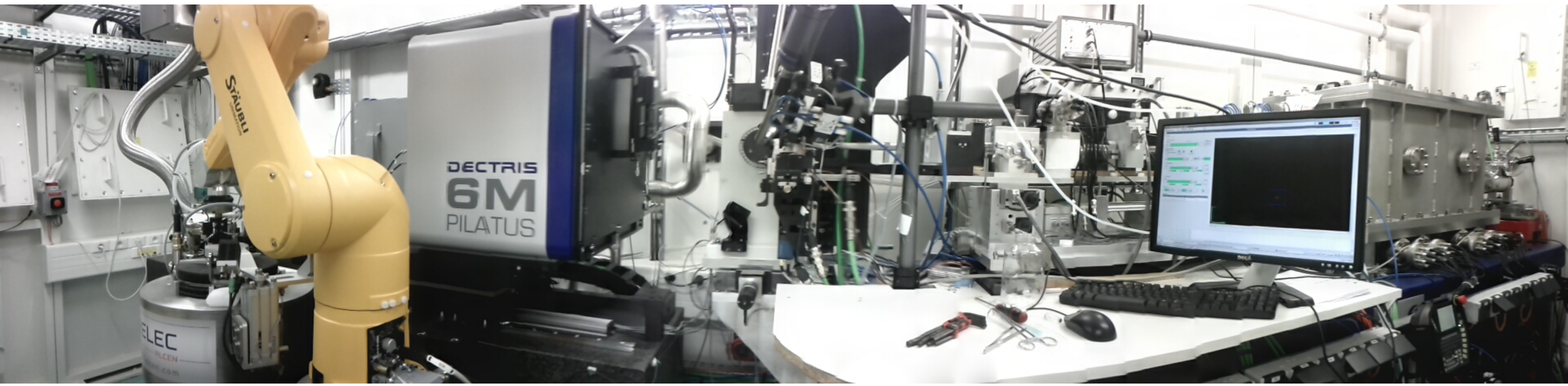
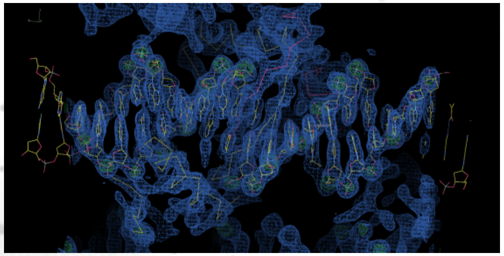


Getting the most from the SOLEIL Beamlines

A. Thompson : "Getting the best from your structural data : Beyond black boxes", IGBMC, 5 – 8 October, 2016.



Macromolecular X-Ray Crystallography at a Synchrotron Radiation Source.

Most Common Reasons for coming to Synchrotron.

- Large unit cell sizes (up to many hundreds of Å).
- Need for high resolution.
- Large volume of crystals to collect or screen.
- Phase problem, need for to choose a specific wavelength / energy.
- Variability of crystals.
- Radiation sensitive crystals.
- Tiny crystals or weakly diffracting crystal (don’t see diffraction at home).
- Increasingly, access to infrastructure! No facilities at home…..

» The most time consuming step is frequently preparing and handling the biological material and getting good crystals.

» You don’t have time to master everything, so clever software helps you in your choices.

» But : some objectives may require compromises, and some choices made by the beamline staff have already made some for you!

» And some potential crystallographic problems don’t reveal themselves immediately.

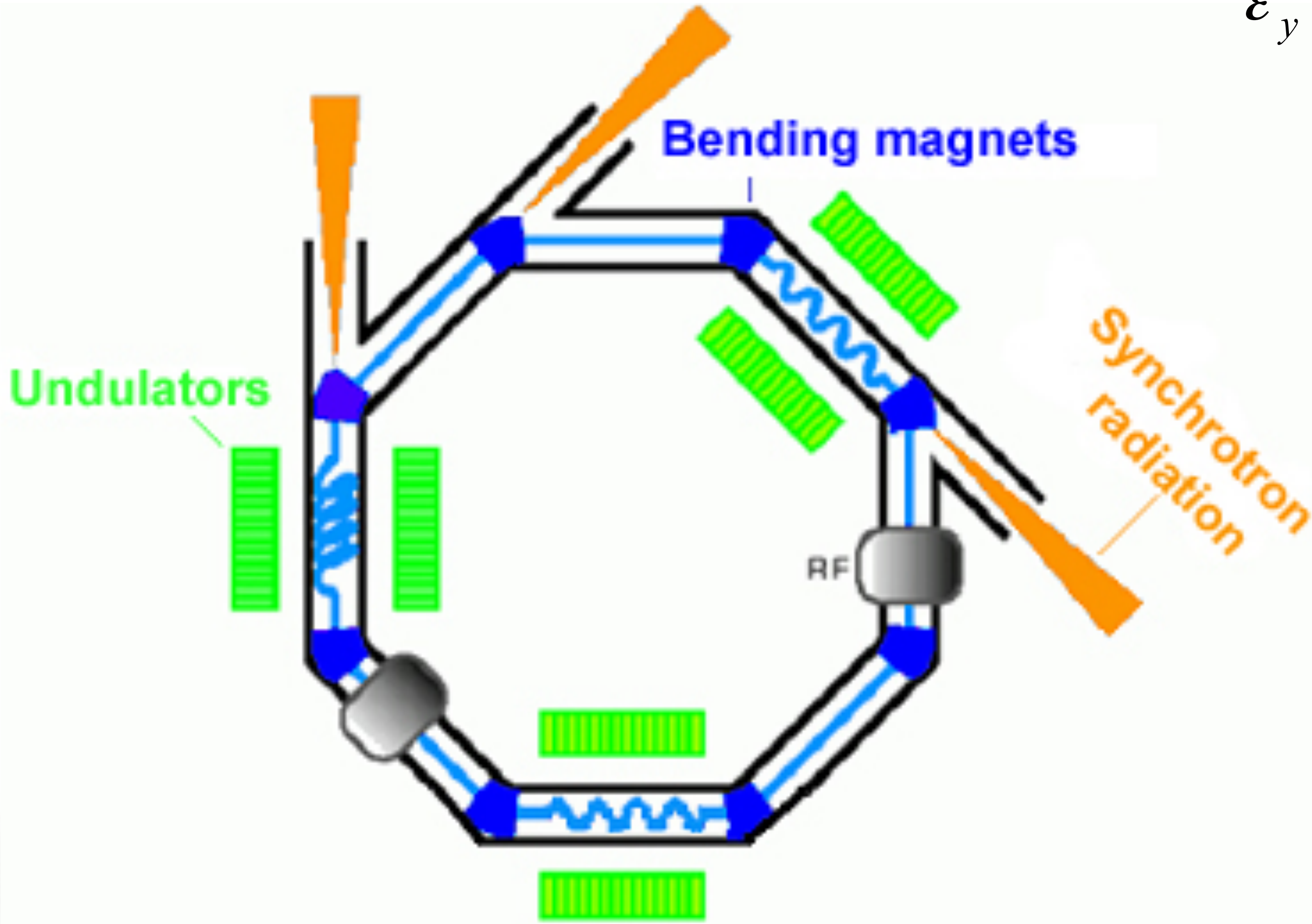
So understand something of what is behind your beamline visit, think about data collection and where these compromises may be.

SOLEIL SYNCHROTRON

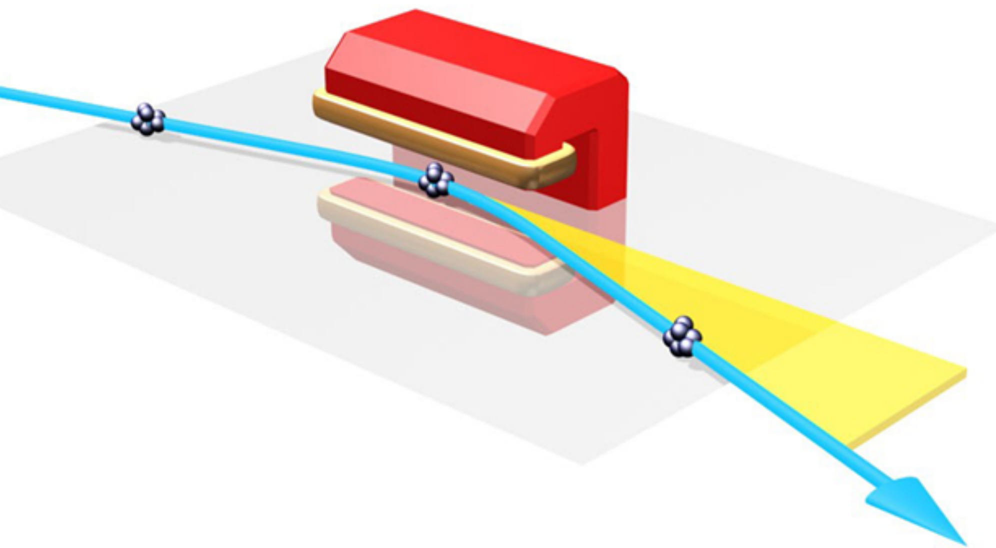
A very short lesson in Synchrotron Radiation beamlines.

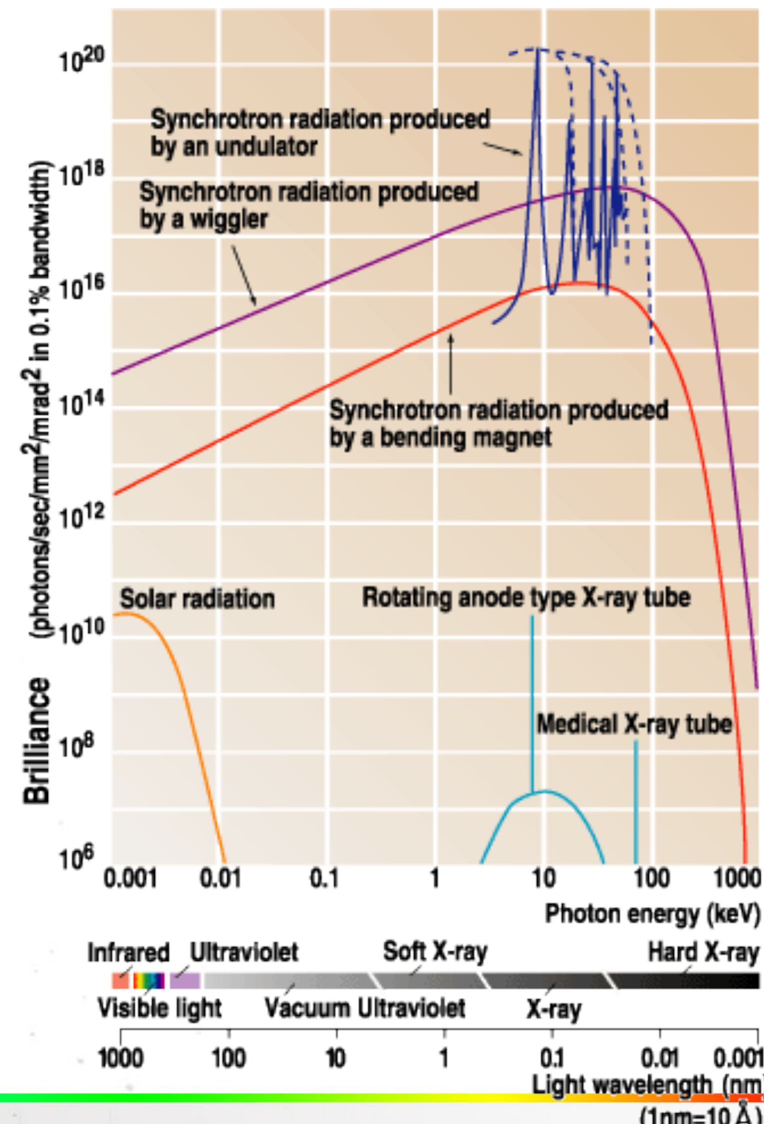
$$\varepsilon_x = \sigma_x \sigma_x^{'}$$

$$\varepsilon_y = \sigma_y \sigma_y^{'}$$



Synchrotron Radiation Source Points.

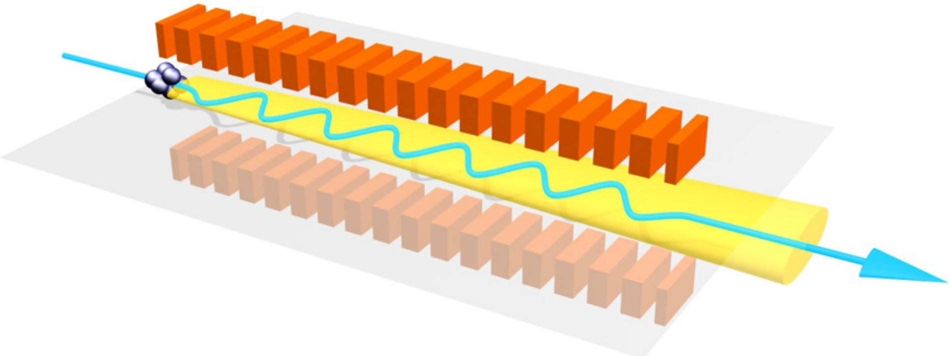


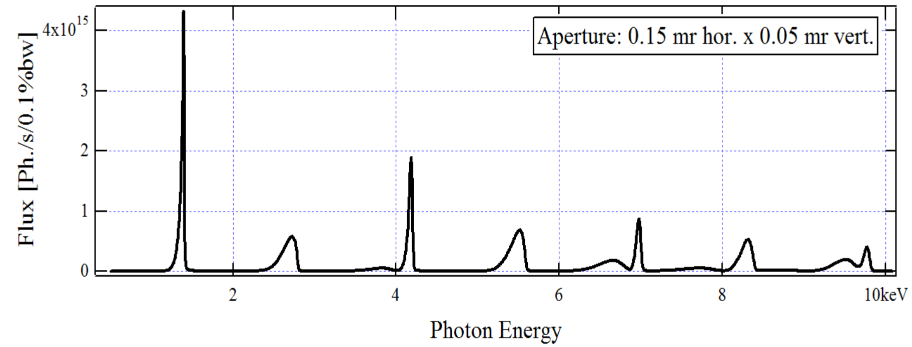


Bending Magnet.

$$\lambda_c = \frac{4\pi\rho}{3\gamma^3} = \frac{5.59\rho}{E^3} = \frac{18.6}{BE^2} \qquad \gamma = \frac{E}{m_e c^2}$$

SOLEIL SYNCHROTRON

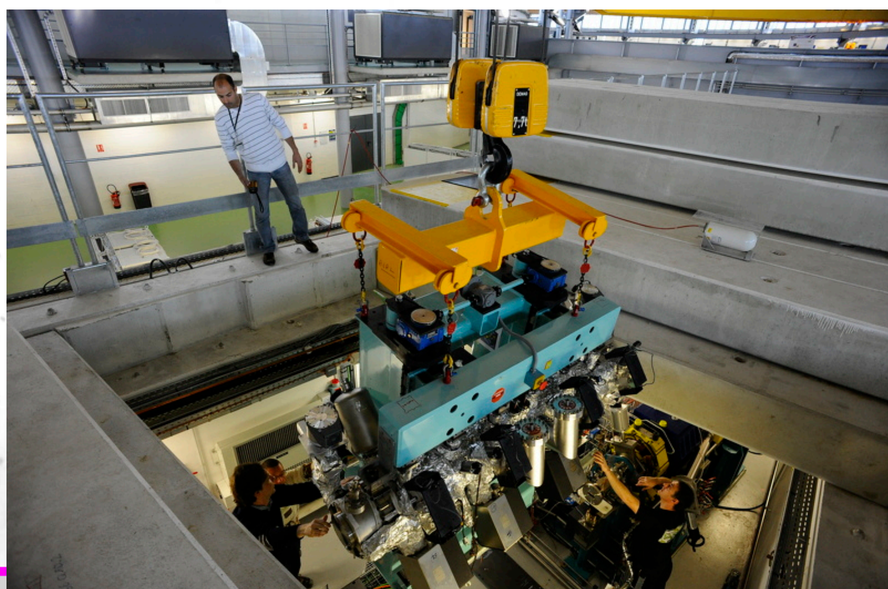


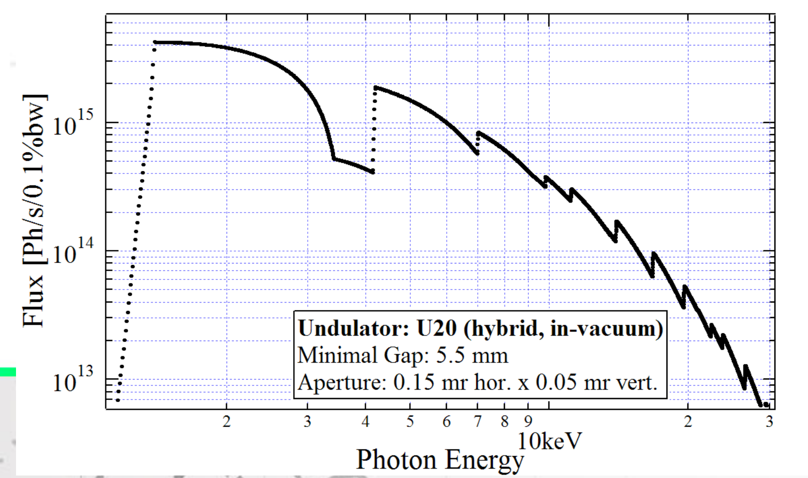


Wiggler or Undulator.

$$k = 0.934 \lambda_u B_0$$

$$\lambda_1 = \frac{13.056 \lambda_u}{E^2} \left(1 + {k^2}/{2} \right)$$





SOLEIL SYNCHROTRON

Macromolecular X-Ray Crystallography at a Synchrotron Radiation Source.

Most Common Reasons for coming to Synchrotron.

- Large unit cell sizes (up to many hundreds of Å).
- Need for high resolution.
- Large volume of crystals to collect or screen.
- Phase problem, need for to choose a specific wavelength / energy.
- Variability of crystals.
- Radiation sensitive crystals.
- Tiny crystals or weakly diffracting crystal (don't see diffraction at home).
- Increasingly, access to infrastructure! No facilities at home…..

» Very high intensity.

» Very broad energy spectrum (X ray – IR).

» Naturally highly collimated

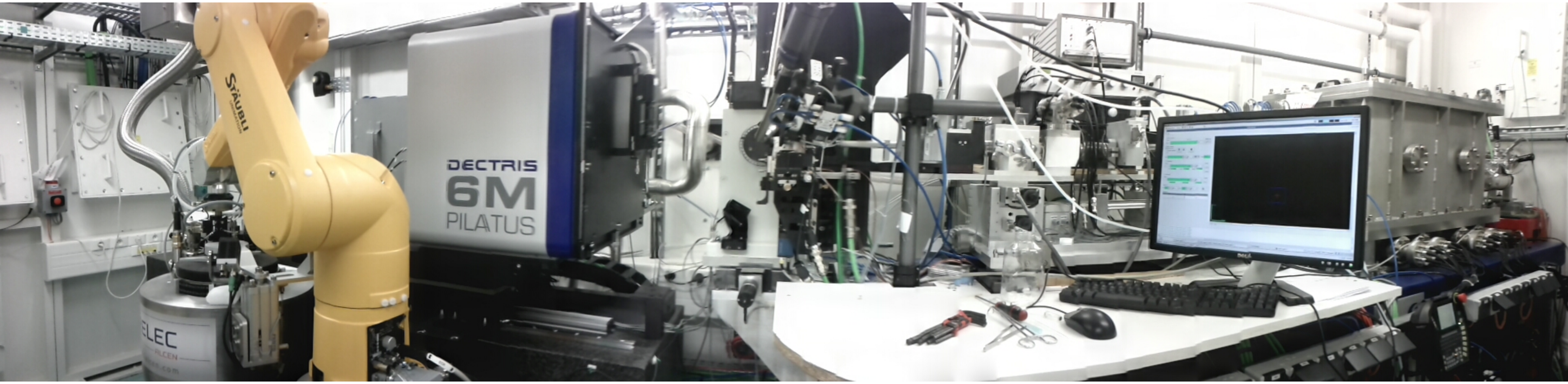
» Small source size.

» High degree of polarisation.

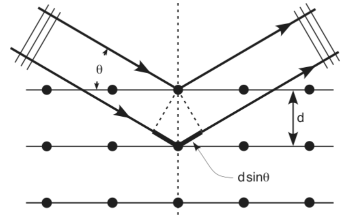
» Pulsed time structure.

