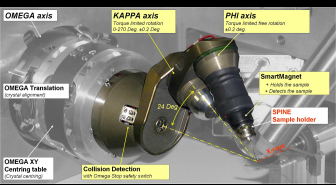
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collision maps  
Summary



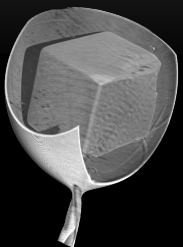
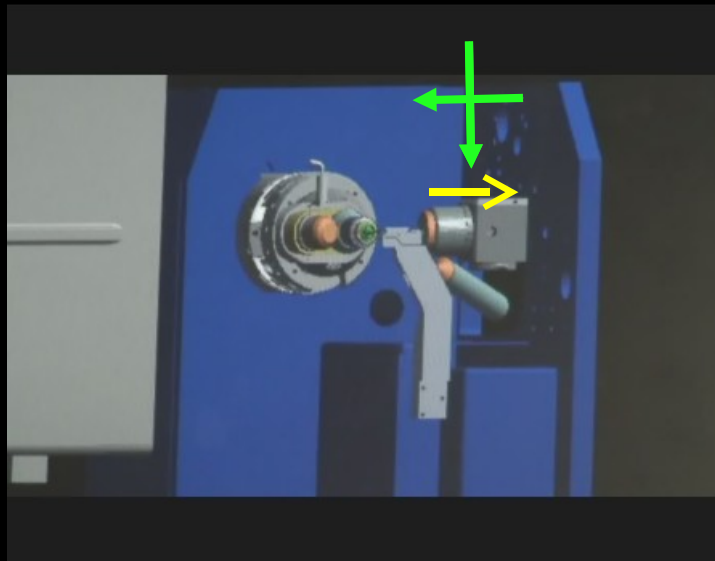
# Virtual Beamline Simulator



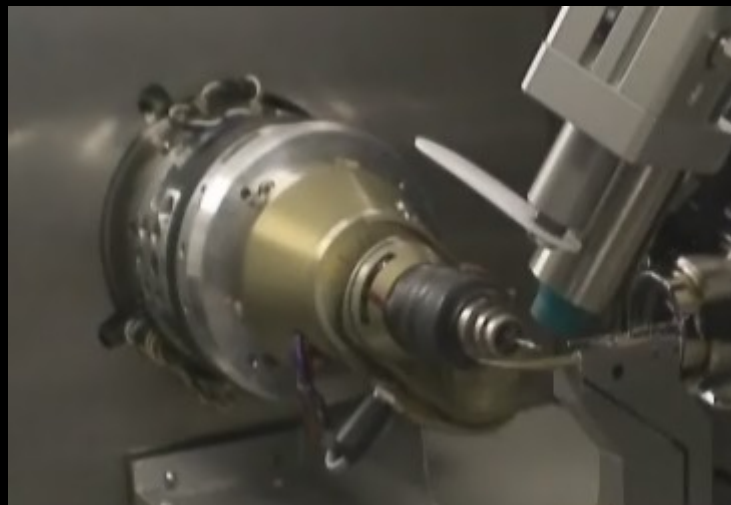
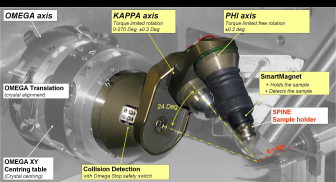
Reorientation  
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## Collision

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Summary



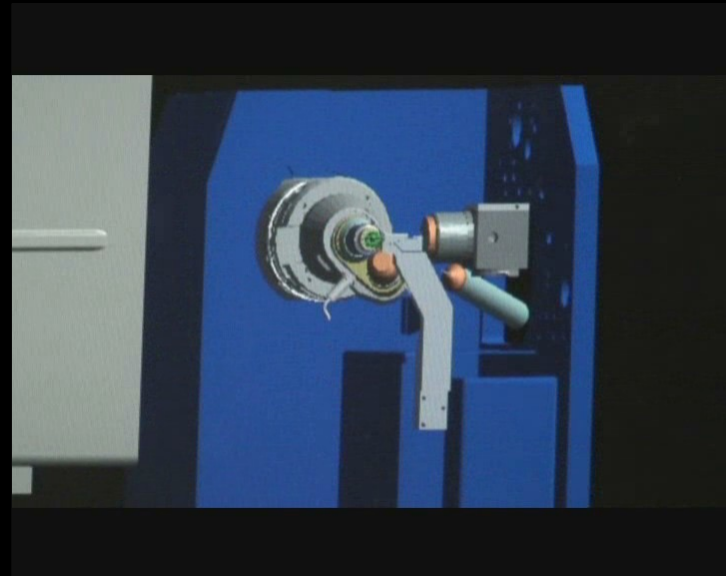
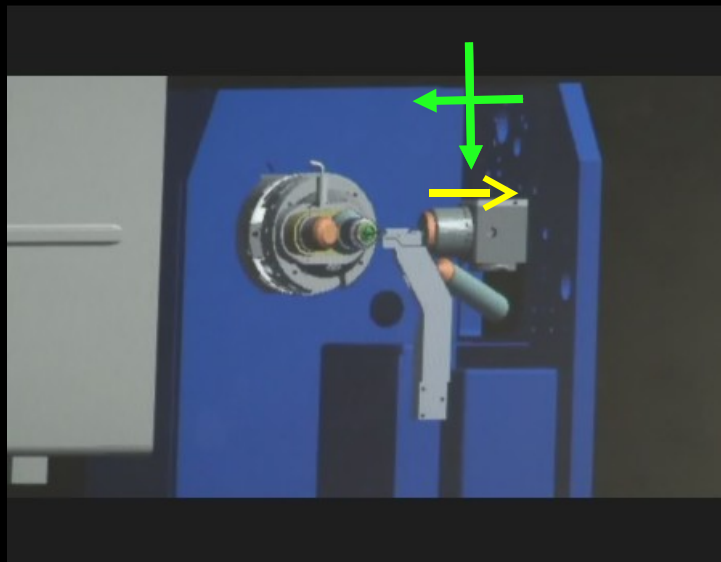
# Virtual Beamline Simulator



