MAX IV

Simulations and design for soft X-ray beamlines at MAX IV

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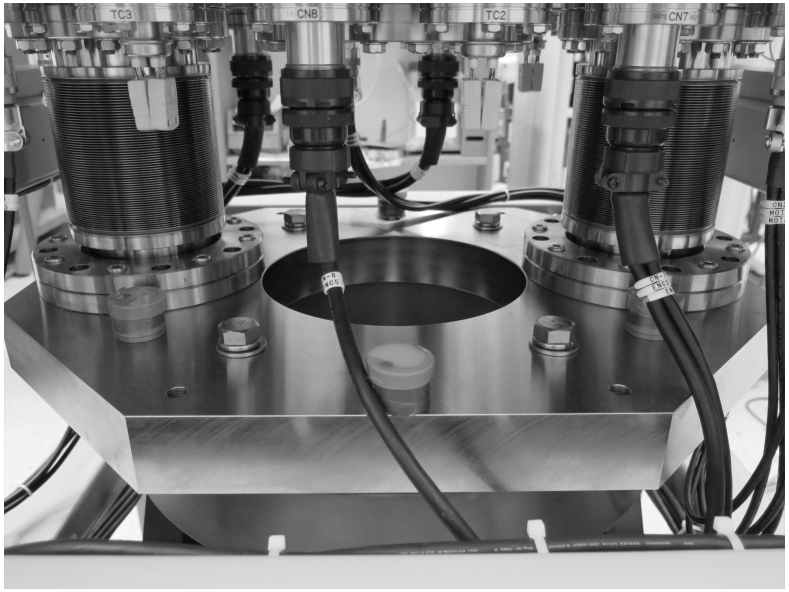
MAX IV

Outline

- MAX IV Laboratory
- Description of the beamlines
- Needs in simulations
  - Performance
  - Power, cooling and stability
  - The source
  - Coherence
- Results and conclusions