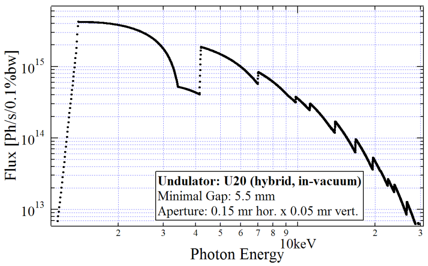
» High brilliance machines give partly coherent beam.

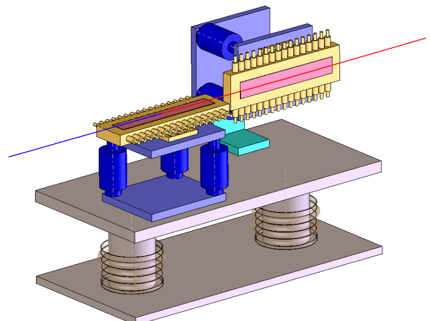
SOLEIL SYNCHROTRON

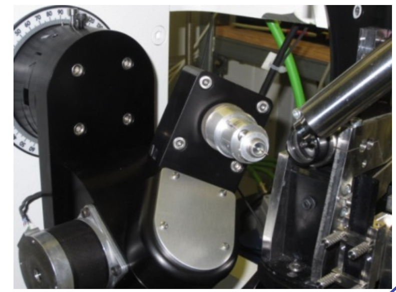


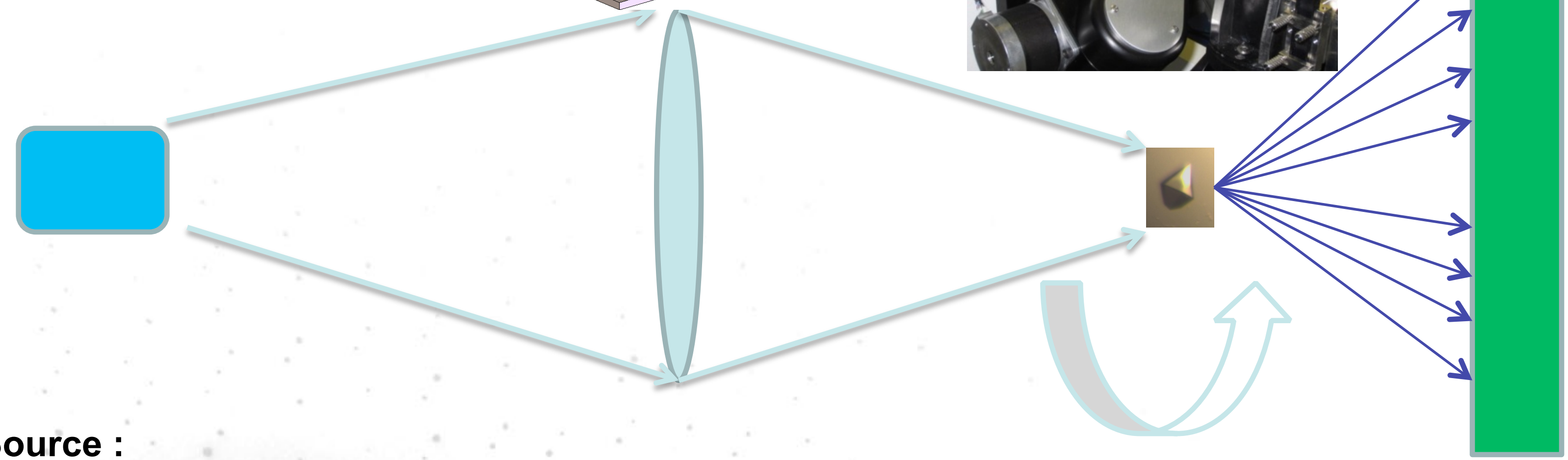
PROXIMA 1 : Larger focus, lower flux density, highly parallel beam : large unit cells.
PROXIMA 2a : Micro-focussed beam, higher flux density : micro-crystals or scanning applications.











Source : Bending magnet, undulator, wiggler

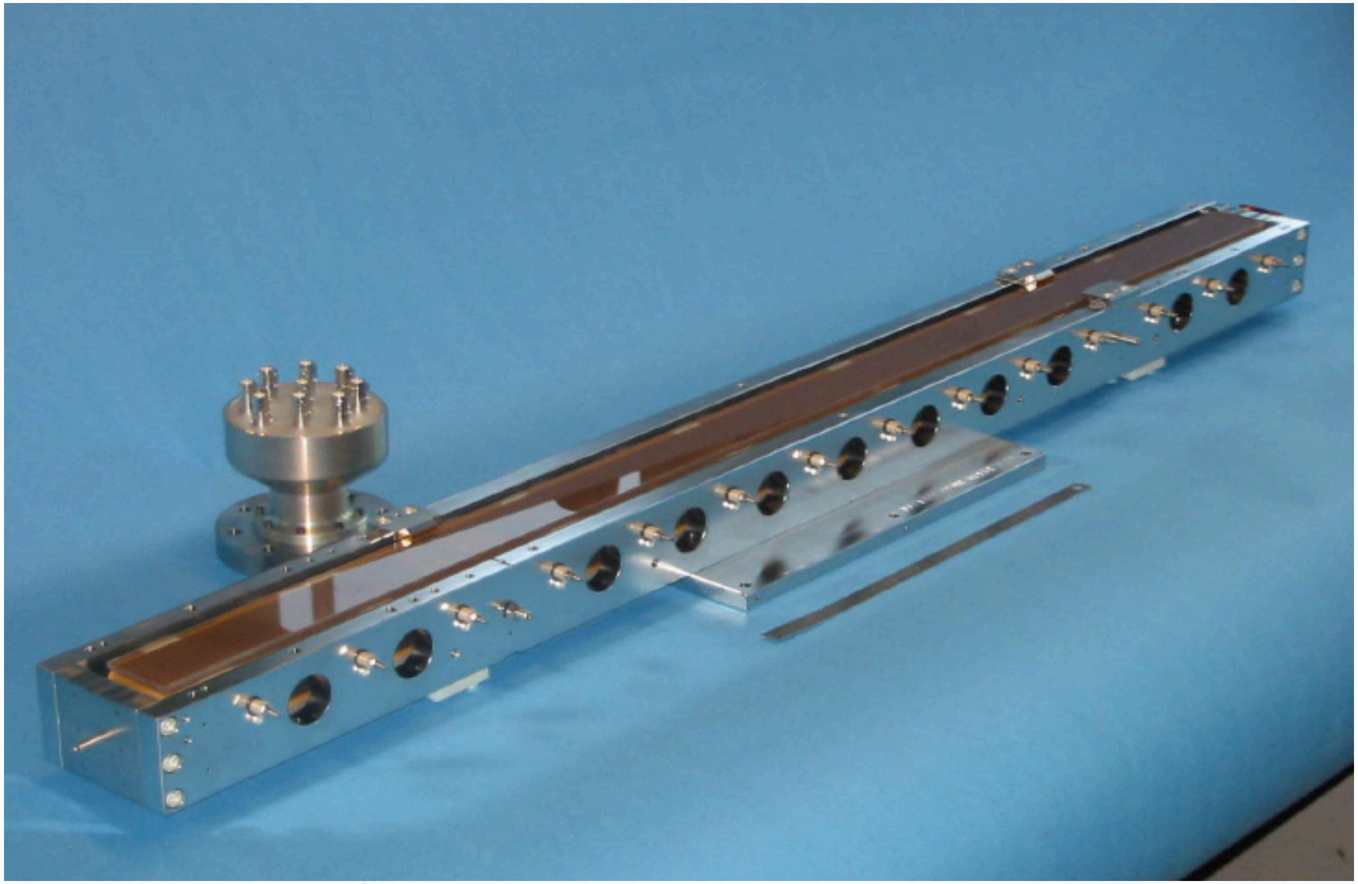
Optics : Monochromator, « mirrors »

Sample : goniometry

Detector : distance

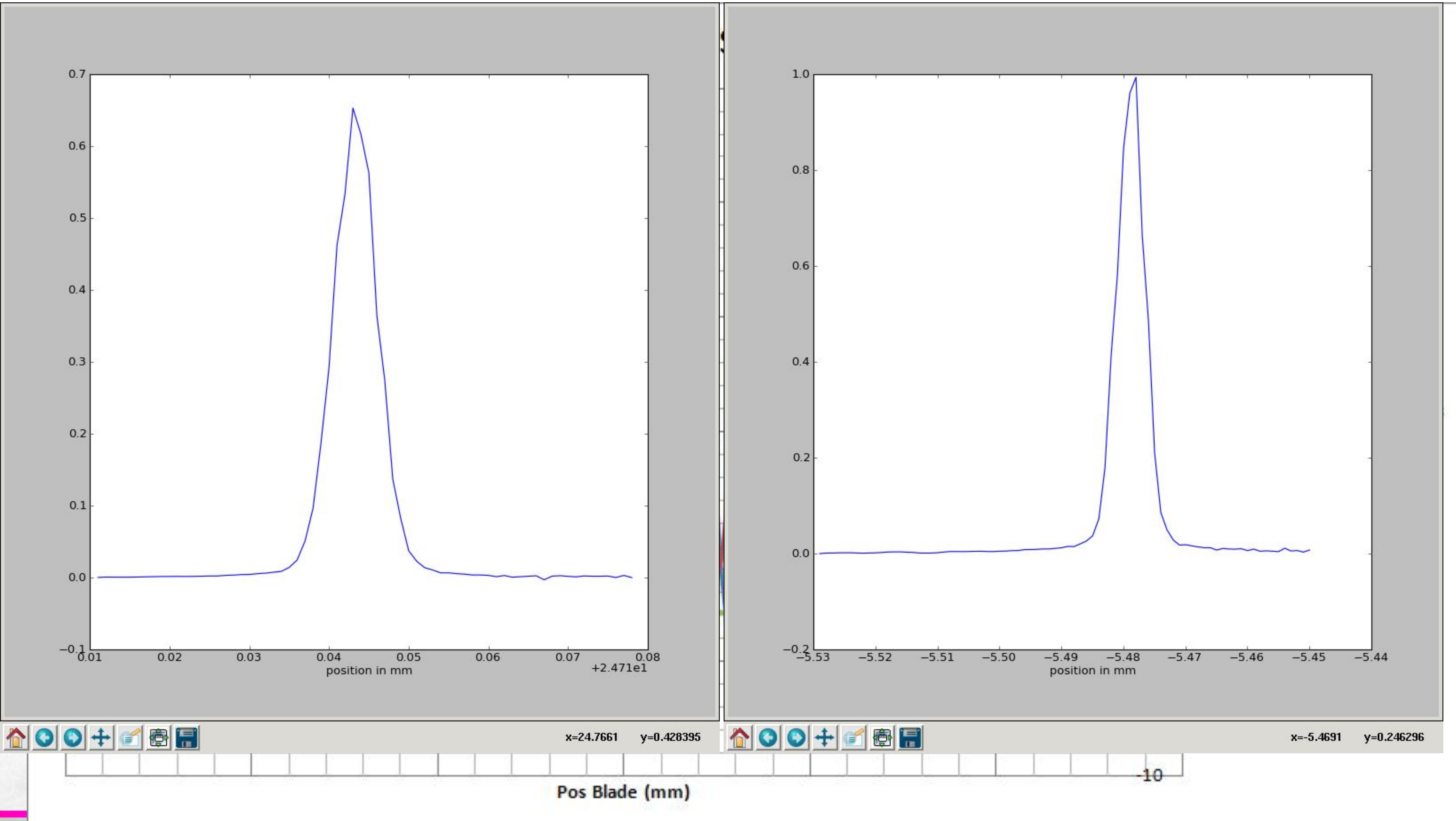
SOLEIL SYNCHROTRON

A beamline – a minimalist view (and vastly distorted)



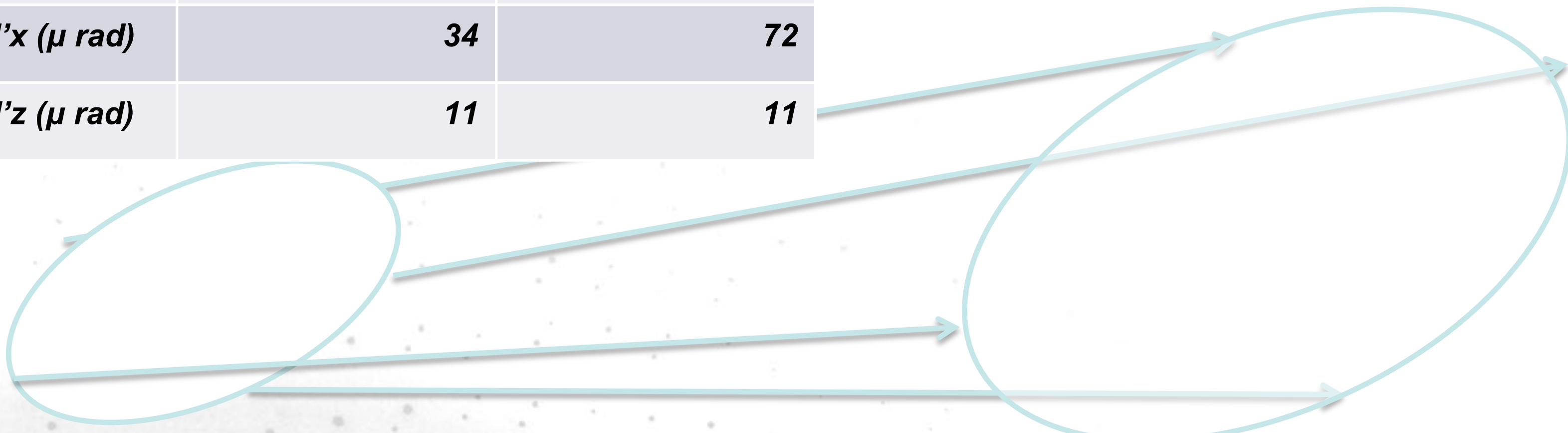
Bimorph (multi segment) mirror. Each part of the mirror surface is locally curved to ensure beam « bits » come to a (near) perfect focus at sample.

Focal Spot Optimisation of PROXIMA 2a Using Bimorphs



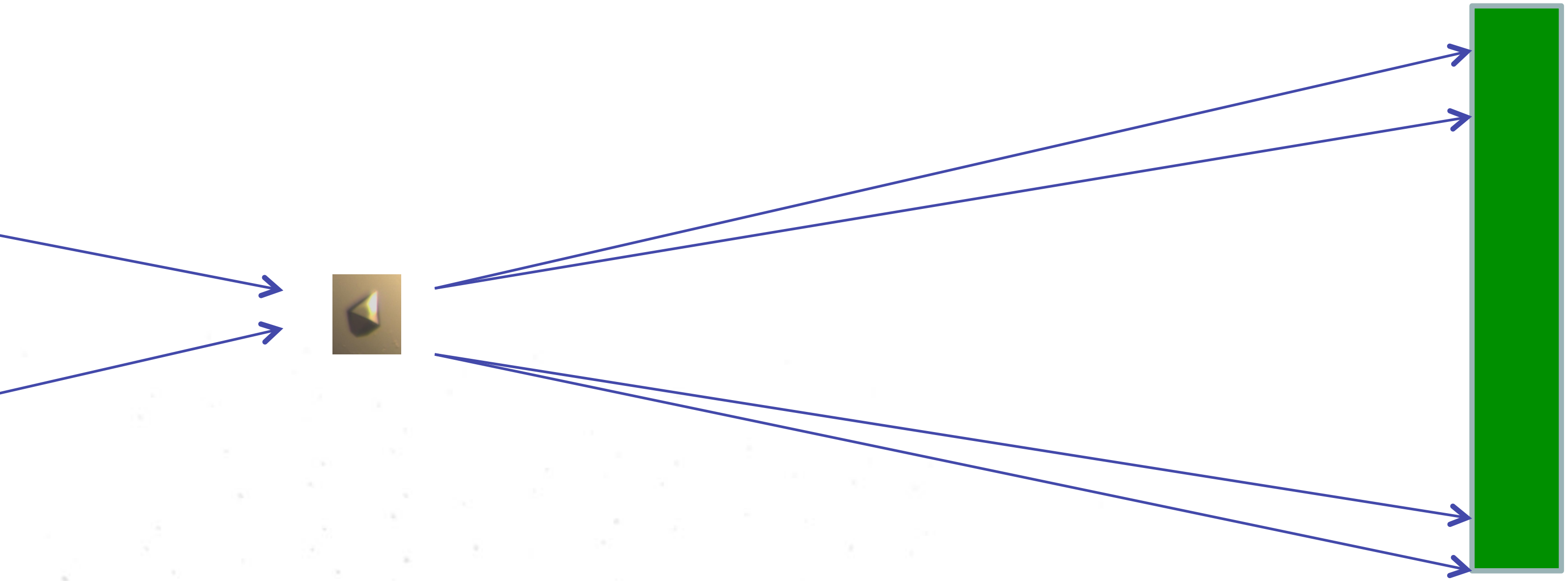
Source Parameter	PROXIMA 1	PROXIMA 2	BM
σx (µm)	388	182	60.1
σz (µm)	8.08	8.11	24.9
σ'x (µ rad)	14.5	30.5	134.8
σ'z (µ rad)	4.6	4.6	2.1

Source Parameter	PROXIMA 1	PROXIMA 2
FWHMx (µm)	912	428
FWHMz (µm)	19	19
FWHM'x (µ rad)	34	72
FWHM'z (µ rad)	11	11



Now apply this to MX data collection

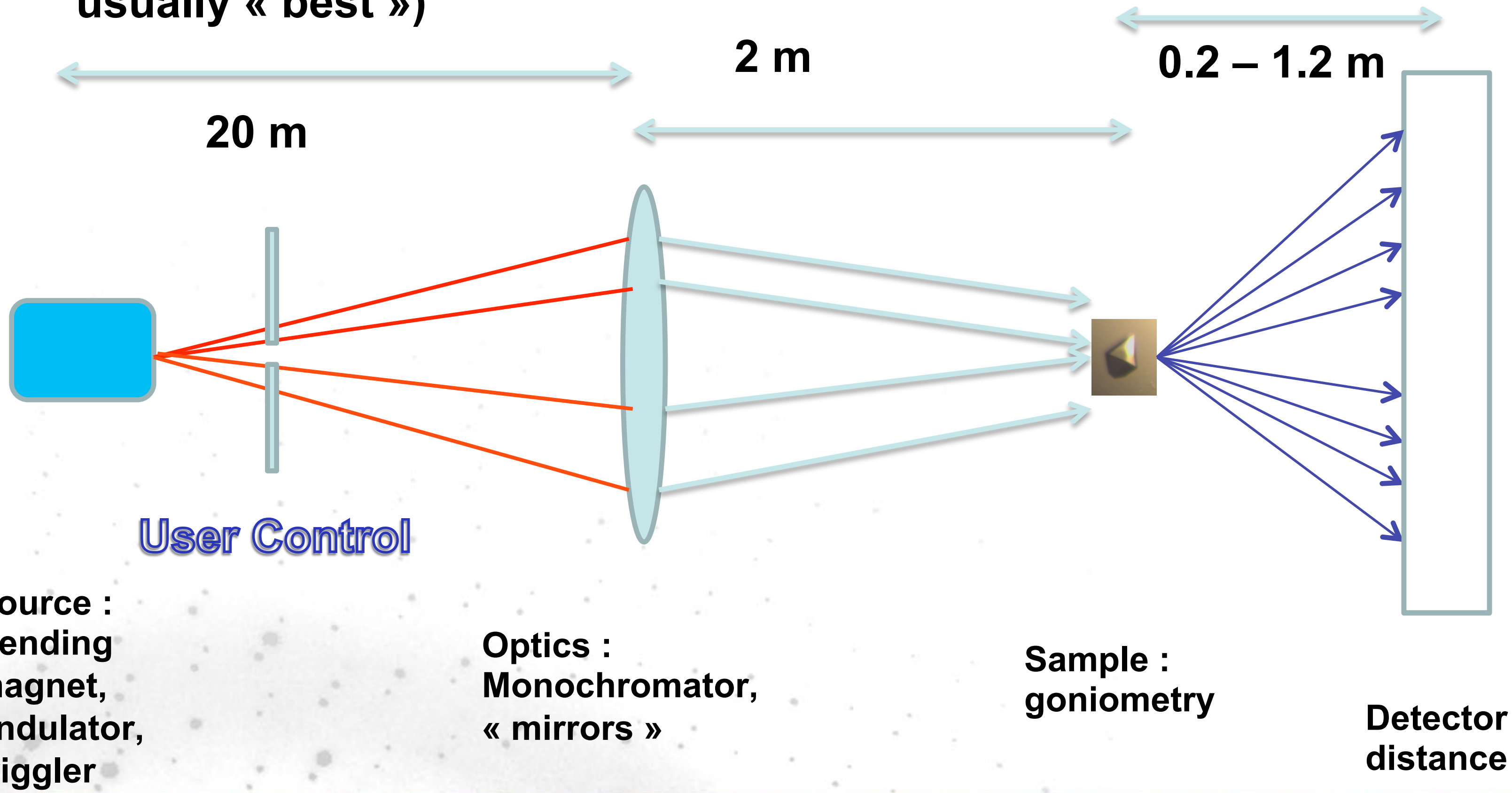
PROXIMA 1, horiz beam FWHM = 2.35 x 388µm = 912µm, actual focal spot is approximately 80µm. Demagnification of source 12. If size is decreased by 12, divergence is multiplied by 12 i.e; 400 µrad
PROXIMA 2 focuses from 428 to 10 µm. Demagnification of source about 42 x, divergence is multiplied by 42, i.e; 3 mrad.