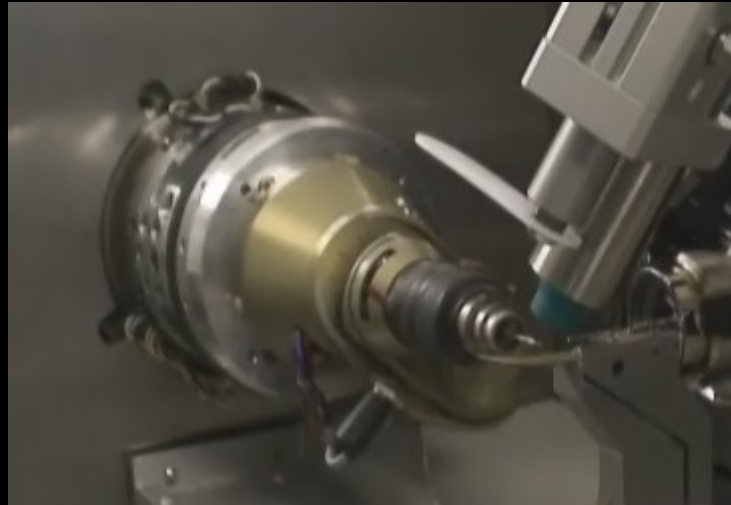
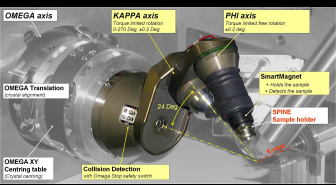
Reorientation  
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## Collision

virtual gonio  
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Summary



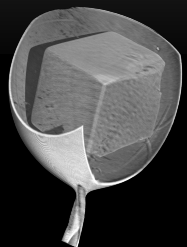
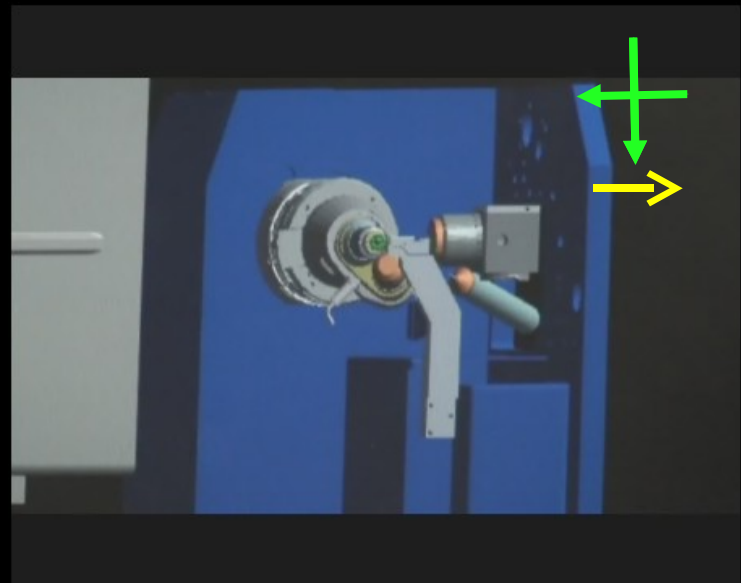
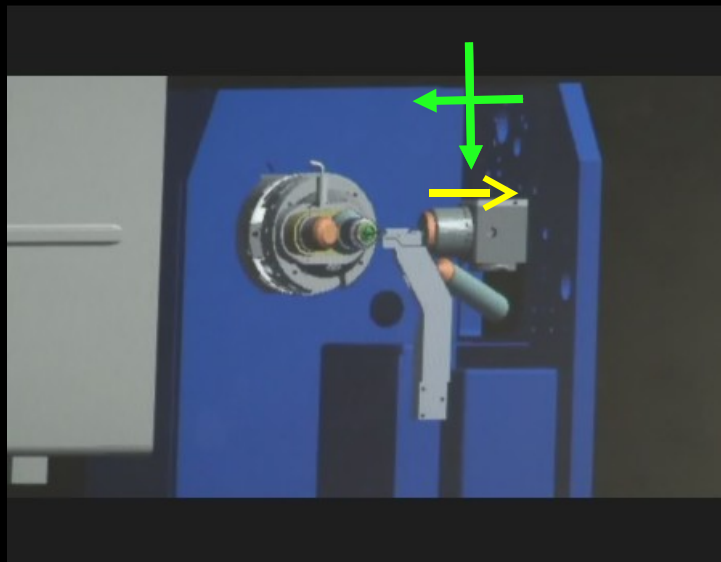
# Virtual Beamline Simulator