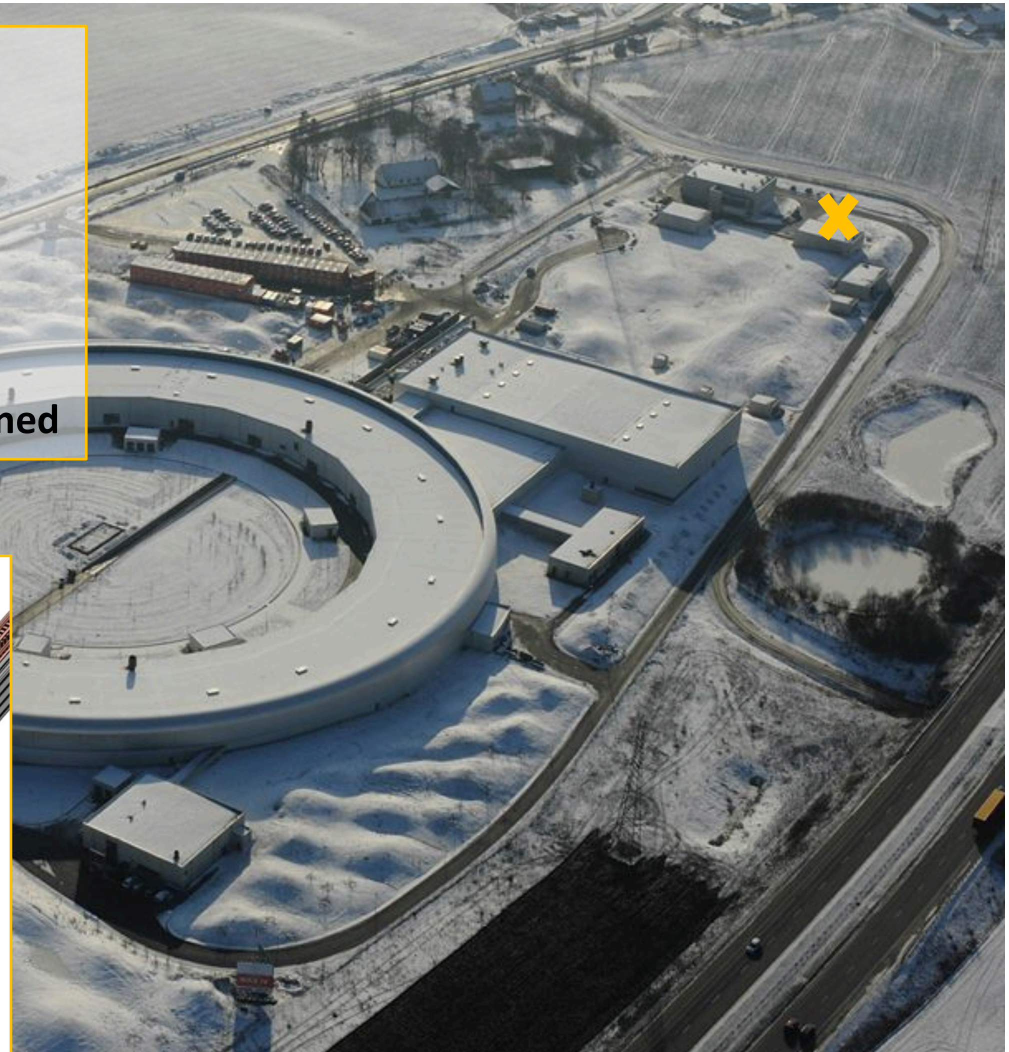
Overwiew

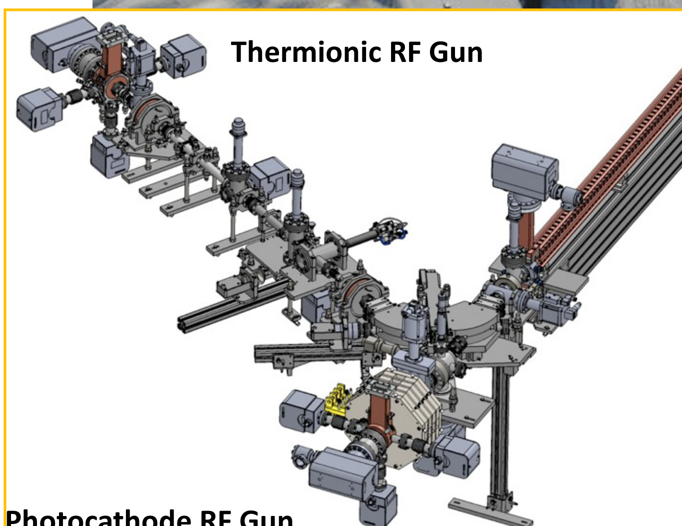
Injection

Two injection system
Thermionic RF Gun
1 nC @ 10 Hz

Photocathode RF Gun
100 pC @ 100 Hz

Status: In operation ≠ Fully commissioned



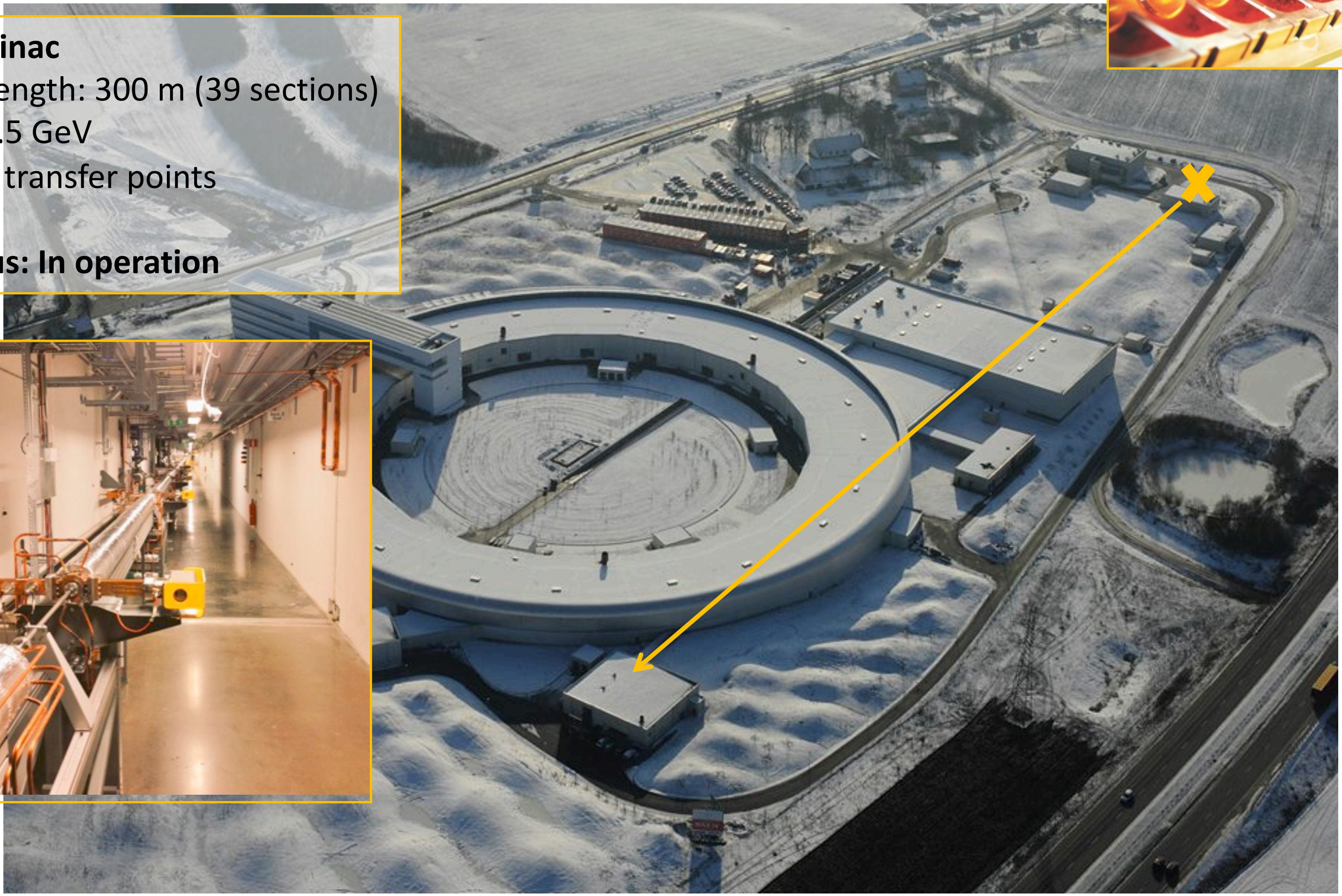