The beam continues to diverge AFTER the sample. So (as shown by James) large beam divergences give large spots on the detector. This may be a good thing for precise measurement, but not if spots overlap or are so close that they cannot be integrated nicely.
If you would like to resolve a large unit cell, it might be a « good idea » to reduce the beam divergence and / or move the detector back to separate spots.

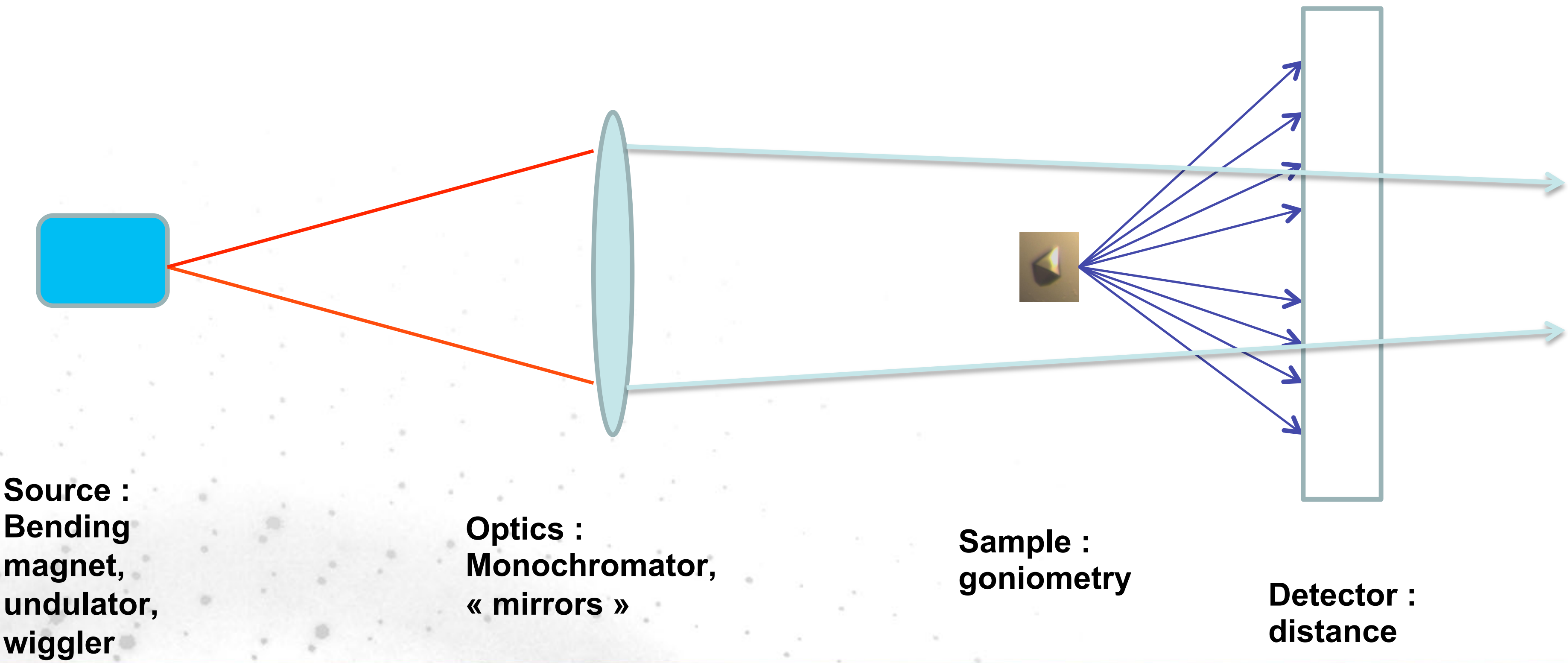
Adding a set of slits near the source does several things :

- Primarily reduces the beam divergence in the relevant direction
- Reduces the flux on the sample
- Changes the beam size (because the « middle » of a mirror is usually « best »)



Distances for PROXIMA 1.

We can also change bimorph to focus on the detector and get the smallest possible beam size , or move the detector further back to let the angle between spots separate the beam more Or focus « behind the detector » to get the most parallel beam possible.

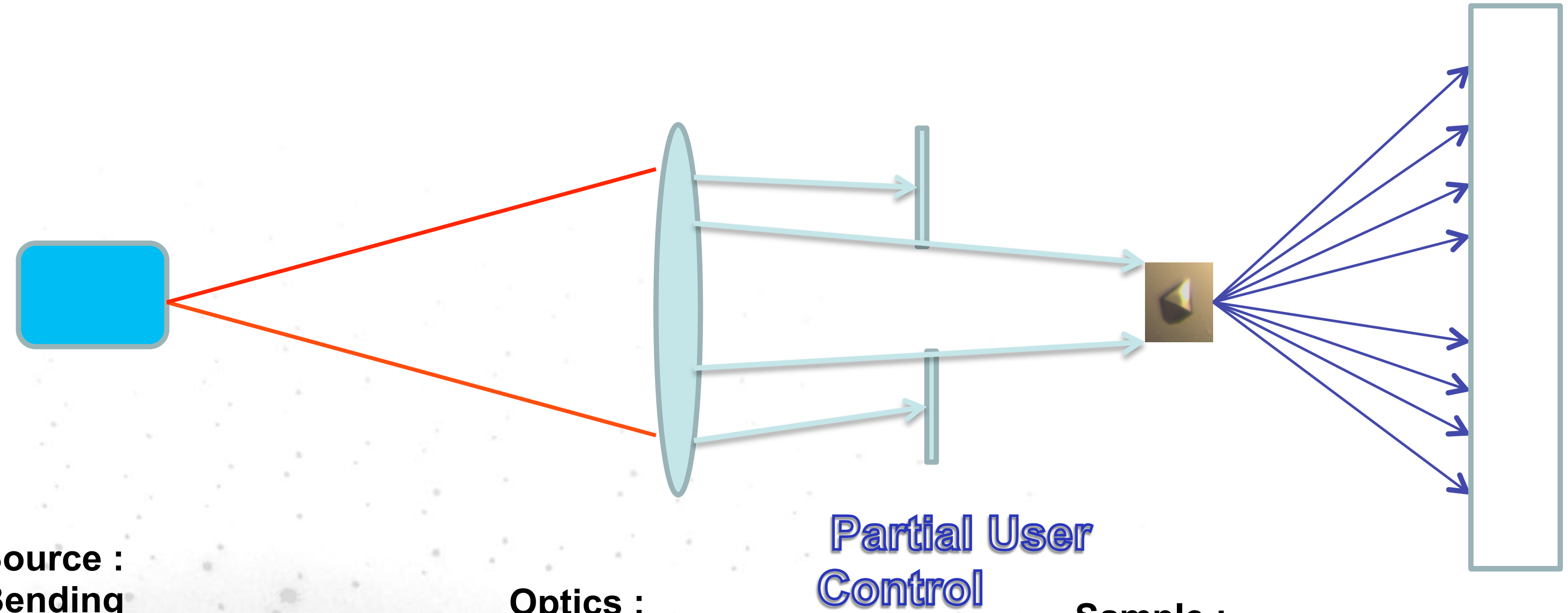


With such a parallel beam, adding a set of slits near the sample does slightly different things :

- Primarily reduces the size in the relevant direction
- Reduces the flux on the sample

This strategy was suggested to us by (copied from!!) Gleb Bourenkov @ EMBL Hamburg.

We employ this strategy for VERY large unit cells, i.e. ribosome data collection



Source : Bending magnet, undulator, wiggler

Optics : Monochromator, « mirrors »

Sample : goniometry

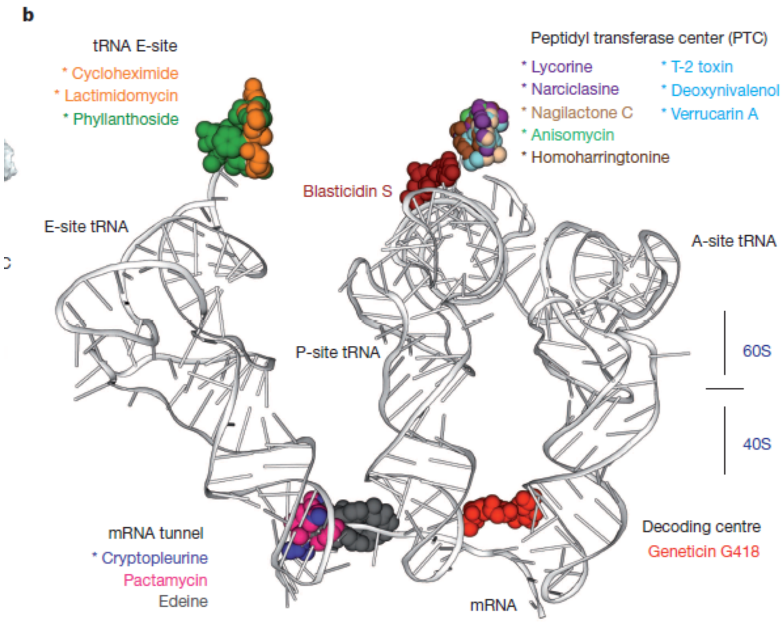
Detector : distance

For every change of configuration, the beam size and flux at sample is given in MXCUBE GUI….you can write it down.

Structural basis for the inhibition of the eukaryotic ribosome

Nature 2014

Nicolas Garreau de Loubresse[1], Irina Prokhorova[1], Wolf Holtkamp[2], Marina V. Rodnina[2], Gulnara Yusupova[1] & Marat Yusupov[1]



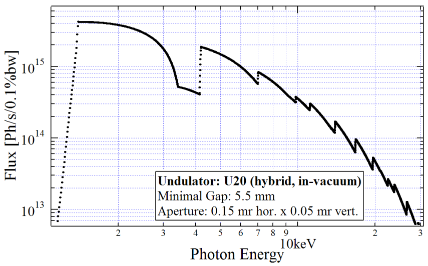
- 3.3 MDa yeast ribosome, significantly bigger than bacterial ribosomes.
- Optimisation of crystal treatment (cryo-protection, preparation in cold room). $P2_1$ 303 x 286 x 435 Ǻ, β=99°. Soaking of different naturally occuring inhibitors, some broad spectrum, some eukaryotic specific.
- « Gentle data collection », translating small, parallel beam across crystal offset cf rotation axis.
- Structure of 16 ribosome inhibitor complexes measured up to 2.8 Å resolution.

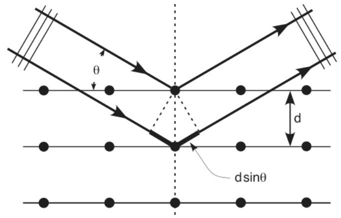
The bottom line ……

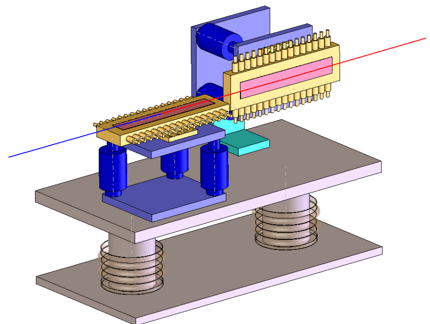
» If you need more spatial resolution :

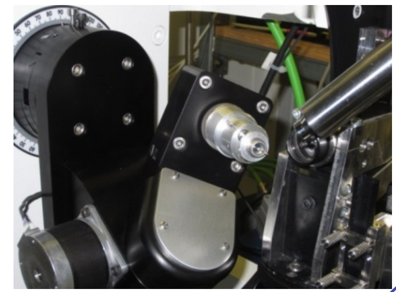
- you can move your detector back but then maybe you have to sacrifice some resolution (or have a huge detector and they are $$$$$$$$$)
- You can focus the beam on the detector to fit in the « maximum number of spots » or focus behind the detector. But the beam at the « sample position » will be bigger so you will lose intensity on the crystal.
- You can cut the beam divergence (and intensity) with slits. You can also cut with attenuators, but also broadens focus!

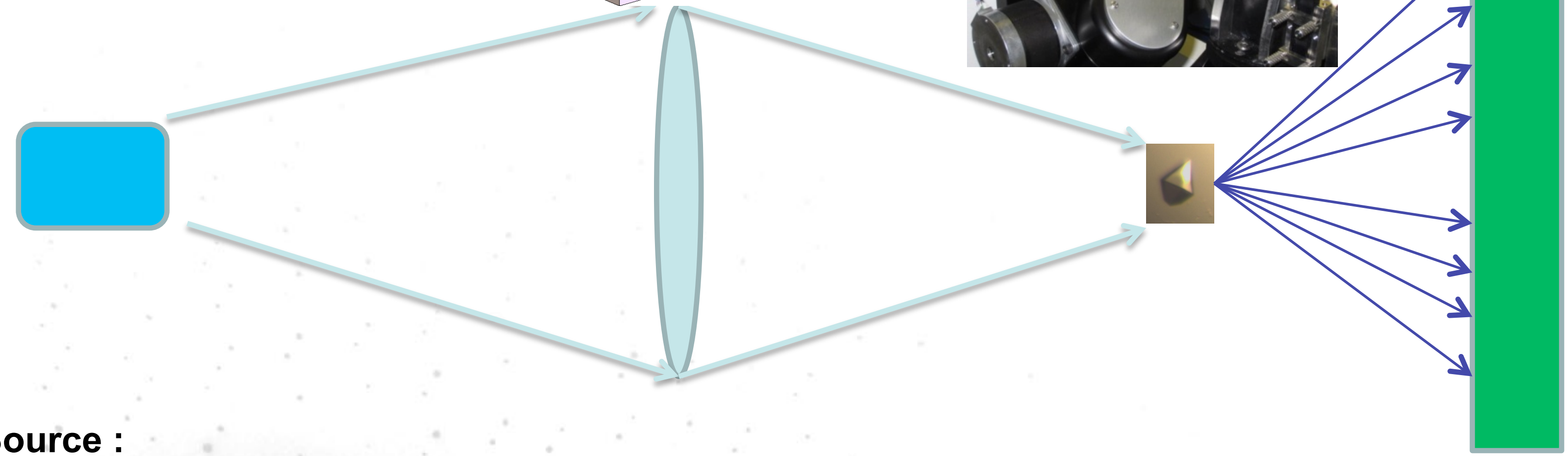
Data collection is like this – a set of sometimes conflicting requirements where you have to make choices.











Source : Bending magnet, undulator, wiggler

Optics : Monochromator, « mirrors »

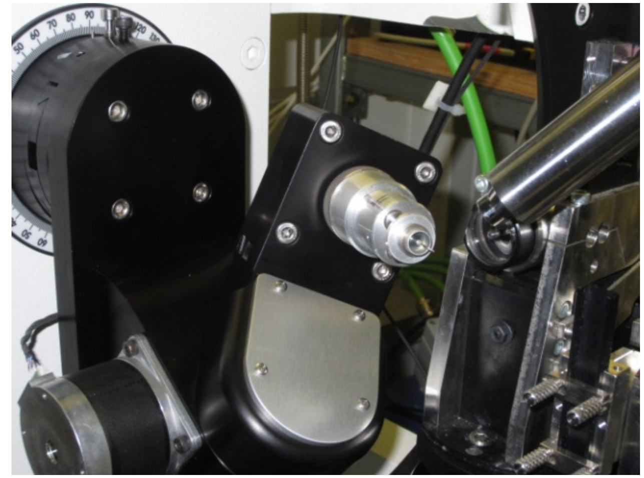
Sample : goniometry

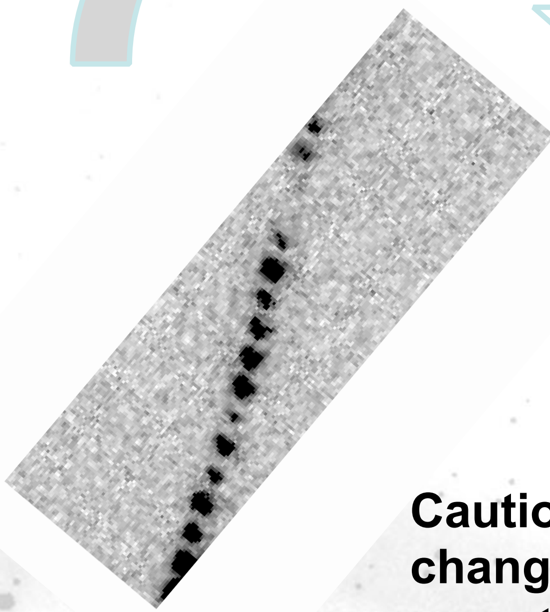
Detector : distance

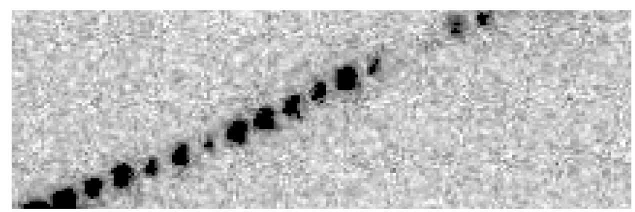
Things around the goniometer…….

Use of 3 circle κ geometry goniostat

- Movement of κ combined with focussing helps deal with complicated unit cells (CNRS Marseilles, 78 x 78 x **723** Å space group P $3_1 21$, to 2.9 Å resolution)



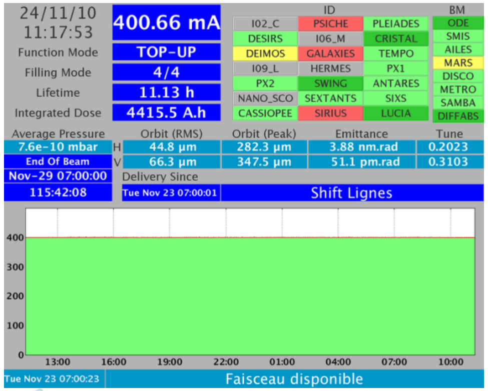


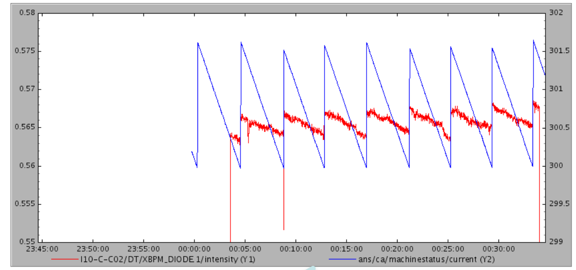


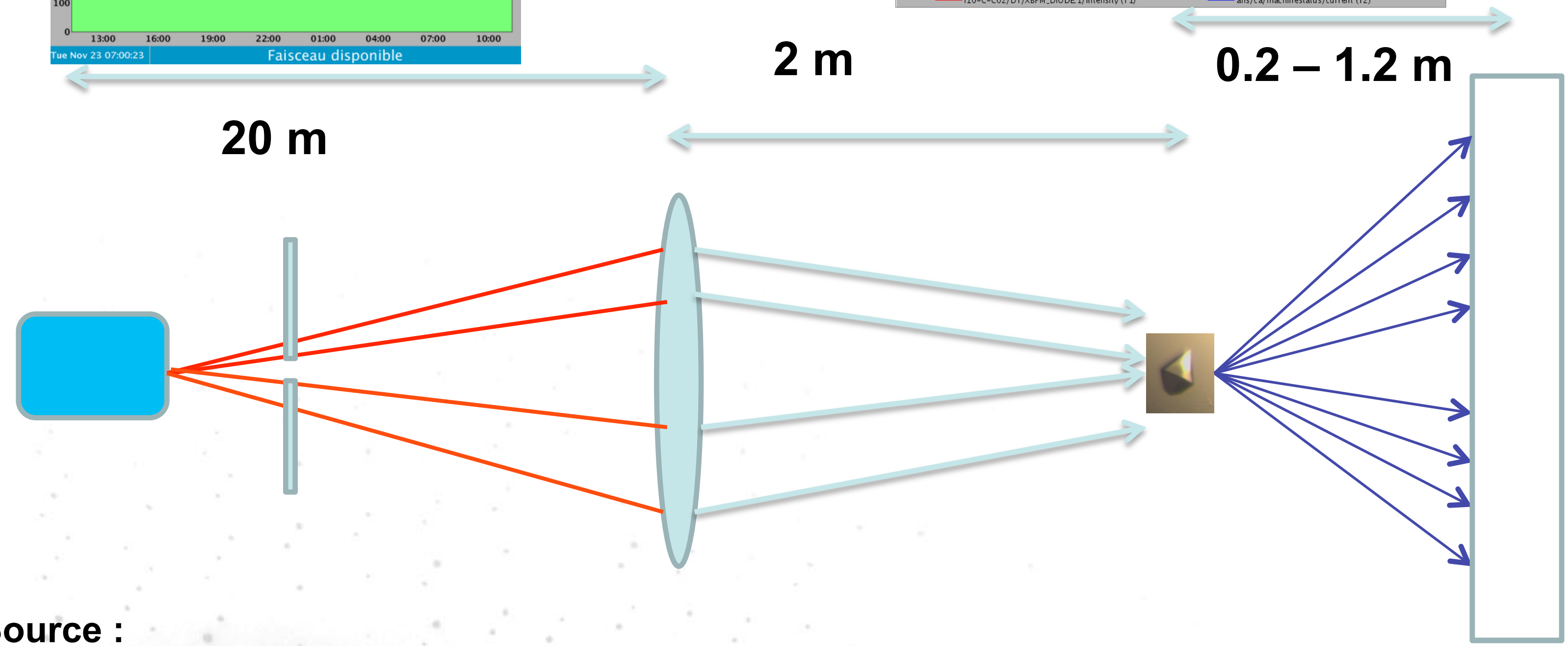
Caution – changing goniometer angle changes orientation of loop w-r-t cryostream : beware crystal movements in gas flow. Alkire et al 2013

SOLEIL SYNCHROTRON

A parenthesis – the systematic error of beam flicker







Source : Bending magnet, undulator, wiggler

Optics : Monochromator, « mirrors »

Sample : goniometry

Detector : distance

Beam strongly demagnified – we are very INSENSITIVE to SOURCE position. We are very SENSITIVE to SAMPLE position.