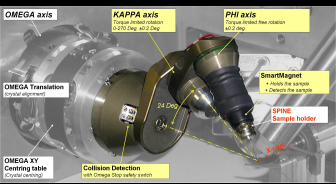


Reorientation  
problem  
solution  
RotCalib  
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xyz ?  
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solution

## Collision

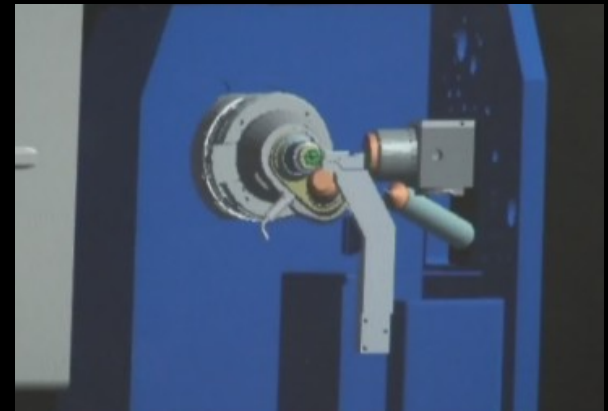
virtual gonio  
adjustment  
collision maps  
Summary





# Virtual Beamline Simulator

- Flexible model generation
- VRML library elements are transformed to the space of actual model
- Model description at arbitrary motor positions
- Automatic adjustment of VBS to *REAL* settings
- Instrument simulation/monitoring
- Fast collision map generation for experiment optimisation



Reorientation  
 problem  
 solution  
 RotCalib  
 method  
 xyz ?  
 TranCalib  
 method  
 solution

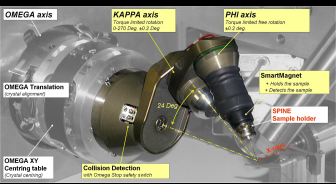
## Collision

virtual gonio  
 adjustment

## collision maps

Summary





# Collision Map Generation

## Collision Map Calculation

produced by

Sandor Brockhauser

[brockhauser@embl.fr](mailto:brockhauser@embl.fr) -

April, 2008

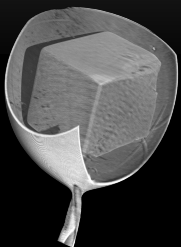
Reorientation  
problem  
solution  
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xyz ?  
TranCalib  
method  
solution

Collision

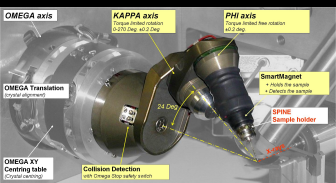
virtual gonio  
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collision maps