Linac

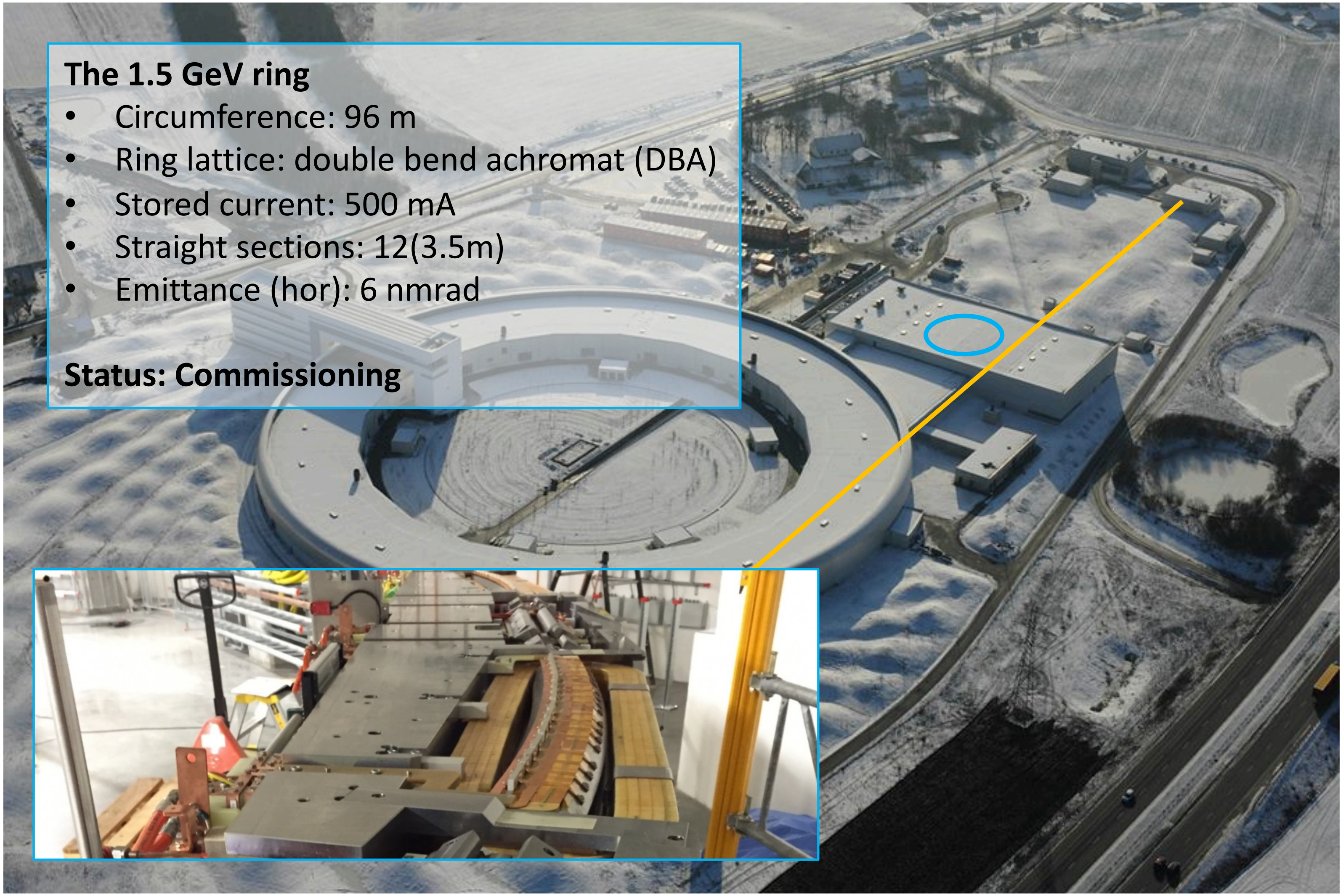
The linac

- Length: 300 m (39 sections)
- 3.5 GeV
- 2 transfer points

Status: In operation



The 1.5 GeV ring



The 1.5 GeV ring

- Circumference: 96 m
- Ring lattice: double bend achromat (DBA)
- Stored current: 500 mA
- Straight sections: 12(3.5m)
- Emittance (hor): 6 nmrad

Status: Commissioning

The 3.0 GeV ring

The 3.0 GeV ring

- Circumference: 528 m
- Ring lattice: 7 bend achromat (MBA)
- Stored current: 500 mA
- Straight sections: 20(5m)
- Emittance (hor): 0.2-0.3 nmrad