SOLEIL beam is at 1.4 m from the ground.

High Frequency
Tiny vibrations that cause angular changes to equipment can give rise to large offsets in the 30 – a few hundred Hz domain.

Low Frequency

Remember some high school physics?
Coefficient of linear expansion about 7 µm per m per C
For steel 12 µm per m per C

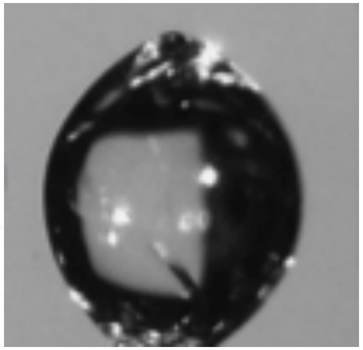
So beam height drift is between 10 and 16 µm « per optical or storage ring component » (a differential effect).

This is why we have air conditioning, leave lights on, and re-measure the intersection of the beam and goniometer centre every day at roughly the same time.

SOLEIL SYNCHROTRON

McSweeneys rule?

Getting your crystal into the beam depends on the beamline (thermal drift, alignment of goniometer to beam, sphere of confusion etc….). But believe it or not, it depends mostly on YOU!



Macromolecular X-Ray Crystallography at a Synchrotron Radiation Source.

Most Common Reasons for coming to Synchrotron.

- ✓ Large unit cell sizes (up to many hundreds of Å).
- ✓ Need for high resolution.
- Large volume of crystals to collect or screen.
- Phase problem, need for to choose a specific wavelength / energy.
- Variability of crystals.
- ✓ (Radiation sensitive crystals – sort of).
- Tiny crystals or weakly diffracting crystal (don't see diffraction at home).
- Increasingly, access to infrastructure! No facilities at home.....

» Very high intensity.

» Very broad energy spectrum (X ray – IR).

» Naturally highly collimated

» Small source size.

» High degree of polarisation.

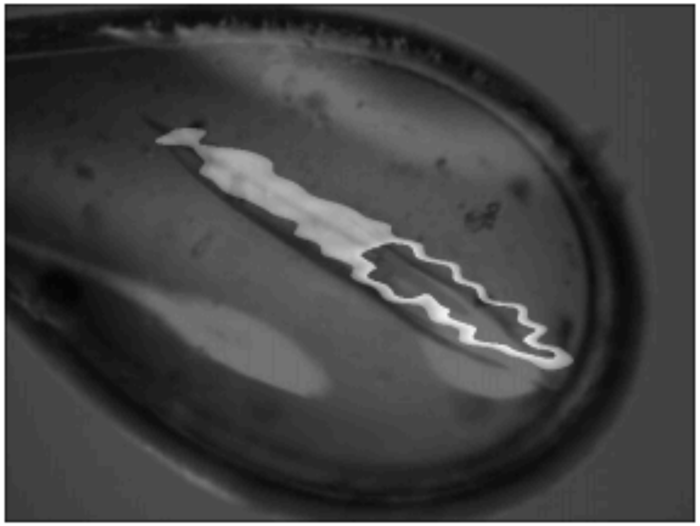
» Pulsed time structure.

» High brilliance machines give partly coherent beam.

PROXIMA 2 – Making use of MD2 goniometer and speed of EIGER 9M detector.

Raster scans

- 5x10 micrometer beam
- 40 Hz default frame rate
- fast axis speed ~0.5 mm/s
- typical grid size 0.1 mm^2 ~1000 images
- typical acquisition time 40 seconds
- processing time 20 seconds
  - dials.find_spots ~ 0.02s/image
  - native support for HDF5



EIGER 9M User Operation since December 2015.
Full size 238 Hz, 4M region of interest 750 Hz.

Accessible X-ray absorption edges PX1/2a.

Element	*Edge*	*Energy (keV)*
Light elements		
S	**K**	**2.472**
Transition metals		
V	K	5.464
Cr	K	5.989
Mn	K	6.537
Fe	K	7.111
Co	K	7.709
Ni	K	8.331
Cu	K	8.980
Zn	K	9.660

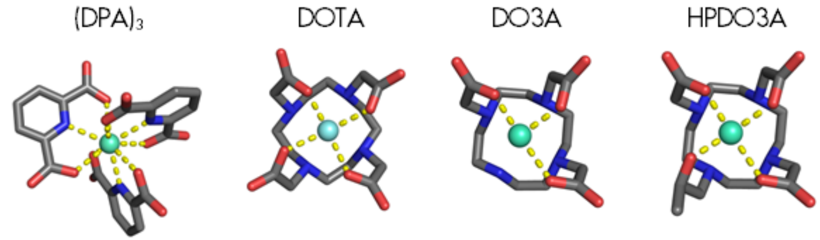
Middle-weight		
Ga	K	10.368
Ge	K	11.103
As	K	11.864
Se	K	12.654
Br	K	13.470
Kr	K	14.324

Intermediate		
Xe	L2	5.104
Cs	L3	5.011
Ba	L3	5.247

Element	*Edge*	*Energy (keV)*
Lanthanides		
La	L3	5.483
Ce	L3	5.724
Pr	L3	5.963
Nd	L3	6.209
Pm	L3	6.460
Sm	L3	6.717
Eu	L3	6.980
Gd	L3	7.243
Tb	L3	7.515
Dy	L3	7.789
Ho	L3	8.067
Er	L3	8.357
Tm	L3	8.649
Yb	L3	8.944
Lu	L3	9.249

Element	*Edge*	*Energy (keV)*
Conventional heavy atoms		
Hf	L3	9.557
Ta	L3	9.876
W	L3	10.200
Re	L3	10.531
Os	L3	10.868
Ir	L3	11.212
Pt	L3	11.562
Au	L3	11.921
Hg	L3	12.286
Tl	L3	12.660
Pb	L3	13.040
Bi	L3	13.426
Po	L3	13.814
At	L3	14.214
Rn	L3	14.619

Actinides
Th, Pa, U: no



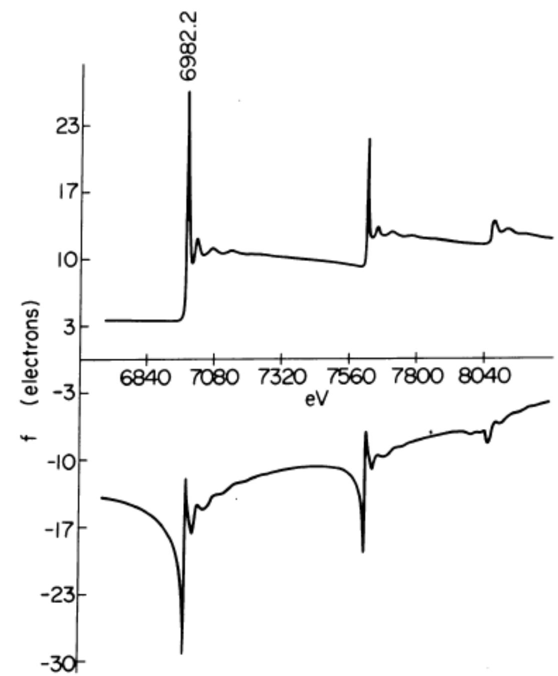


FIG. 2. Values of f'' and f' for Eu(PhAcAc)$_3$. The values of f' were obtained by using a Kramers–Kronig transform as discussed in the text. The vertical scale is calibrated from tabulated values of f' and f'' at CrKα and CuKα. The L_3 edge is the lowest in energy (to the left) and L_1 is the highest. The similarity between the L_3 and L_2 edges is apparent; the L_1 lacks the white line. These effects are discussed in the text.

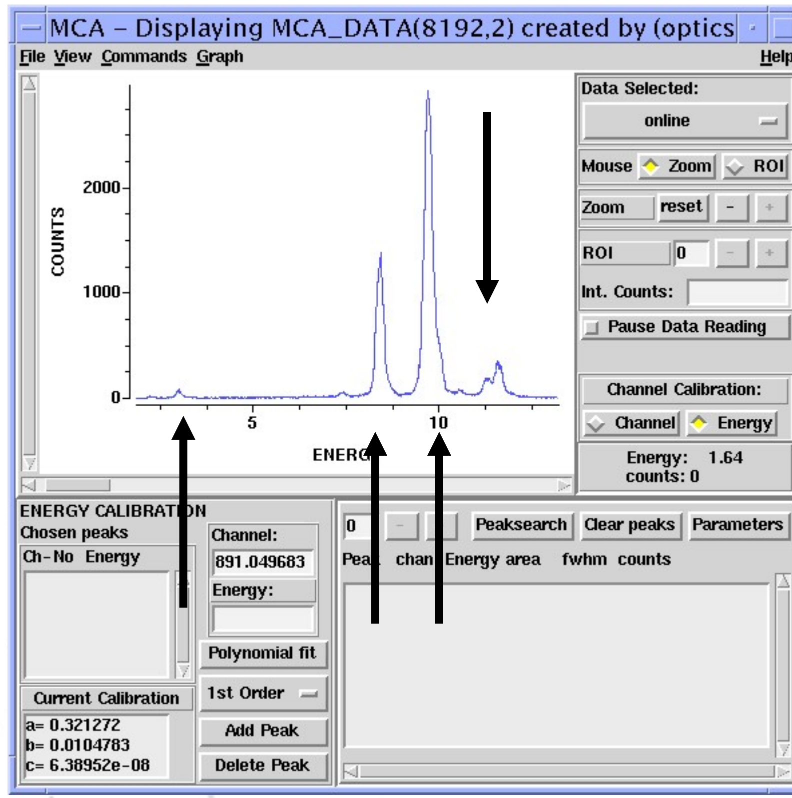
Lye et al, PNAS 1980

Measurement of fluorescence from sample.

» Inelastic scatter from sample.

- **Fluorescence – emission lines.**

- **These lines have to be interpreted – some may be useful to you! But the presence of a line does not (necessarily) indicate an ordered site!**



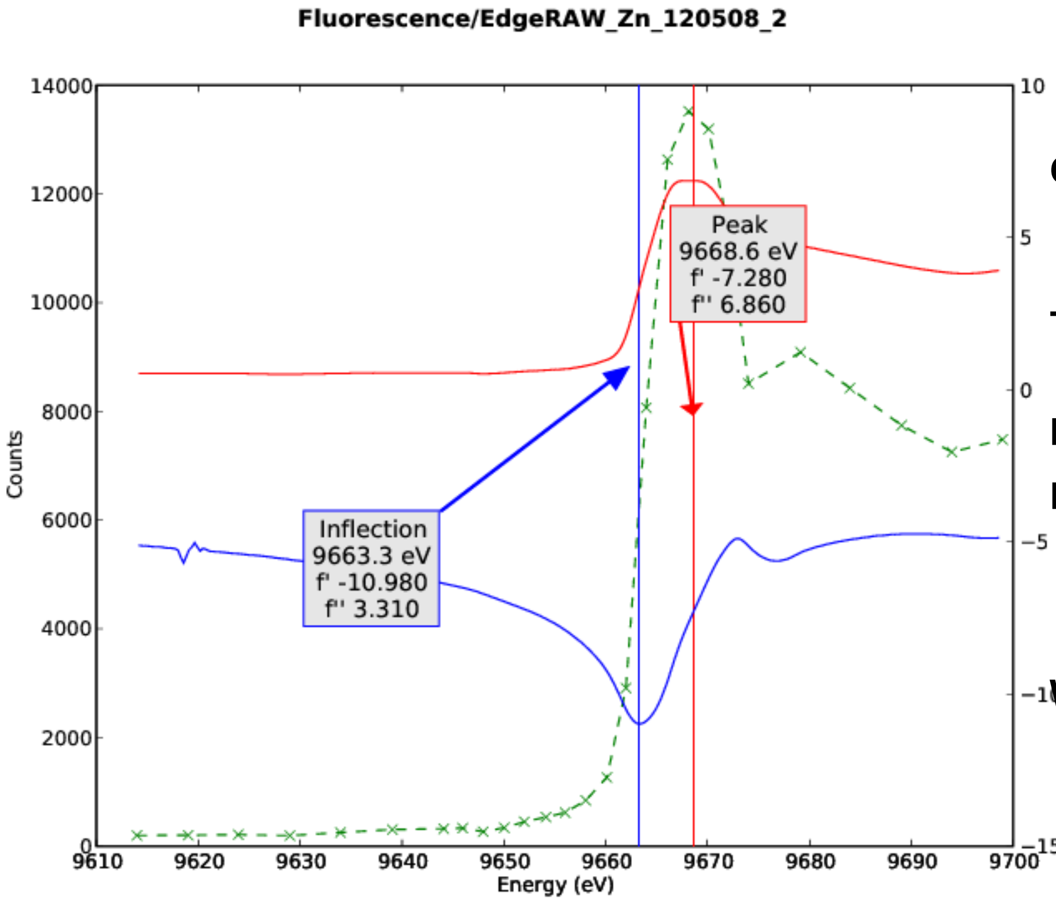
SOLEIL SYNCHROTRON

(A short parenthesis)

MAD is a possibility – don't always be SAD.

- SAD phasing gives a bimodal phase distribution, with slight bias of probability towards the correct solution.
- In order to choose the correct phase for each reflection, « wrong » atom positions have to be eliminated (usually via solvent flattening).
- SAD phasing works (extremely) well when we have sufficently well measured anomalous signal, high resolution, « normal » solvent content, NCS. This is « most of the time » for Se-met.

SOLEIL SYNCHROTRON



Crystals supplied by Ahmed Haouz. Collaboration SOLEIL, SLS, Global Phasing, Institut Pasteur.

Tetragonal space group, 378 residues + 5 Zn per a.u.

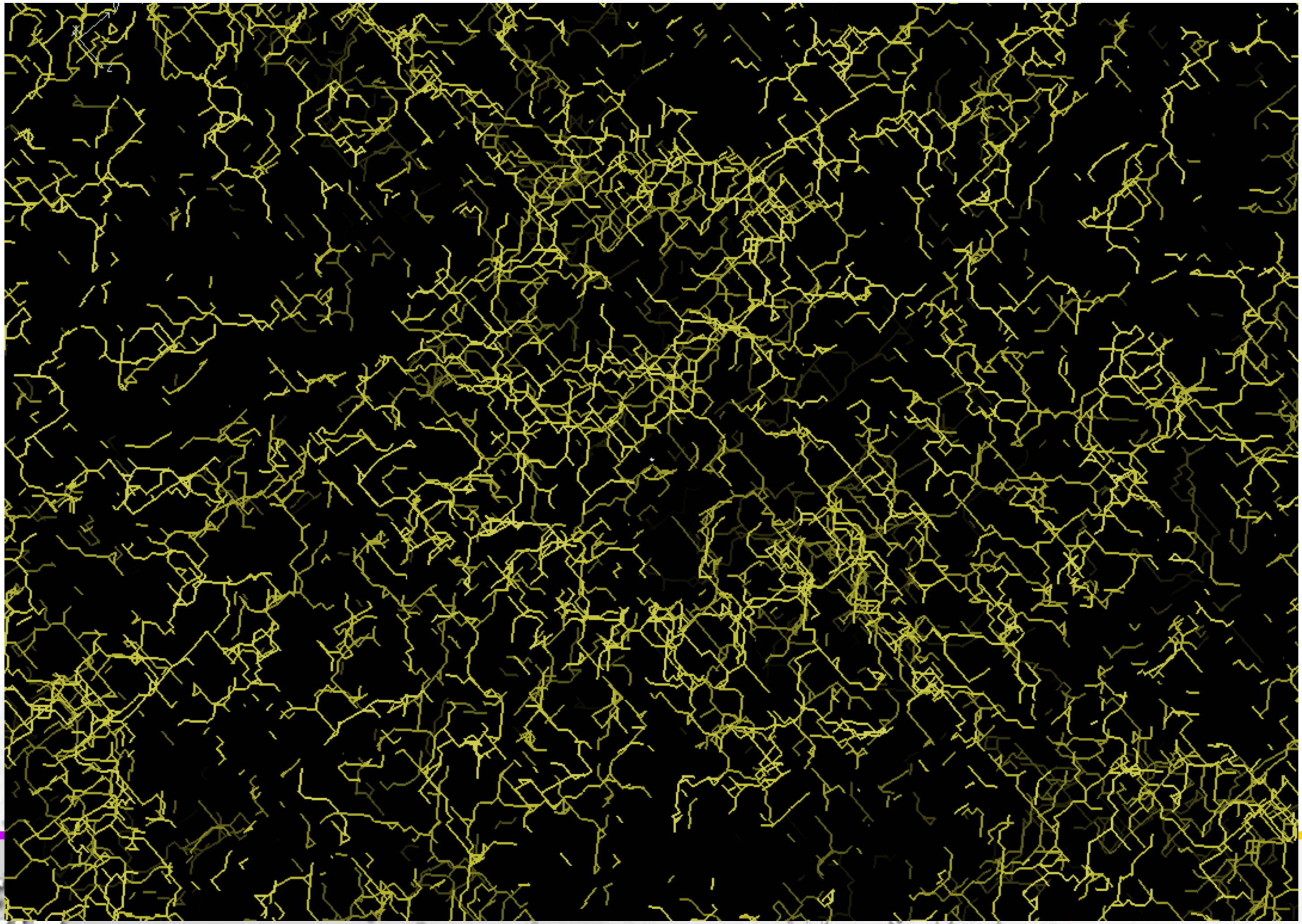
Possibility of alignment of 2-folds

Large crystals, 2 chunks of equal quality : an exact comparison could be made between SAD and 2-wvl MAD (aligned or not) with identical total doses.