Summary

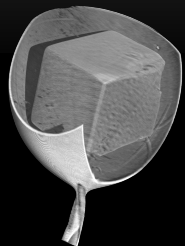
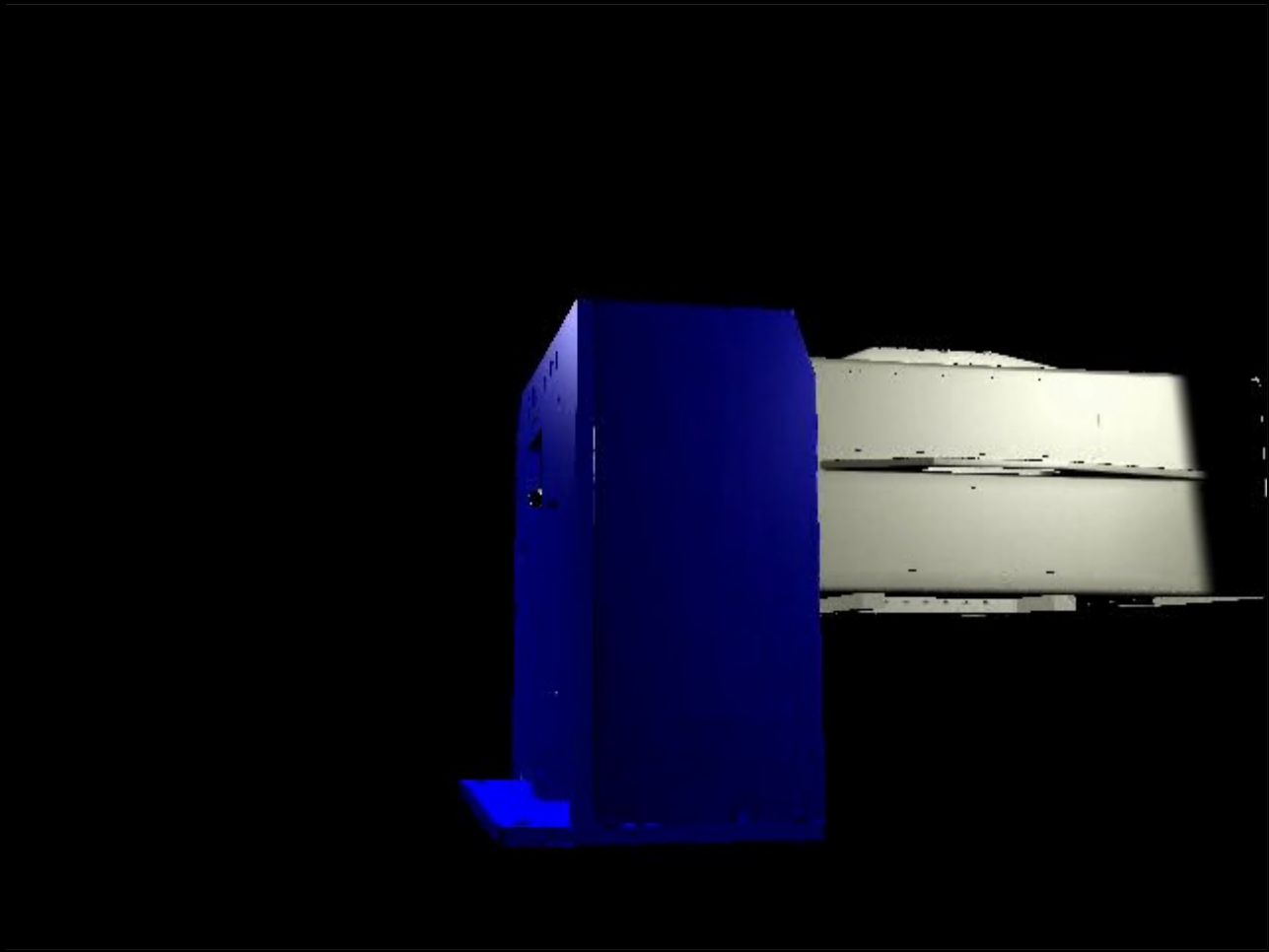


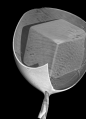
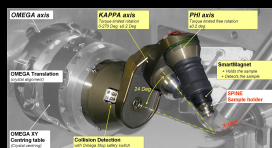
# VBS in Action



Reorientation  
problem  
solution  
RotCalib  
method  
xyz ?  
TranCalib  
method  
solution  
Collision  
virtual gonio  
adjustment  
collision maps

## Summary





# Acknowledgements

## **EMBL-Grenoble**

*Florent Cipriani, Franck Felisaz, Julien Huet, Alexandre Gobbo, Bernard Lavault, Andrew McCarthy, Raimond Ravelli*

## **Kappa Workgroup**

*Doug du Boulay, Gerard Bricogne, Gleb Burenkov, Ralf Flaig, Pierre LeGrand, Krister Larsson, Uwe Muller, Sasha Popov, Clemens Schulze-Briese, Takashi Tomizaki, Peter Turner, Johan Unge, Thomas Ursby*

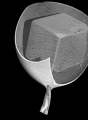
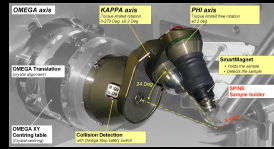
## **BioXDM and CCPN**

*Wayne Boucher, Rasmus Fogh, Peter Keller*

## **ESRF MX and support Groups**

*Marco DiMichiel, Claudio Ferrero, Matias Guijarro, Mario Lentini, Gordon Leonard, Sean McSweeney, Jens Meyer, Didier Nurizzo, Vicente Rey-Bakaikoa, Daren Spruce, Olof Svensson, Martin Walsh*

## **BIOXHIT Sections 3 and 4**



Thank you for your attention!