Status: In operation

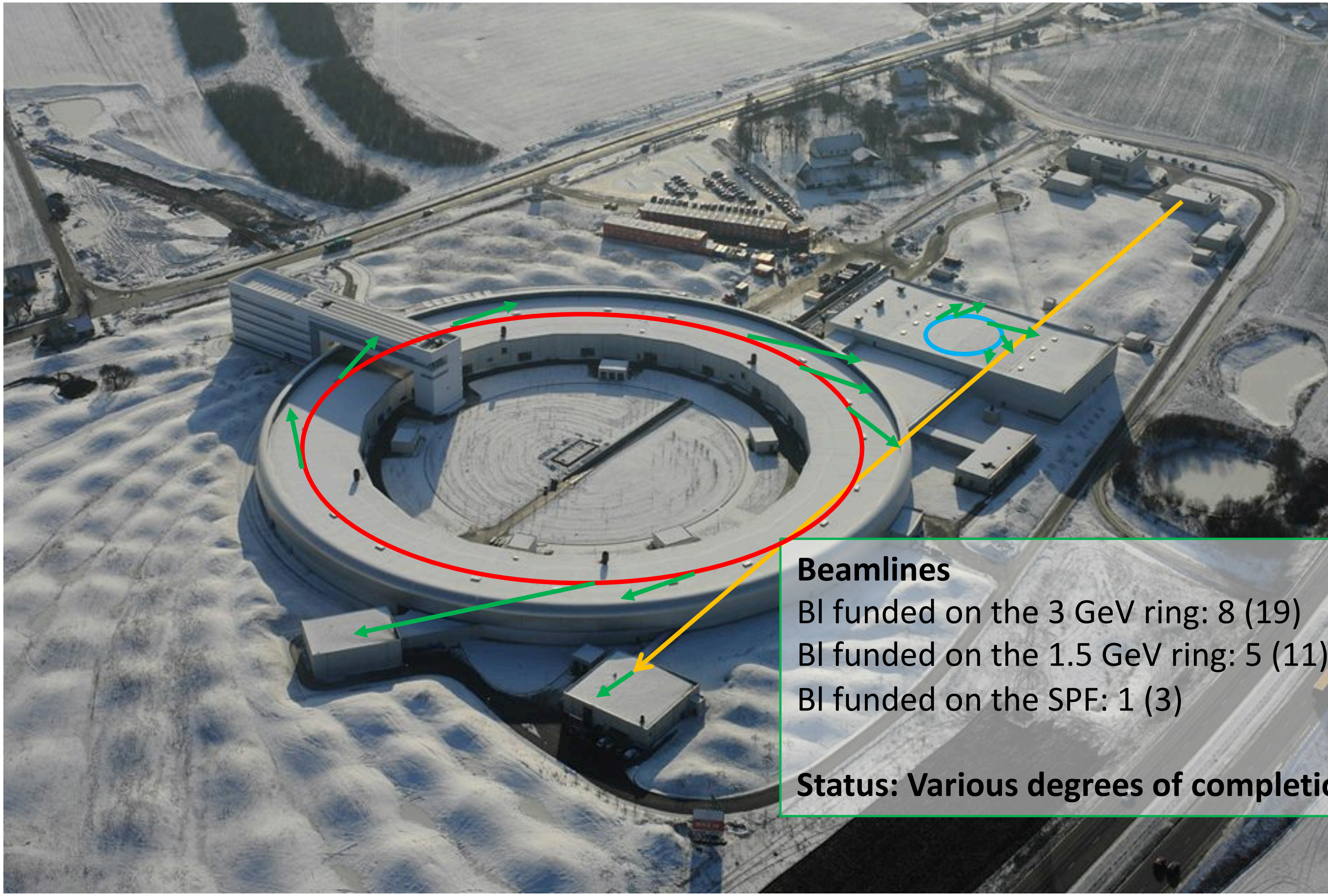
The SPF

The Short Pulse Facility
- Pulses > ≈ 100 fs
- Repetition rate: 100 Hz

FemtoMAX beamline
- Energy range: 1.8 – 20 keV
- Photons/ pulse: 10^7

Status: Commissioning

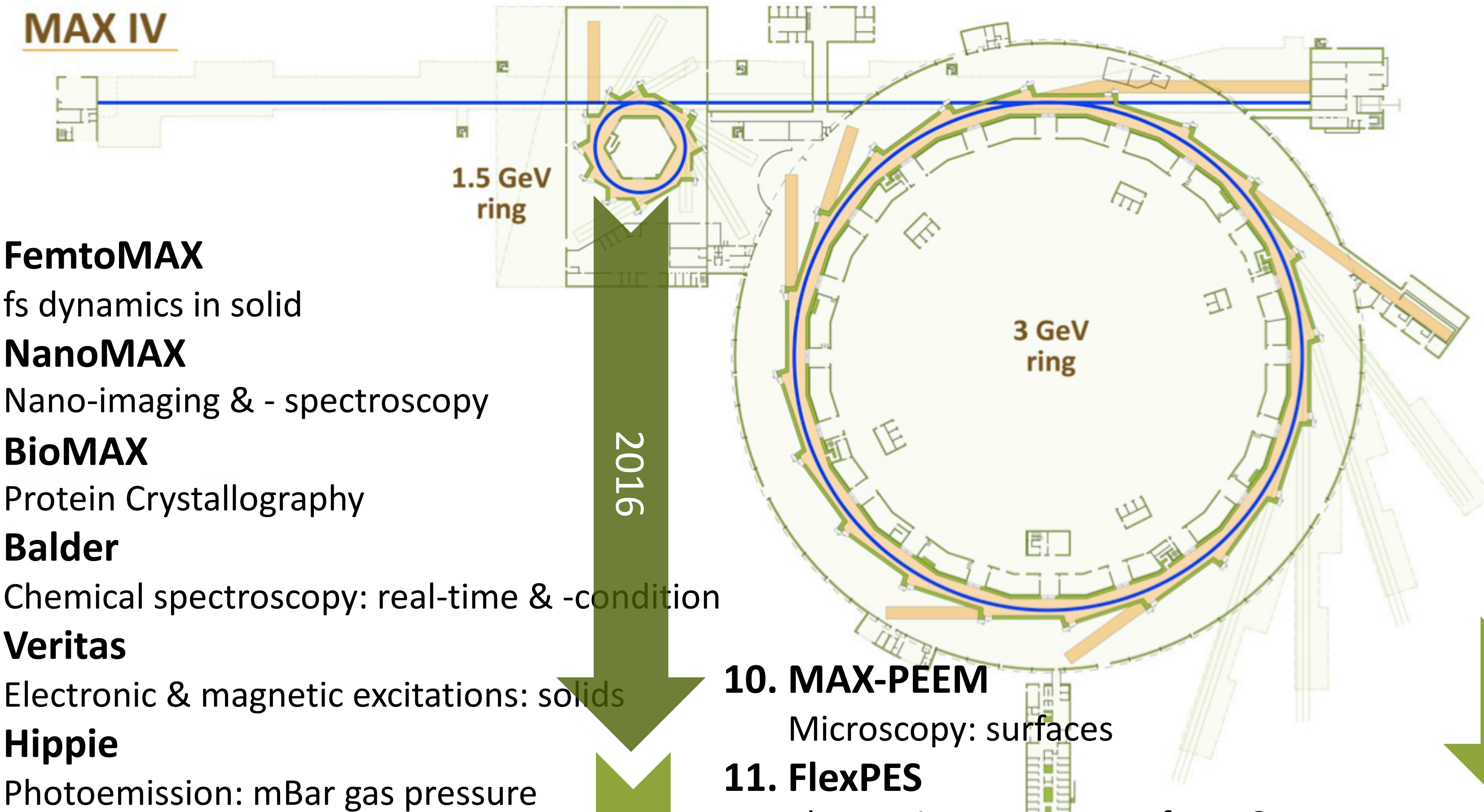
Beamlines



Beamlines
Bl funded on the 3 GeV ring: 8 (19)
Bl funded on the 1.5 GeV ring: 5 (11)
Bl funded on the SPF: 1 (3)

Status: Various degrees of completion

Beamlines



1. **FemtoMAX**
   fs dynamics in solid
2. **NanoMAX**
   Nano-imaging & - spectroscopy
3. **BioMAX**
   Protein Crystallography
4. **Balder**
   Chemical spectroscopy: real-time & -condition
5. **Veritas**
   Electronic & magnetic excitations: solids
6. **Hippie**
   Photoemission: mBar gas pressure
7. **ARPES**
   Electronic structure: solids
8. **FinEstBeaMS**
   Electronic structure: gases, aerosols
9. **SPECIES**
   Electronic & magnetic excitations: surfaces
10. **MAX-PEEM**
    Microscopy: surfaces
11. **FlexPES**
    Electronic structure: surfaces & gases
12. **CoSAXS**
    Geometric structure & correlation: (bio) liquids
13. **Soft*i*MAX**
    Microscopy & method development
14. **DanMAX**
    Powder diffraction & imaging: materials science