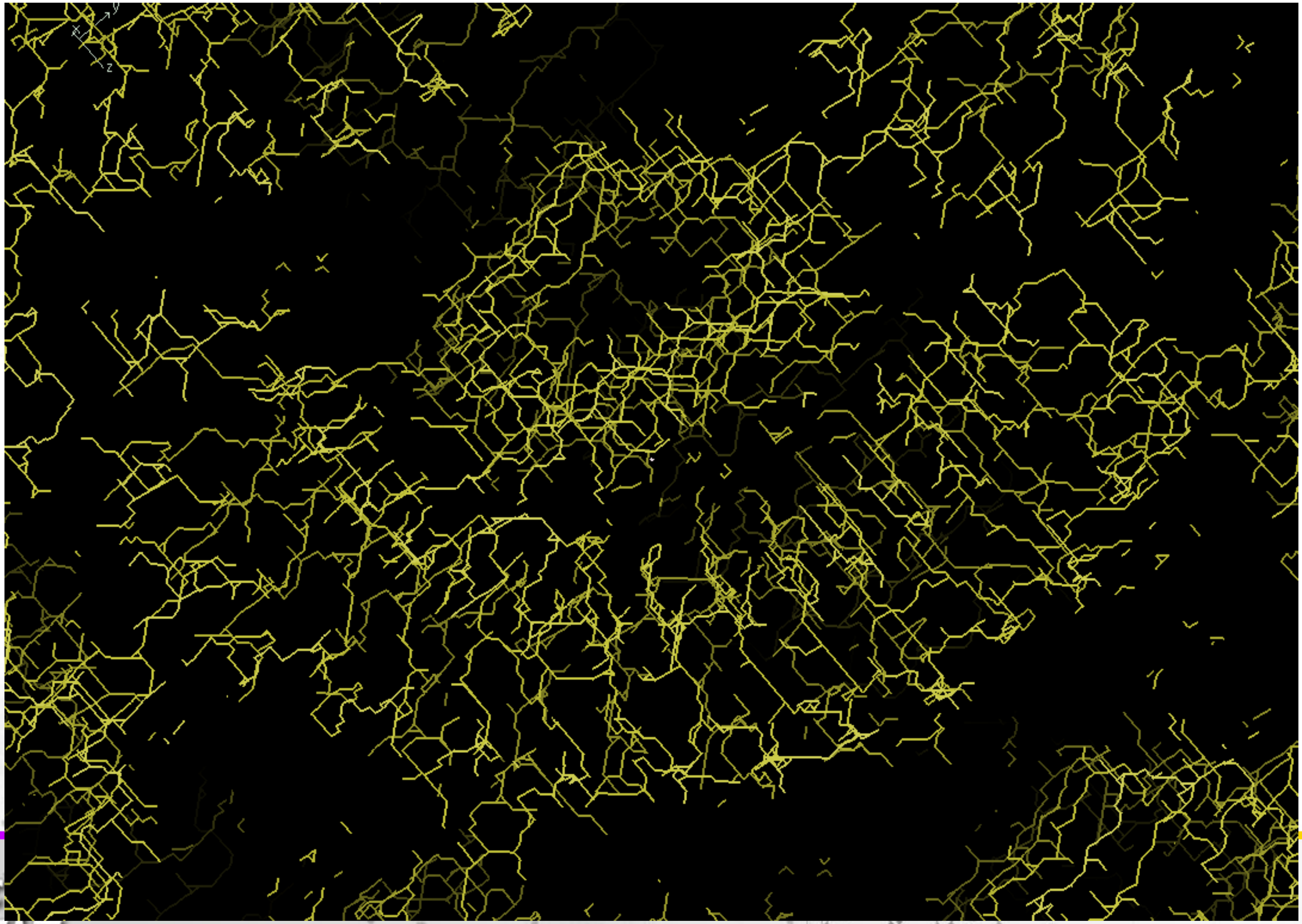
Will report on the very first one (unaligned).

Falling Inflection: 9673 eV

« Double redundancy » SAD Skeleton, With Solvent Flattening.



Equivalent dose 2 wavelength MAD Skeleton, With Solvent Flattening.



SOLEIL SYNCHROTRON

(End of parenthesis)

Two messages :–

- If you have a reason, go to a high energy and check fluorescence for heavy atoms in your crystal. I have phased a number of times on things that were not supposed to be there...(usually Zn, As)
- Second – if you have low solvent content and need phases, MAD is a good bet.

Macromolecular X-Ray Crystallography at a Synchrotron Radiation Source.

Most Common Reasons for coming to Synchrotron.

- ✓ Large unit cell sizes (up to many hundreds of Å).
- ✓ Need for high resolution.
- • Large volume of crystals to collect or screen.
- ✓ Phase problem, need for to choose a specific wavelength / energy.
- • Variability of crystals.
- ✓ Radiation sensitive crystals.
- • Tiny crystals or weakly diffracting crystal (don't see diffraction at home).
- • Increasingly, access to infrastructure! No facilities at home…..

» Very high intensity.

» Very broad energy spectrum (X ray – IR).

» Naturally highly collimated

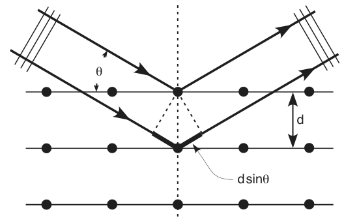
» Small source size.

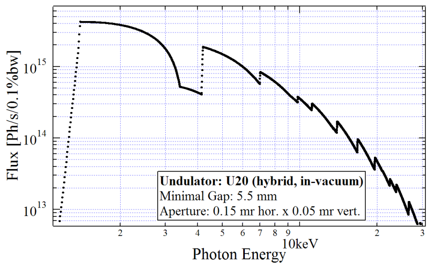
» High degree of polarisation.

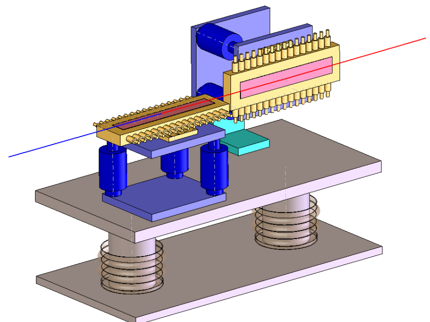
» Pulsed time structure.

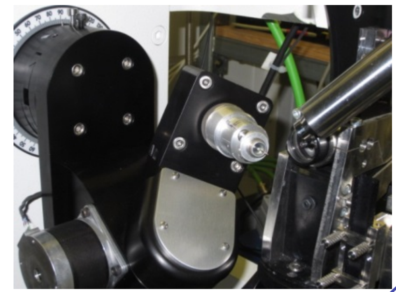
» High brilliance machines give partly coherent beam.

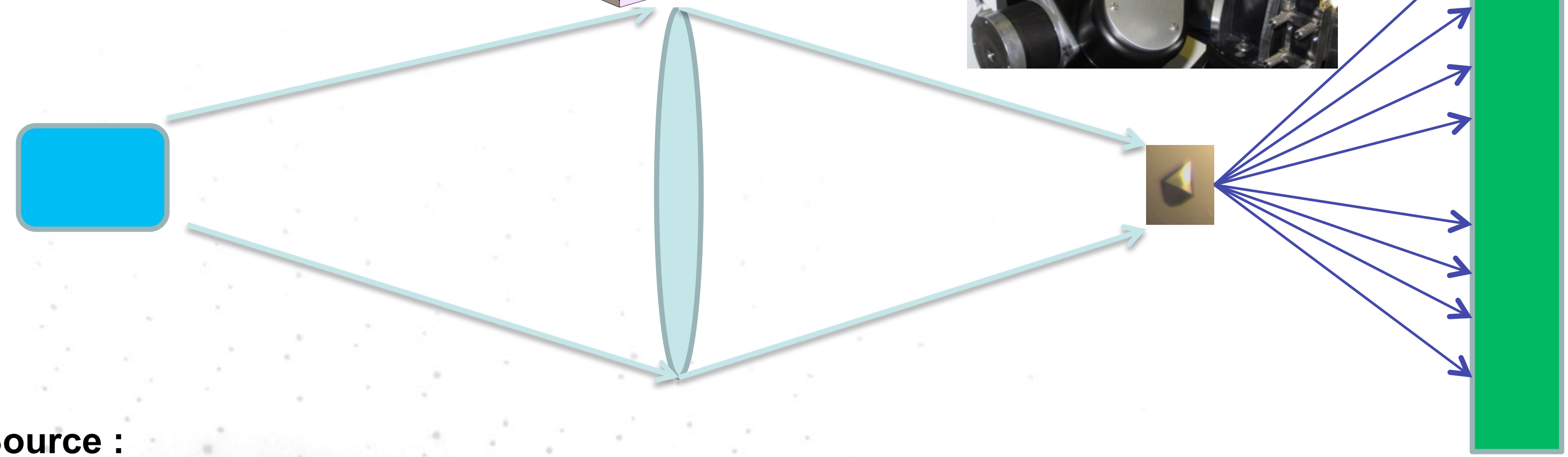
SOLEIL SYNCHROTRON











Source : Bending magnet, undulator, wiggler

Optics : Monochromator, « mirrors »

Sample : goniometry

Detector : distance

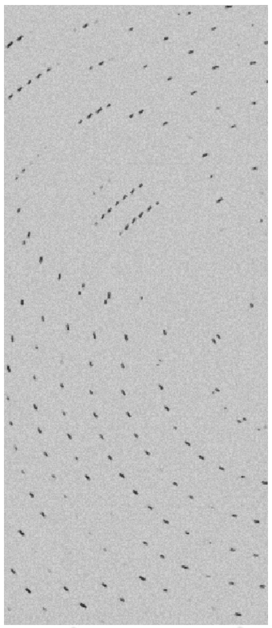
A beamline – a minimalist view (and vastly distorted)

2D X-ray detector characterization

Detectors Group – Proxima 1

Evaluation of the performances to reproduce the photons image

Perfect image



- Nb of photons
- Poisson noise

Detector

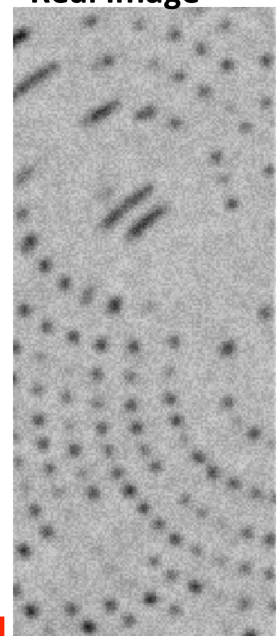
- Efficiency
- Dynamic
- Linearity
- Point spread function
- spatial sampling
- noise

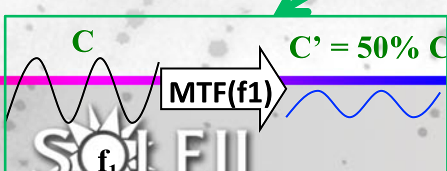
- Contrast reduced
- noise increased

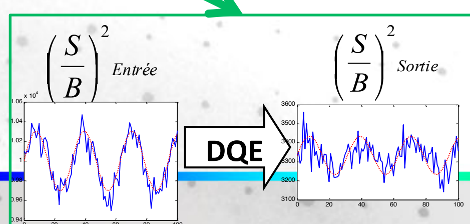
→ Signal/noise reduced

Quantify the degradation of input image with the MTF and DQE

Real image







$$DQE(\nu) = g \times \frac{\bar{S}}{NPS(\nu)} \times MTF(\nu)^2$$

Quantitative evaluation of the performances of a 2-D X-Ray detector

S. Hustache, P. Legrand, A. Thompson and K. Medjoubi.

Imaging performance of 2D X-ray detectors can be described by the linear system transfer theory. In this approach, input-output relationships of an imaging system are expressed in terms of three transfer functions: the modulation transfer function (MTF), the noise power spectrum (NPS) and the detective quantum efficiency (DQE). These functions quantify the propagation quality of the spatial distribution of the incident photons, including statistical fluctuations. More familiar parameters [such as X-ray sensitivity, dynamic range (which includes linearity), spatial homogeneity, spatial linearity, stability, lag effects and, if available, energy resolution] are implicit in these transfer functions. Quantified separately, these parameters improve the understanding of the physical consequences of specific aspects of the MTF, NPS and DQE.In this document, these functions and parameters are defined and methods of measuring them are established.

In the following document only monochromatic beam exposure is considered and measurements are to be performed at different energies. All the relevant quantities will be determined after the usual image corrections (energy dependant flat field corrections, dark current subtraction, spatial distortion correction etc …).

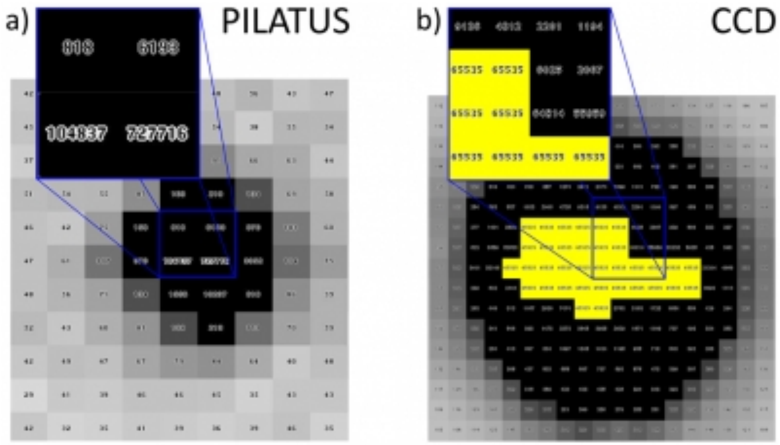
These measurements will be done with different configurations of the detector (Binning, Gain, shaping time, threshold…) potentially used during scientific experiments, on different parts of the detector (including interfaces between modules to examine boundary effects) and at different energies.

- **MTF, NPS and DQE**
- **Linearity and dynamic range**
- **Spatial Homogeneity**
- **Spatial Linearity**
- **Noisy or dead pixels**
- **Imaging stability**
- **Frame rate**
- **Lag effects**
- **Energy resolution**

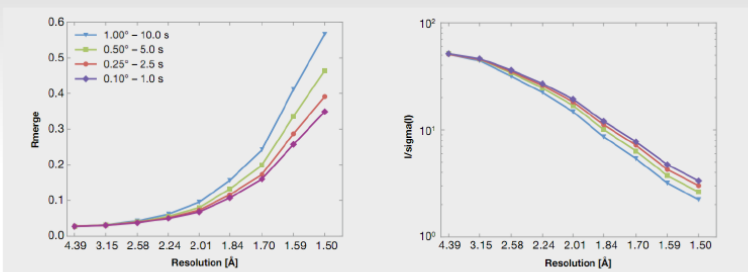
SOLEIL SYNCHROTRON

K. Medjoubi, Detector Group, Synchrotron Soleil

Use of pixel array detector.



3. Data quality improvement at high resolution



Insulin data sets covering 180° of rotation, all collected with the same angular speed.

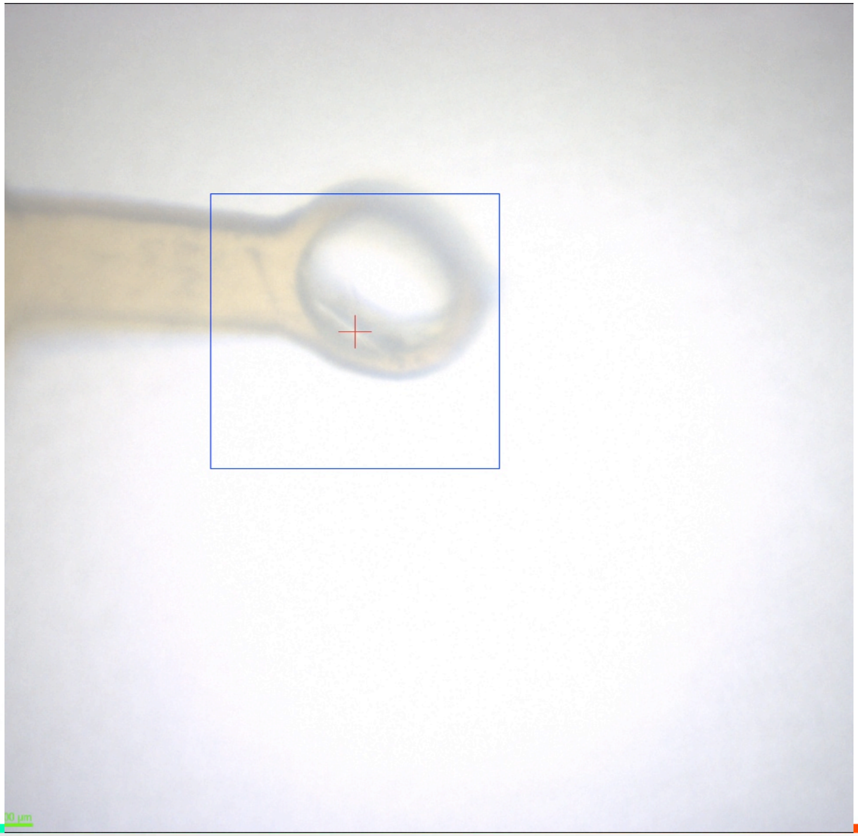
--> Gain in speed & data quality

- Critical advantages :
- Fast : fine phi slicing / shutterless.
- No detection noise – background counts come from your experiment.
- Small PSF helps pull out weak reflections at high angle.
- Allows you to collect with lower dose for the same data quality – more data per crystal.

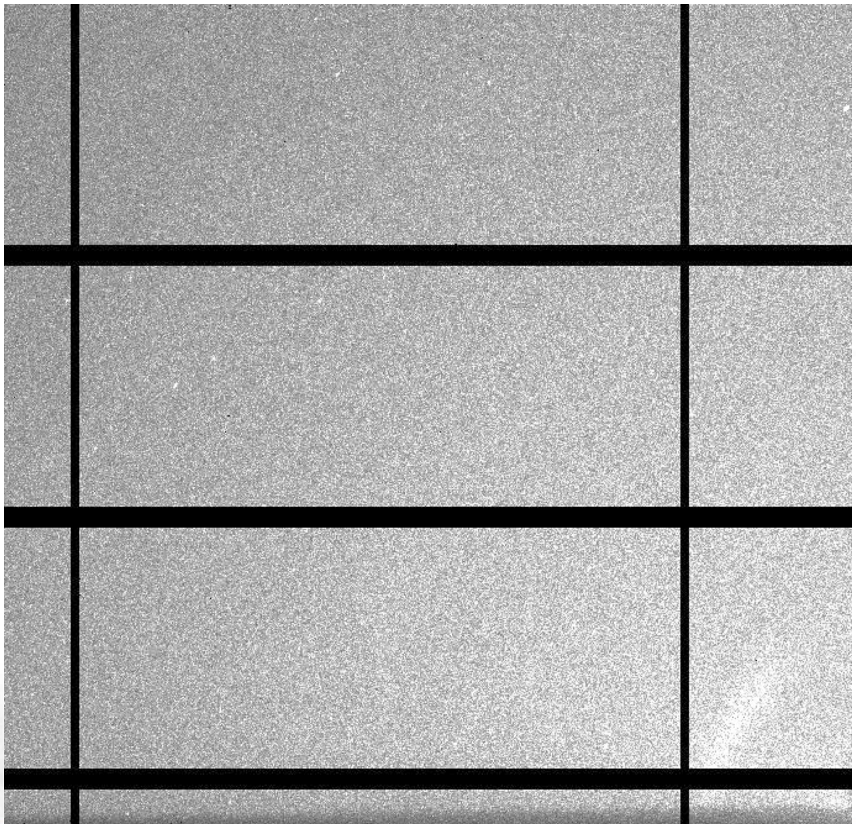
SOLEIL SYNCHROTRON

What crystal do I collect?

- The missing partner from a series of mutants, needed for publication.
- Only sign of crystals was an agglomeration of « sea urchin like » spikes.
- Tried to fish the biggest and caught a fragment – approximately 10 x 10 x 100 µm. Protein small (about 20 kDa), space group tetragonal.



If it was my crystal (this one was!) I would look at images carefully …….



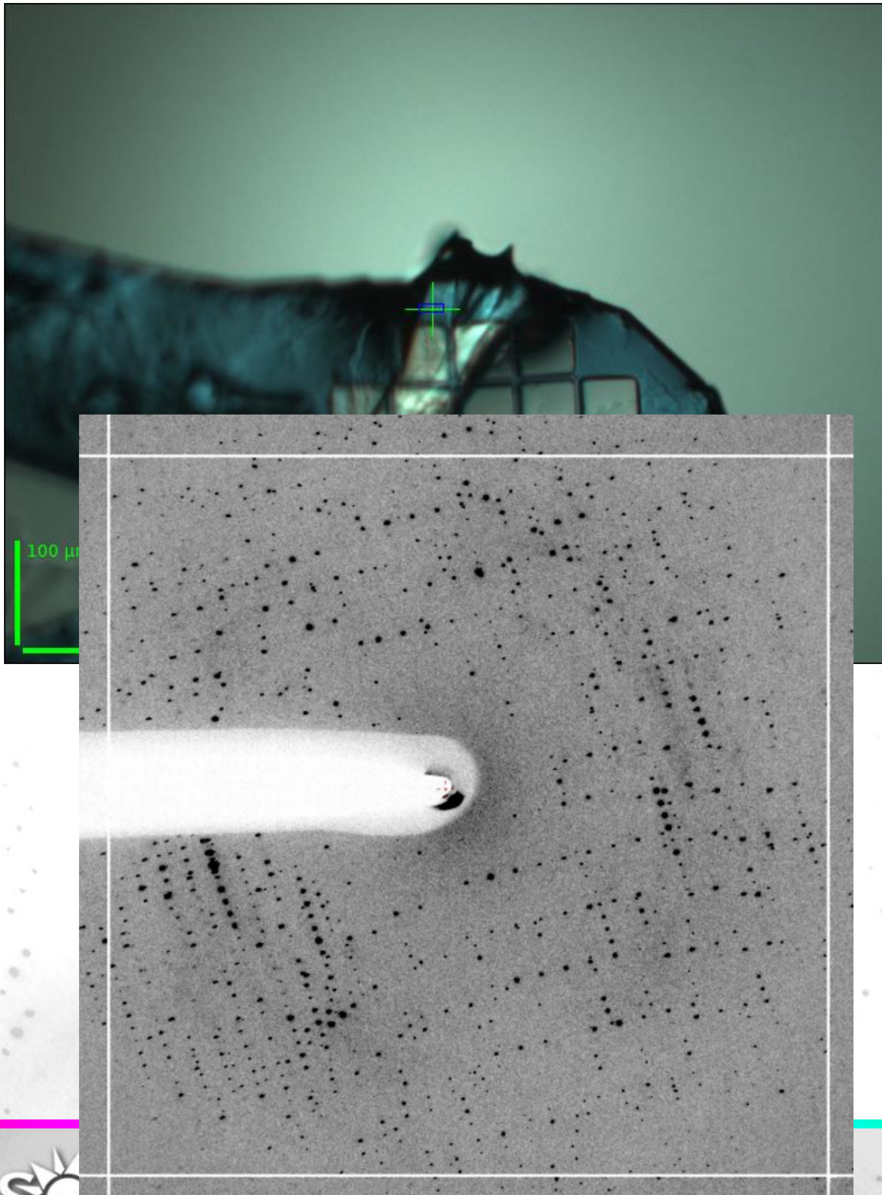
9	11	14	20	17	15	19	18	16	19	19	13	15	21	14	8	11	19	16	17	7	13	14	15	19
21	11	9	13	10	9	14	6	19	12	20	18	19	18	16	15	15	11	14	22	9	10	16	20	13
10	14	12	6	25	17	10	25	12	22	7	13	12	11	19	11	17	15	13	16	14	14	12	9	12
16	16	12	16	11	17	13	12	18	12	10	7	12	18	14	9	18	12	16	13	18	12	21	16	16
18	17	21	14	18	13	13	16	14	14	17	14	13	14	18	11	11	19	8	19	9	12	10	13	11
8	10	17	14	12	17	19	11	12	14	12	17	9	22	12	14	14	16	17	11	18	11	14	11	13
19	13	13	16	16	15	12	21	13	18	9	19	16	15	15	9	13	13	16	21	14	15	10	17	11
15	12	11	20	14	14	10	17	16	18	21	**36**	23	15	12	12	13	18	12	19	12	25	11	16	11
12	15	16	12	12	12	15	16	14	17	**58**	**44**	18	14	15	12	15	16	12	14	16	14	9	24	19
14	16	17	12	13	11	13	17	14	21	**54**	28	16	14	14	12	16	16	11	15	15	15	12	19	16
16	15	17	10	17	12	12	21	16	24	**50**	14	15	12	13	12	16	15	11	14	15	20	15	15	14
13	2	21	17	15	13	16	14	12	17	19	9	17	10	15	11	13	12	16	11	9	17	22	15	9
7	18	15	10	13	16	13	14	18	18	14	16	26	16	14	17	8	8	13	18	17	7	21	25	7
13	14	21	11	15	19	17	11	11	14	16	11	18	7	14	17	12	15	15	17	8	15	17	5	12
16	14	17	18	9	13	10	7	20	13	17	16	15	14	9	13	18	16	20	16	13	9	12	15	8
13	18	14	21	15	15	13	17	12	11	11	15	8	10	18	18	16	10	12	16	11	7	12	23	13
15	19	17	12	10	15	15	13	18	20	18	19	20	11	15	18	11	12	17	13	16	17	15	14	21
13	7	9	11	20	12	10	8	26	14	20	12	13	10	12	14	21	12	17	20	13	18	15	12	12
13	9	11	9	13	13	12	16	6	9	21	16	13	16	12	8	9	17	15	16	17	12	16	12	12
14	14	10	14	15	11	20	22	10	7	10	17	14	9	18	15	12	10	13	16	21	11	9	17	16
14	14	12	12	15	15	13	14	11	14	10	10	7	11	12	11	17	9	5	10	15	14	17	12	11
16	20	19	14	17	9	16	13	9	11	19	13	10	20	10	17	16	13	14	12	14	13	16	11	27
14	15	7	21	17	9	12	9	14	17	8	11	10	12	6	15	16	14	17	6	14	12	9	14	10
7	12	11	10	15	15	19	15	14	11	18	12	12	11	11	10	14	15	18	11	23	15	21	9	13

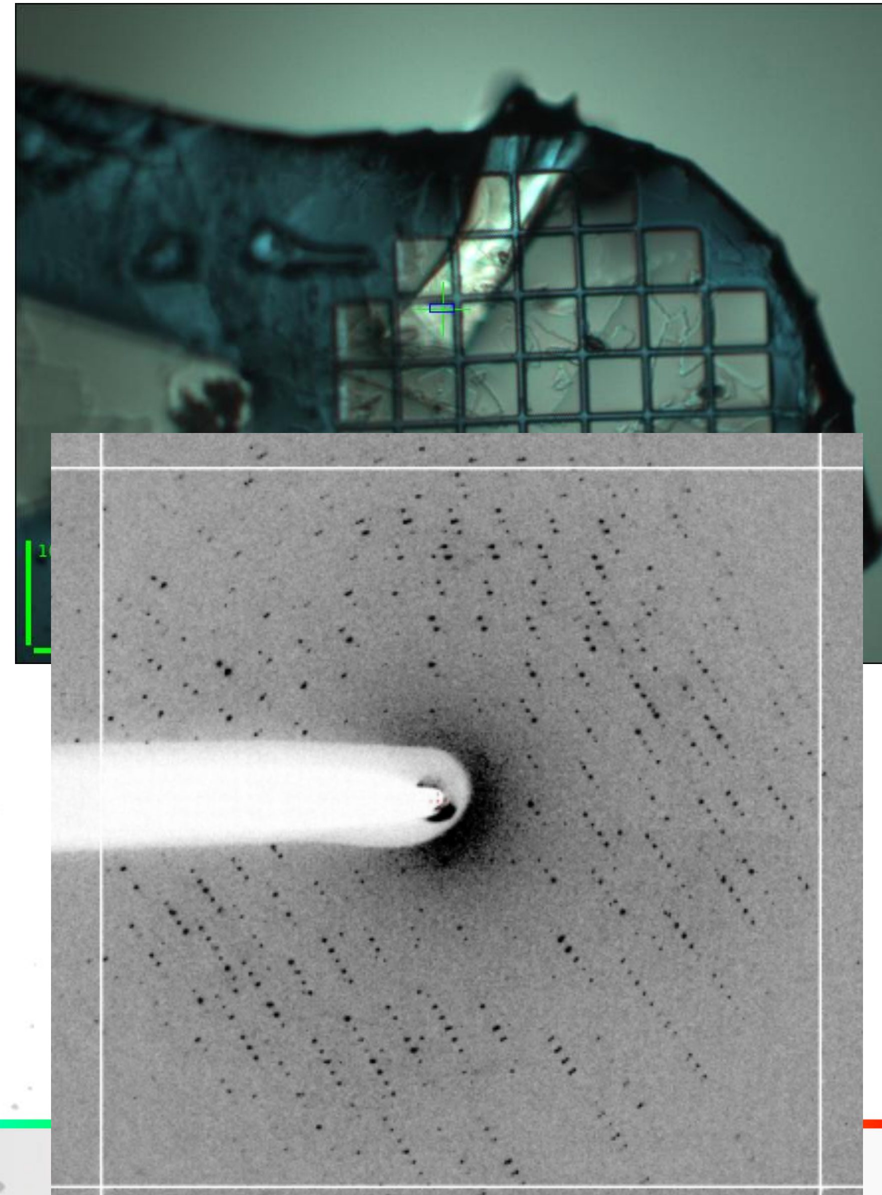
SUBSET OF INTENSITY DATA WITH SIGNAL/NOISE >= -3.0 AS FUNCTION OF RESOLUTION

RESOLUTION LIMIT	NUMBER OF REFLECTIONS OBSERVED	UNIQUE	POSSIBLE	COMPLETENESS OF DATA	R-FACTOR observed	R-FACTOR expected	COMPARED	I/SIGMA	R-meas	CC(1/2)	Anomal Corr	SigAno	Nano
8.39	2477	406	434	93.5%	5.4%	5.3%	2467	26.47	5.9%	99.8*	-7	0.780	223
5.98	4456	652	675	96.6%	12.1%	11.9%	4437	13.90	13.1%	99.3*	-6	0.774	444
4.90	5815	817	838	97.5%	12.9%	12.5%	5803	14.11	13.9%	99.1*	-10	0.762	608
4.25	6954	965	983	98.2%	11.6%	11.2%	6934	15.71	12.5%	99.5*	-12	0.773	734
3.80	7936	1083	1101	98.4%	20.0%	20.0%	7912	9.95	21.6%	98.4*	-6	0.773	840
3.47	8407	1175	1189	98.8%	30.4%	30.8%	8383	6.91	32.7%	96.7*	-2	0.770	913
3.22	9288	1282	1303	98.4%	42.7%	42.2%	9267	5.21	46.0%	94.2*	-5	0.770	1021
3.01	10176	1374	1387	99.1%	75.5%	76.9%	10154	3.02	81.1%	86.6*	-10	0.713	1093
2.84	9849	1409	1469	95.9%	122.8%	130.0%	9799	1.69	132.4%	69.3*	-9	0.663	1088
total	65358	9163	9379	97.7%	23.3%	23.4%	65156	8.58	25.1%	98.9*	-7	0.745	6964

Screenshot from CORRECT.LP. Not data to be proud of, but it rounded off a publication.

Crystal Uniformity : PX2a





PROXIMA 1 – CATS robot, 3x Unipuck, 48 samples
PROXIMA 2 – CATS robot, 7 x Unipuck, 144 samples

At worst, you can screen all your crystals and collect the best (one or two) – robots are pretty reliable nowadays, and they are there to let you do a better experiment, NOT to just to let you do MORE EXPERIMENTS……

Question was asked « how to know what to collect ? »
The answer is it depends on how much you want the answer and how much work you put in !

Blob of ice under pin base, usually from ice in your Dewar. It is cold coming from the robot transfer.

But it warms up and your loop can move « after you centred it ». Always keep an eye on it……..

Another little pitfall for the unwary and corollary to McSweeney's rule.

Robots add to your experiment. But do be careful when centring your crystals :

Macromolecular X-Ray Crystallography at a Synchrotron Radiation Source.

Most Common Reasons for coming to Synchrotron.

- ✓ Large unit cell sizes (up to many hundreds of Å).
- ✓ Need for high resolution.
- ✓ Large volume of crystals to collect or screen.
- ✓ Phase problem, need for tunability
- ✓ Variability of crystals.
- ✓ Radiation sensitive crystals.
- ✓ Tiny crystals or weakly diffracting crystal.
- Increasingly, access to infrastructure!

Solutions proposed

- Highly parallel beams
- Tunable beams for *ab initio* phasing in presence of native or labelled crystals.
- Screening methods (robots, crystal or plate scans)
- Data processing pipelines and book-keeping.
- Micro-beams.
- Very precise and flexible goniometry
- High intensity.
- Highly sensitive (and expensive) detectors and very low background.
- Expertise in data collection.
- Rapidity.

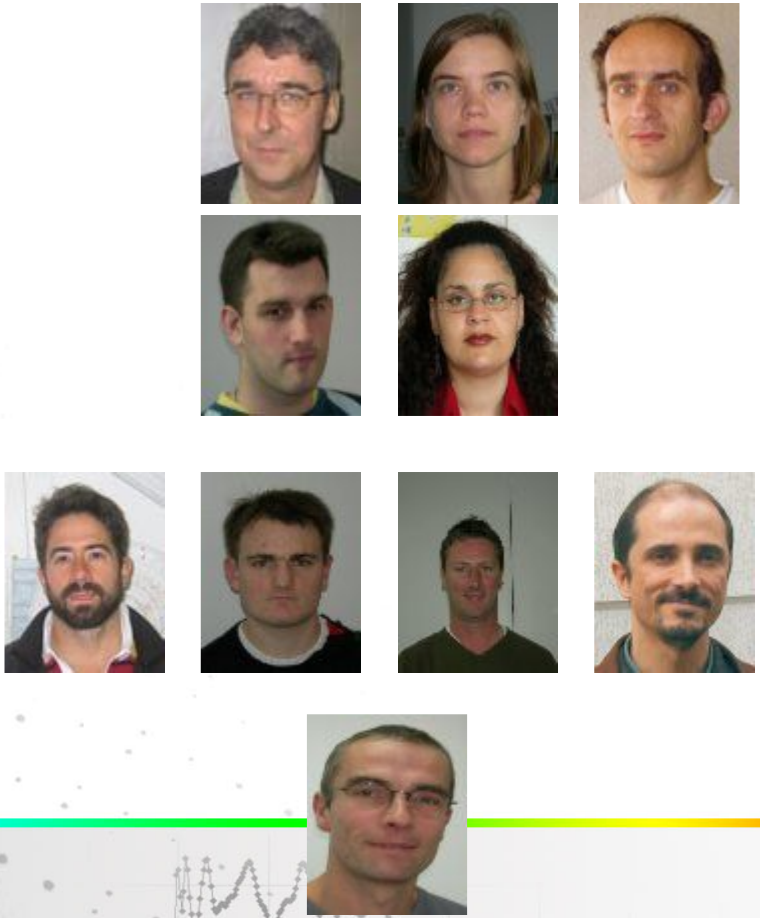
SOLEIL SYNCHROTRON

Acknowledgments.

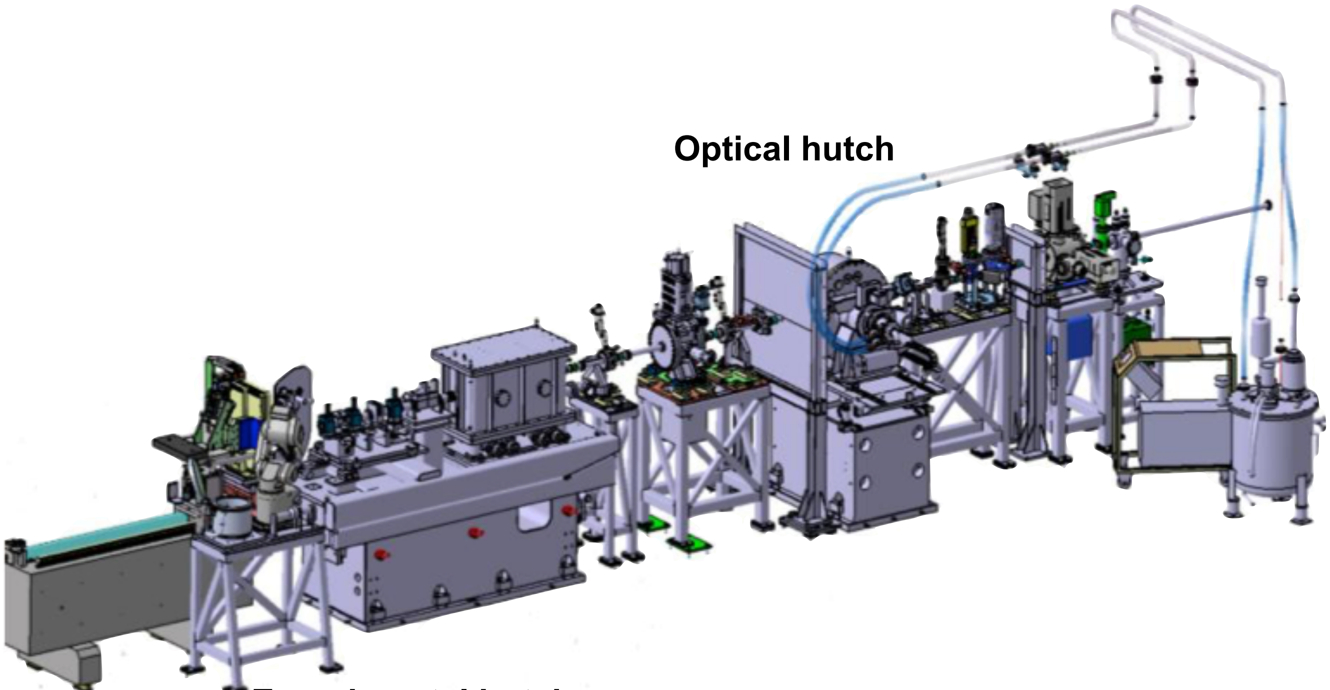
»PROXIMA 1 – L. Chavas, P. Gourhant, (B. Guimaraes), T.Isabet, P. Legrand, (N. Foos), S. Sirigu, F. Blache and S. Pierre-Joseph

»PROXIMA 2a – W. Shepard, G. Fox, (D. Duran), M.Savko,T. Moreno, A. Buteau

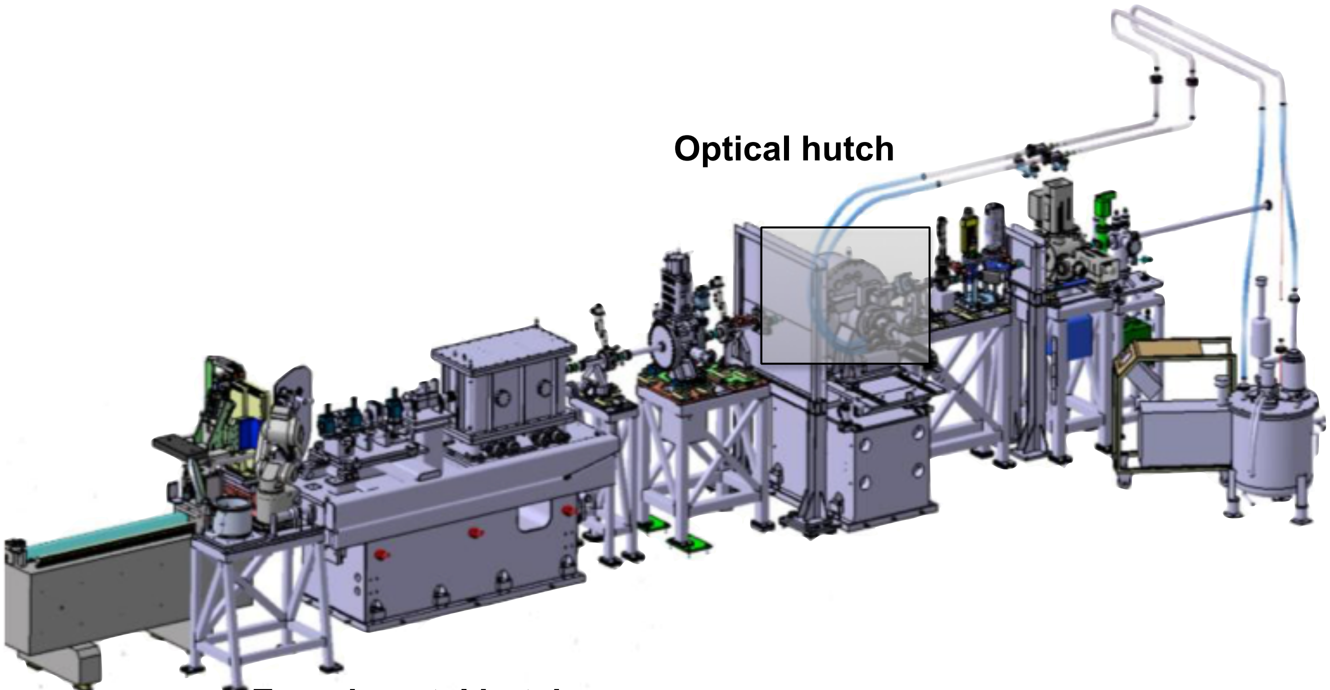
»Also G. Bricogne, C. Vonrhein, V. Olieric