Description of the soft X-ray beamlines

- VERITAS, 3.0 GeV ring
  - Very high resolution RIXS spectroscopy
  - 275-1600 eV
  - R=50 000, 500 eV, $1x10^{12}$ ph/s
  - Small spot, always, <2x10 μm^2
- HIPPIE, 3.0 GeV ring
  - High pressure XPS
  - 263 – 1500 eV
  - R = 40 000, 400eV
  - Medium size spot, 50x30 μm^2

Description of the soft X-ray beamlines

- SoftiMAX, 3.0 GeV ring
  - STXM and CXI
  - 275-2500 eV
  - R ≈ 5000
  - Spot ca. 20-30 nm at STXM branch and ca. 20 x 20 μm^2 at CXI branch

Description of the soft X-ray beamlines

- ARPES, 1.5 GeV ring
  - Very high resolution ARPES
  - 10-200 (1000) eV
  - R < 1 meV up to 100 eV
  - Medium size spot <25x25(40) μm^2
  - High degree of circular polarization and high spectral purity
- FINESTBEAMS, 1.5 GeV ring
  - spectroscopy of solids, liquids and gases, luminescence
  - 4-1000eV (1500eV)
  - R = 5 000 – 10 000
  - Medium size spot <100x100 μm^2

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Description of the soft X-ray beamlines

- SPECIES, 1.5 GeV ring
  - RIXS and AP-XPS
  - 27-1500 eV
  - R ≈ 10 000
  - Spot at RIXS < 5 x 20μm^2
  - Spot at AP-XPS 60 x 100 μm^2
  - Prototype for MAX IV beamlines
  - Complementary, low energy beamline for HIPPIE

Description of the soft X-ray beamlines

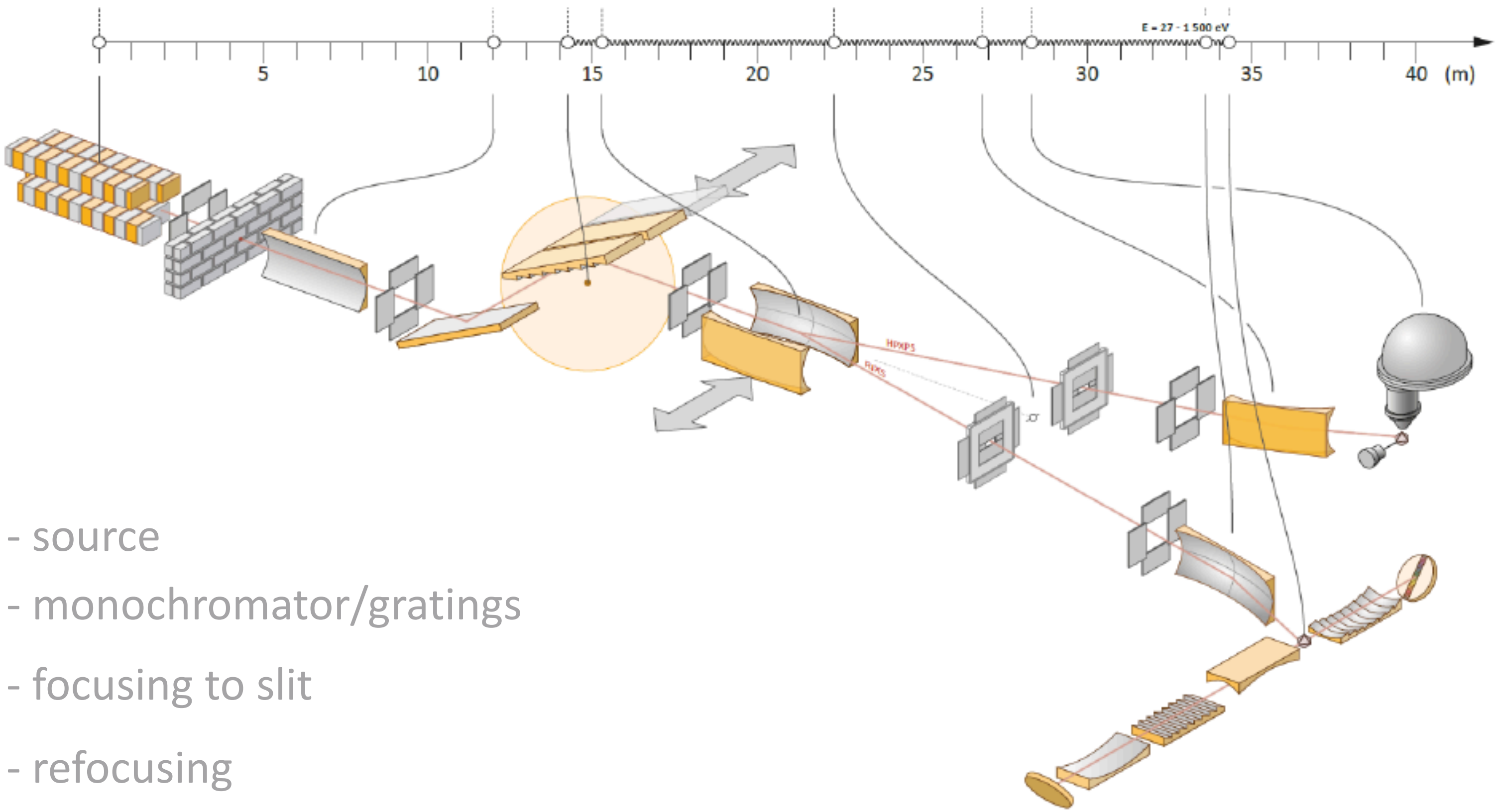
- INSERTION DEVICES
  - 3.0 GeV ring: ca. 3.75m long EPUs
  - 1.5 GeV ring: ca. 2.5m long EPUs