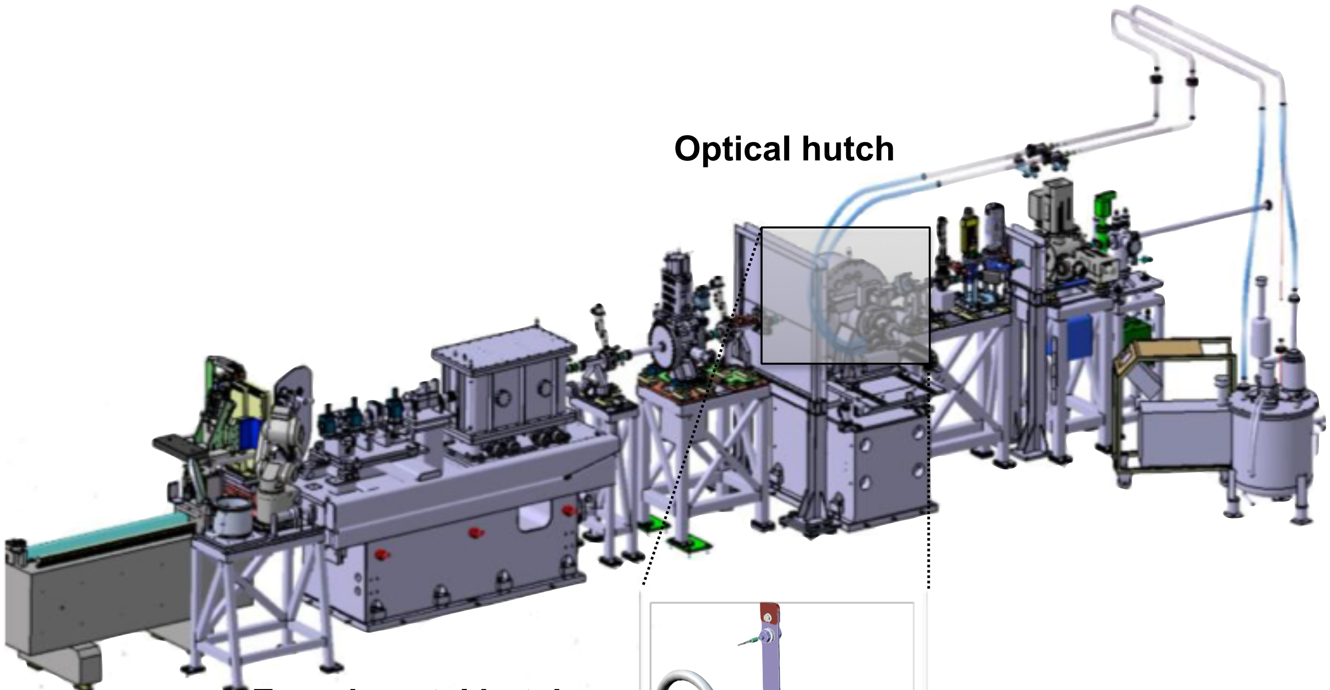
Beamline evolution: present and future

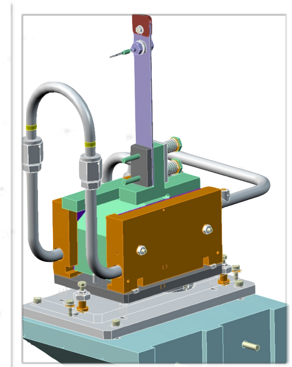


Beamline evolution: present and future



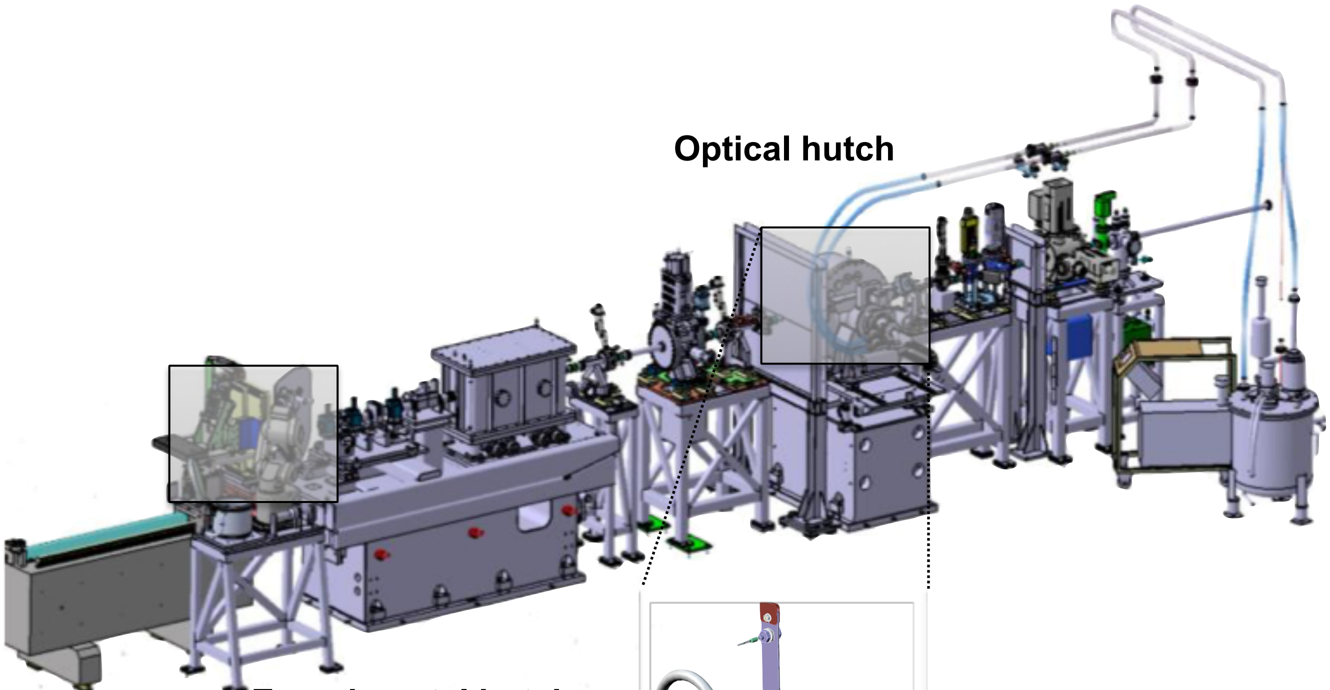
~~Beamline evolution: present and future~~

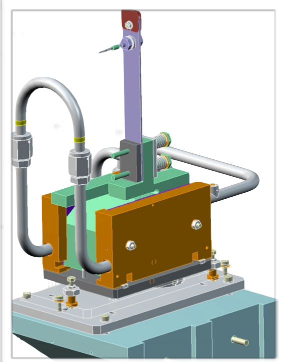




Summer-2016

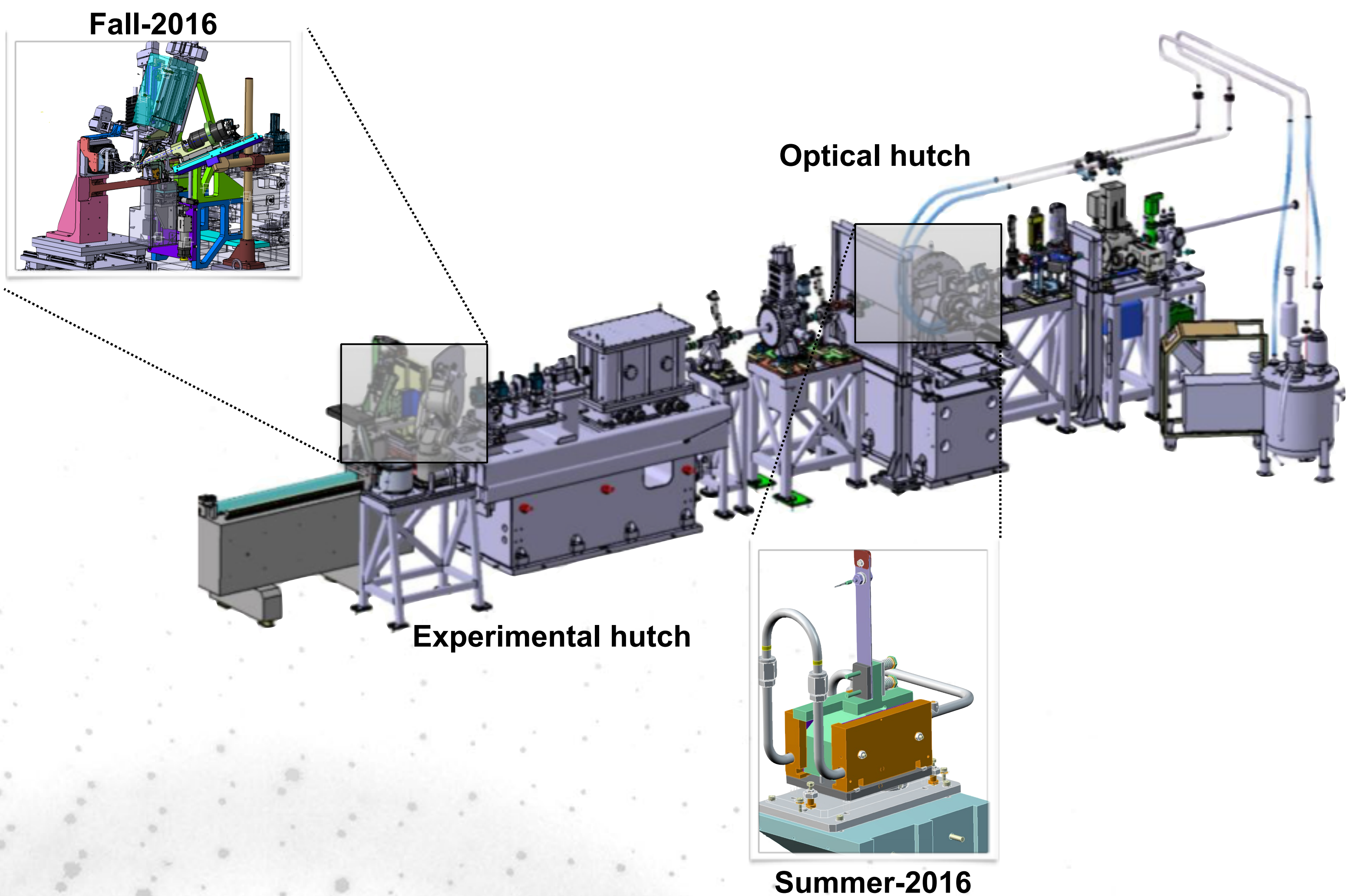
Beamline evolution: present and future





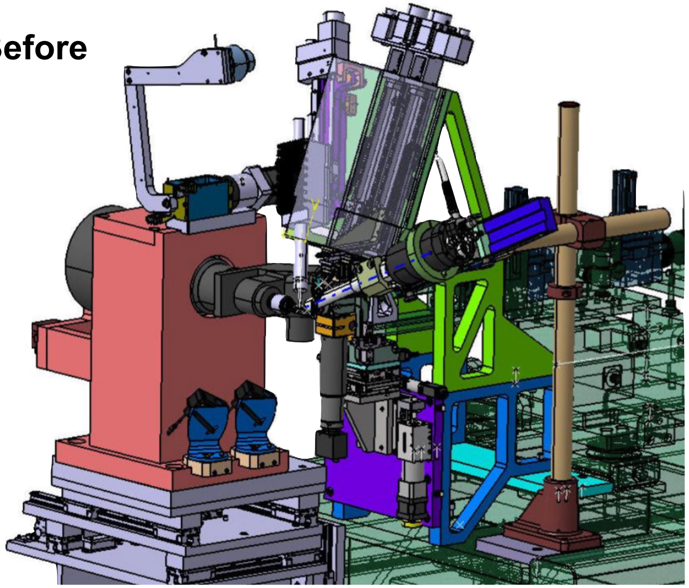
Summer-2016

Beamline evolution: present and future



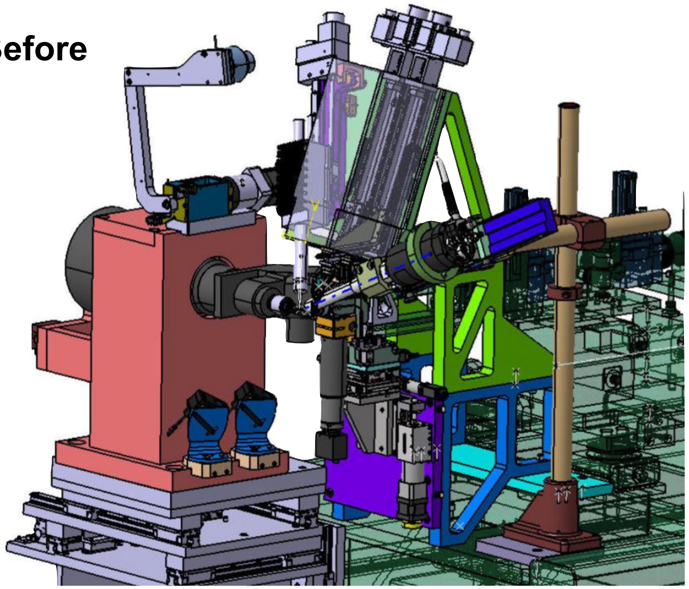
Beamline evolution: present and future

Before

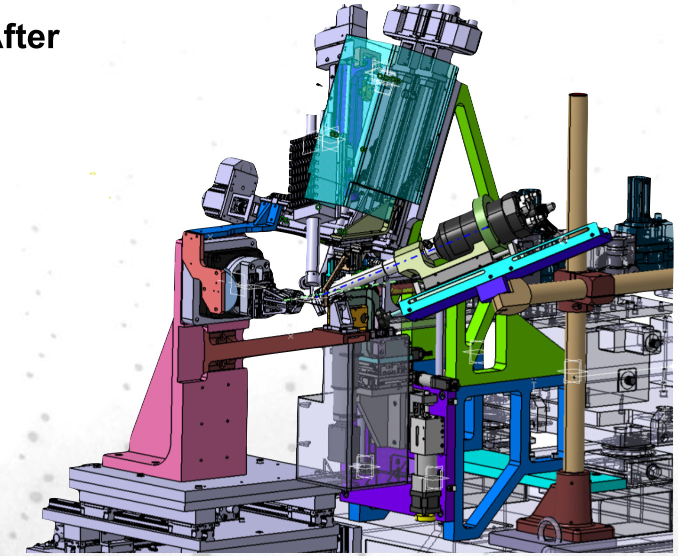


Beamline evolution: present and future

Before

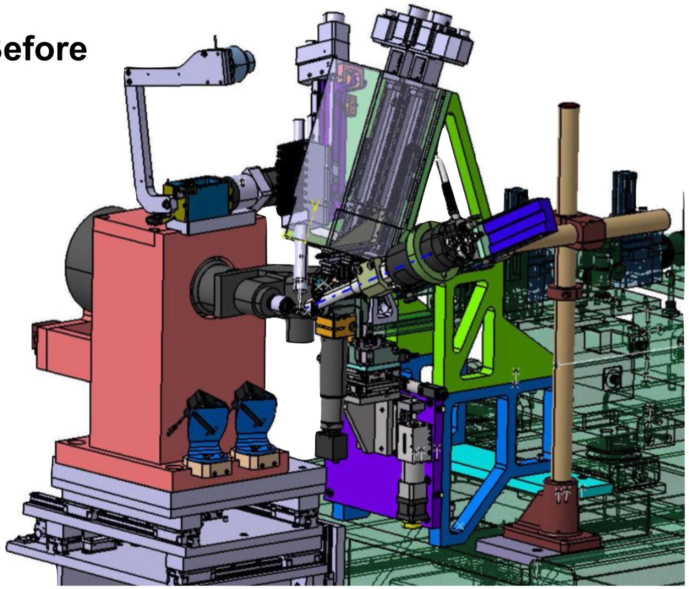


After

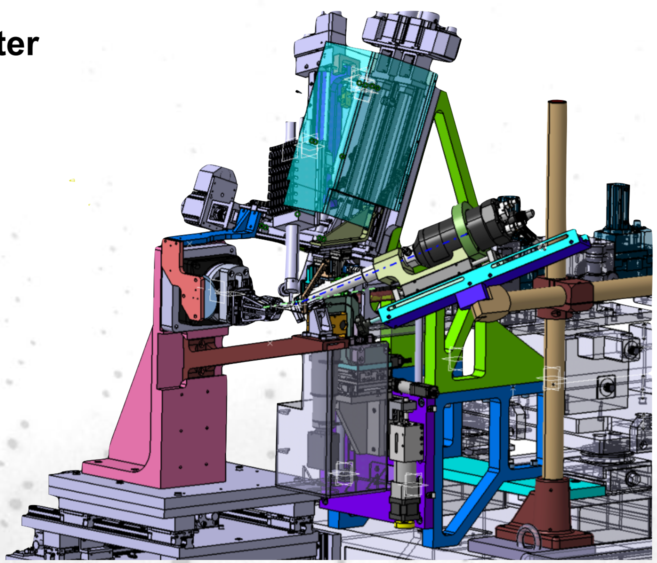


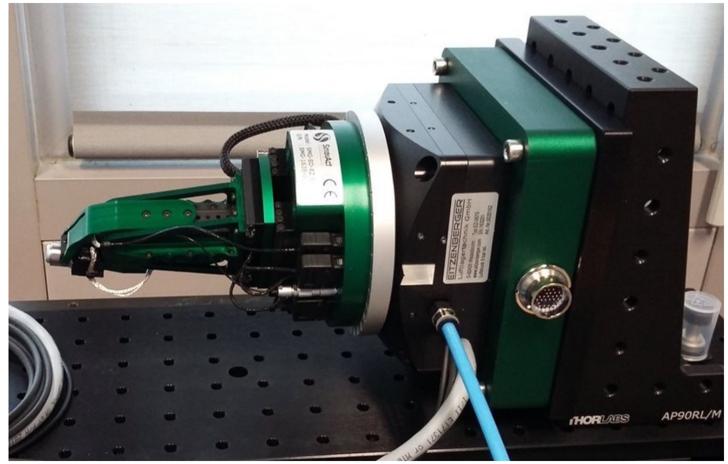
~~Beamline evolution: present and future~~

Before



After



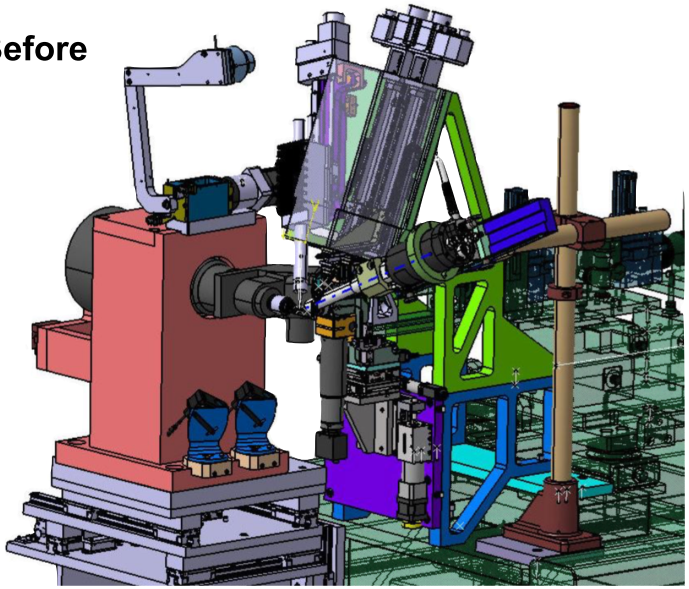


Goniometer in the house.

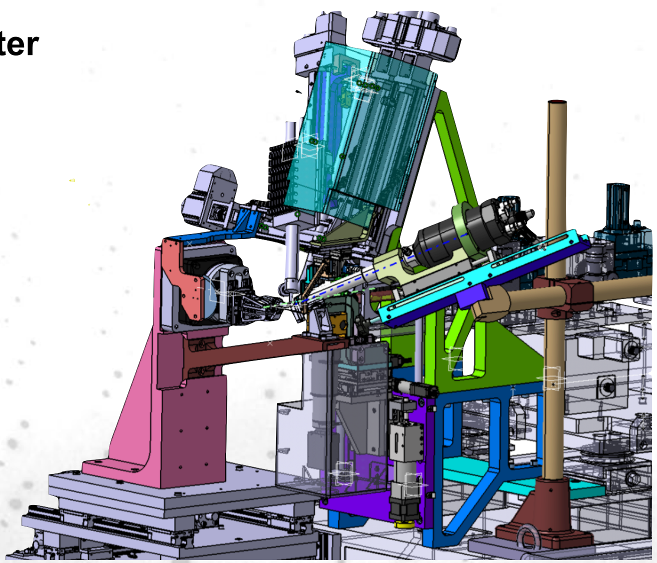
Ready for installation: Fall 2016

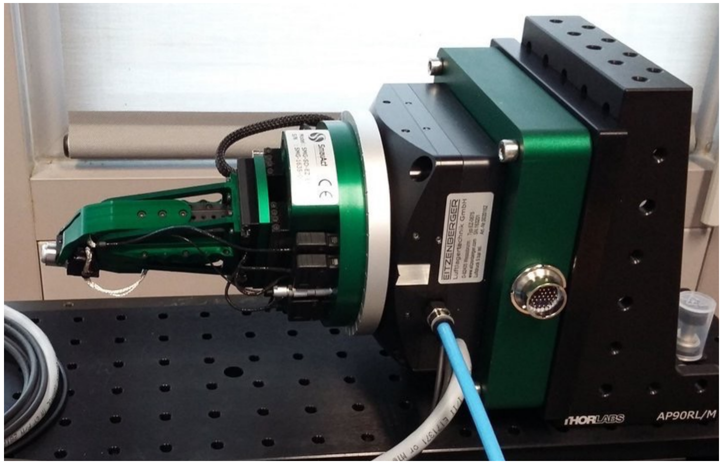
~~Beamline evolution: present and future~~

Before



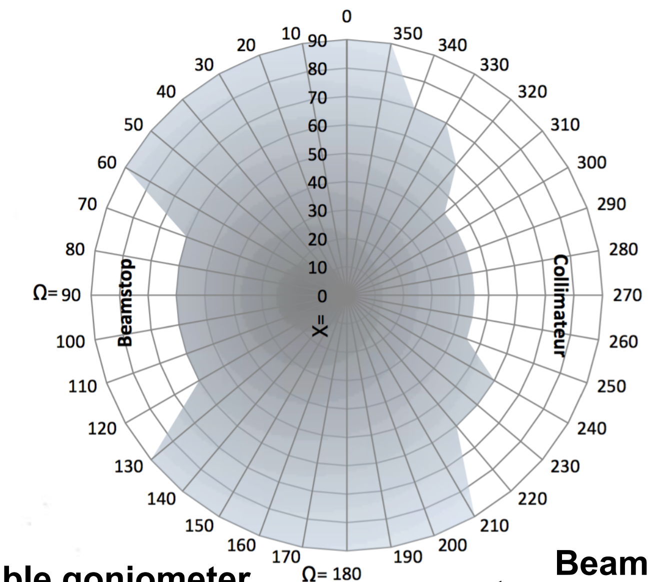
After





Goniometer in the house.

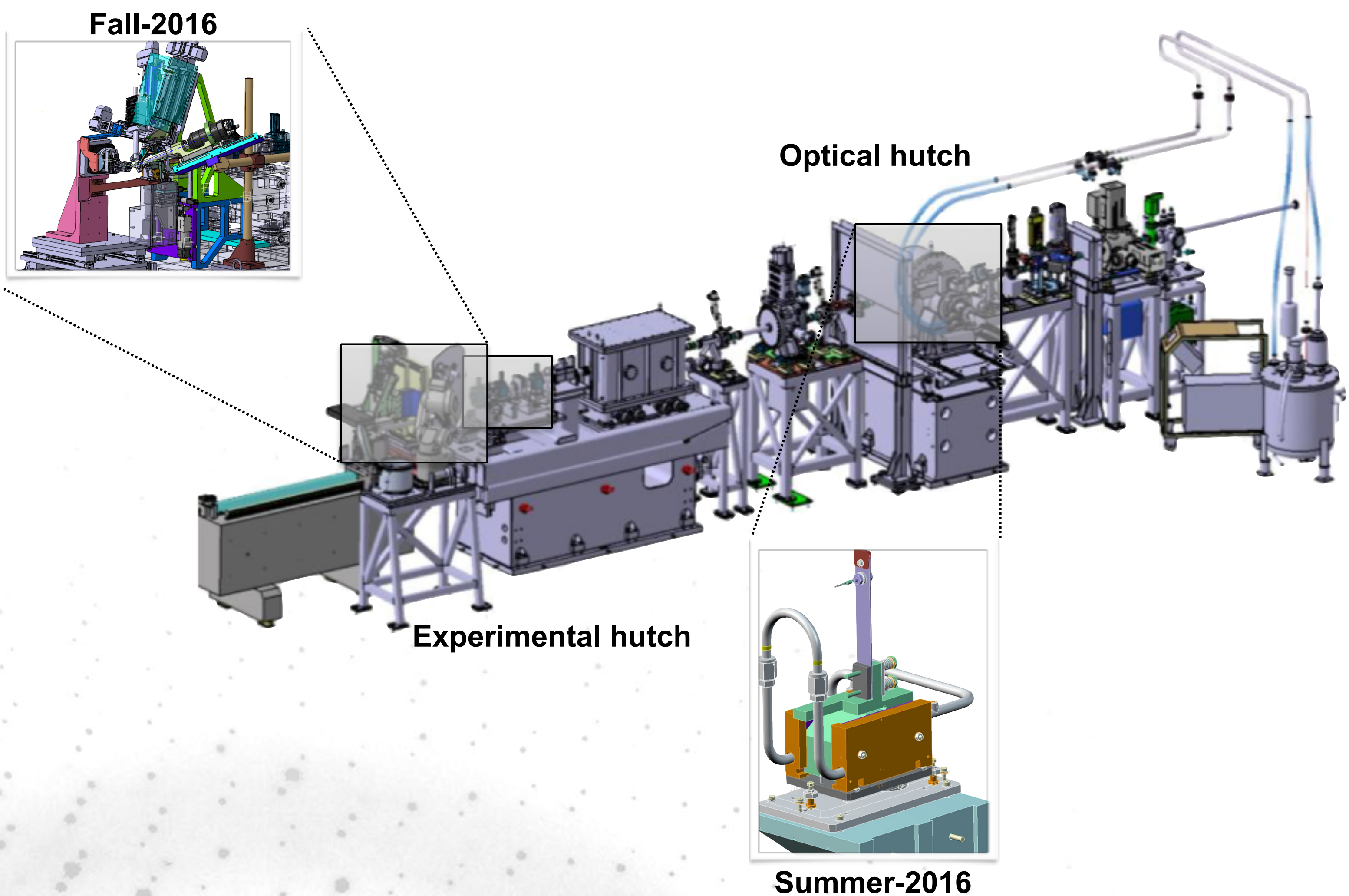
Ready for installation: Fall 2016



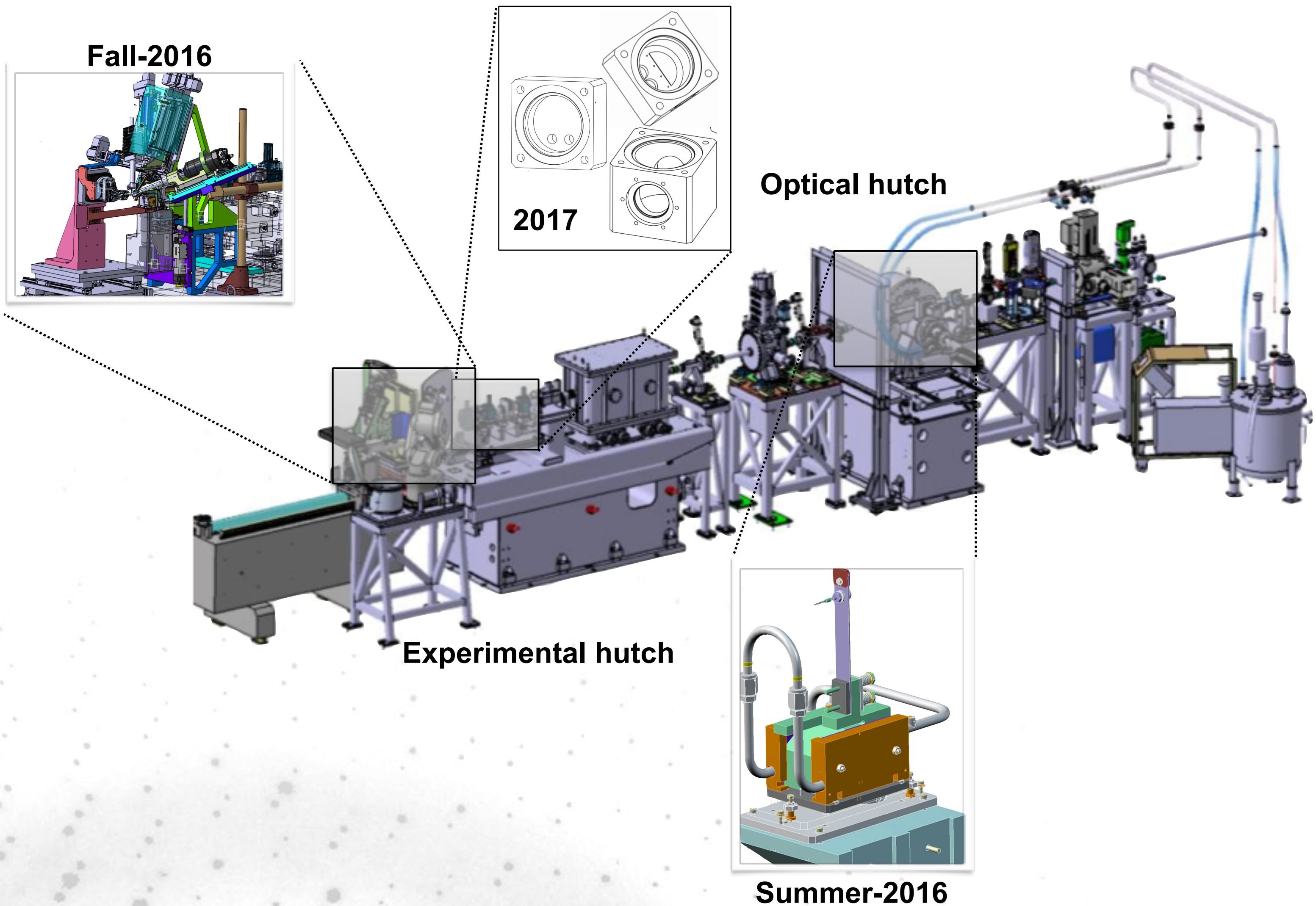
Sphere of possible goniometer movements around the sample position

Beam direction

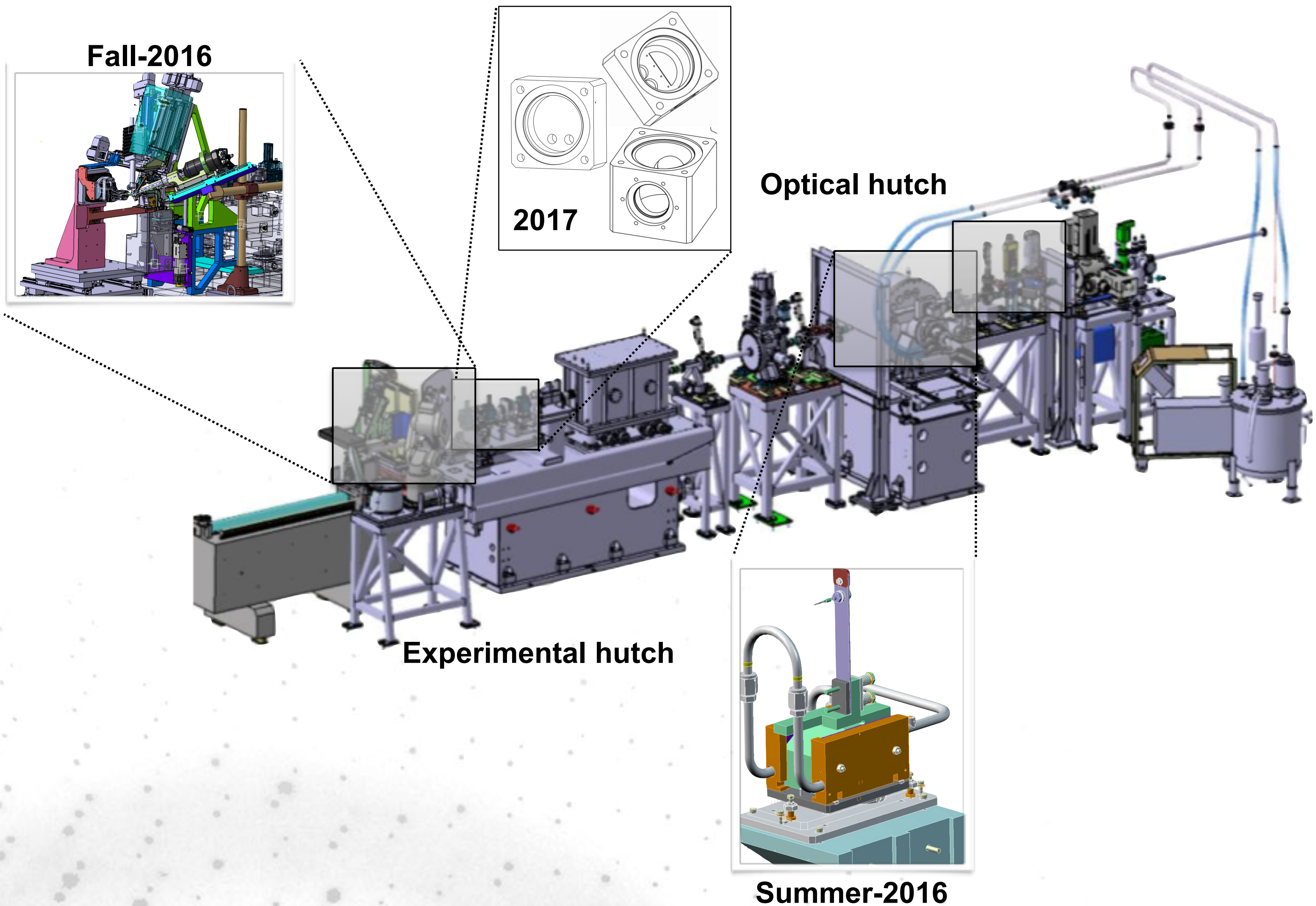
Beamline evolution: present and future



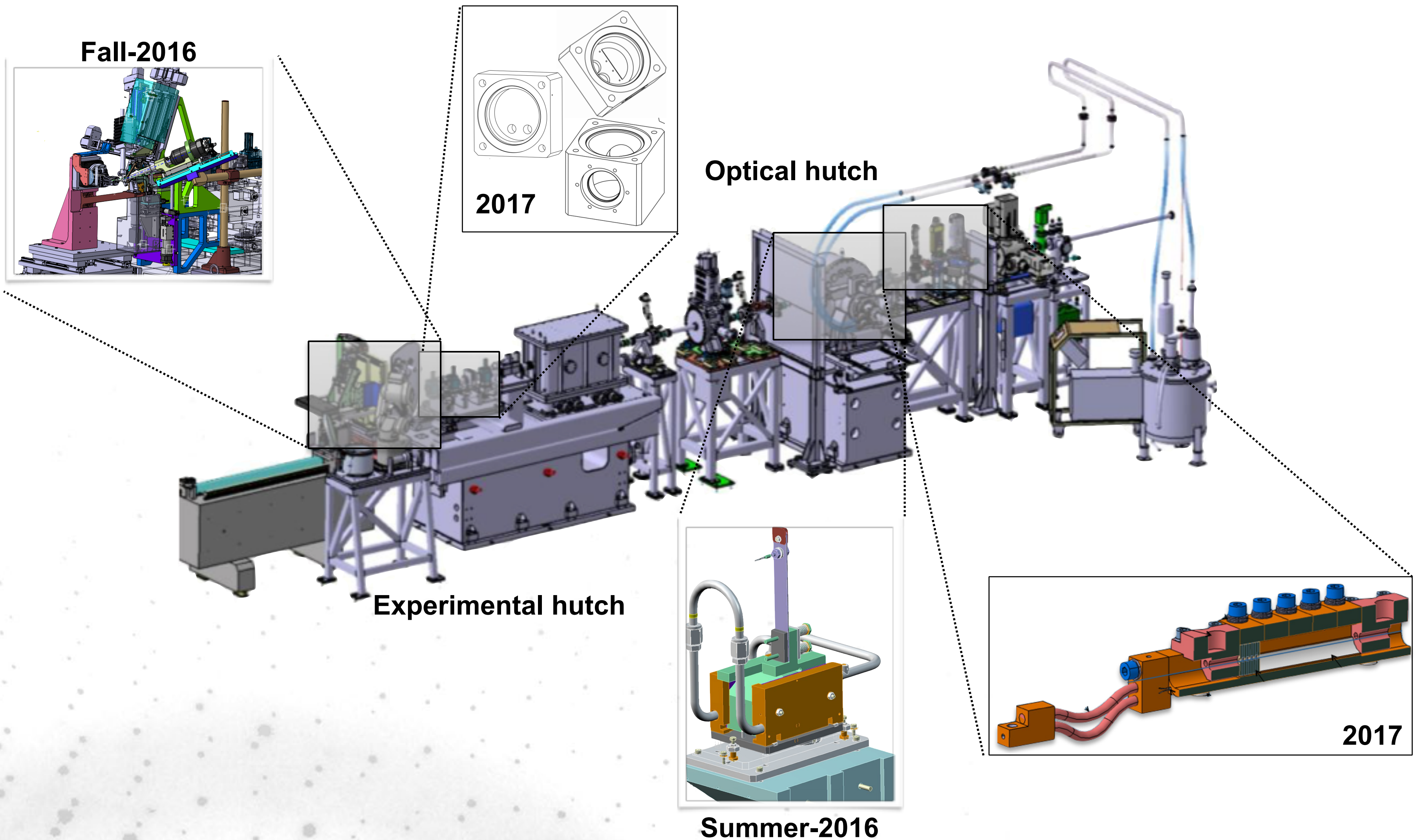
Beamline evolution: present and future



~~Beamline evolution: present and future~~



Beamline evolution: present and future



DLSR – Diffraction limited Storage Ring : MAX – IV, other sources following (ESRF, SLS, ALS? APS? SOLEIL?.......)

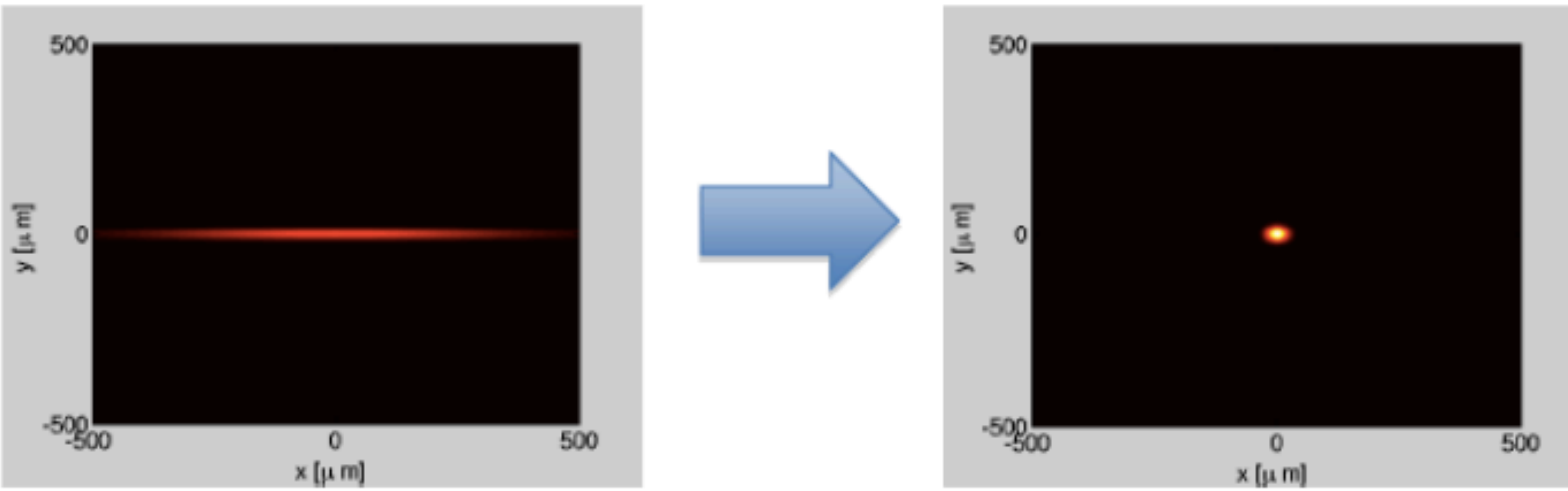


Figure 12: Illustration of typical current beam dimensions in 3rd generation light sources (left) and the big reduction possible in horizontal emittance at DLSRs (right).