- Other specifications
  - 3.0 GeV ring: ca. 50m beamlines
  - 1.5 GeV ring: ca. 30…40m beamlines
  - Horizontal beam at sample(!)
  - Experiment at reasonable height (!)
  - High flux, low flux, high resolution, low resolution, medium spot which can be reduced, or in some cases expanded

Design of the soft X-ray beamlines

- Collecting input from the user communities; convergence to final parameters
- Comparison of various designs – aim in finding local optimum
- Extensive modeling corresponding to final design
  - Reliable estimate of performance
  - Tolerances defined for optical elements
  - Stability/vibrations included for checking the effect

Design of the soft X-ray beamlines



- source
- monochromator/gratings
- focusing to slit
- refocusing

Design of the soft X-ray beamlines

Practically all VUV - soft X-ray monochromators at MAX-lab were based on plane gratings

- Experience on working with them
- Blazed plane gratings available for reuse
- Flexible and yet easy to use

Plane grating monochromator illuminated with collimated light chosen in the end for all present soft X-ray beamlines.

Design of the soft X-ray beamlines

Having also the horizontal focus at the exit slit plane increases achievable resolving power.

- Focusing with first mirror results in highest resolving power but lowest demagnification
- Focusing horizontally (and vertically) with the focusing mirror increases demagnification
- Having a collimation-focusing pair by first mirror and focusing mirror gives a bit of both advantages

- Stigmatic focus at exit slit allows using ellipsoidal refocusing mirrors

Design of the soft X-ray beamlines

Single refocusing mirror, ellipsoidal or toroidal used for all except coherent scattering beamline

- Single reflection, less losses
- Easy to keep beam horizontal at experiment
- Sagittal focusing in vertical direction
- Aberrations (low)

- Rotation around the normal of a toroidal mirror (yaw) allows to enlarge the beam
- Beam position can be changed along horizon (pitch) and perpendicular to it (roll)

Design of the soft X-ray beamlines

Astigmatic focus for refocusing toroidal mirror allows to change its source size (exit slit opening) without affecting the image size which is now dictated by the beam divergence.

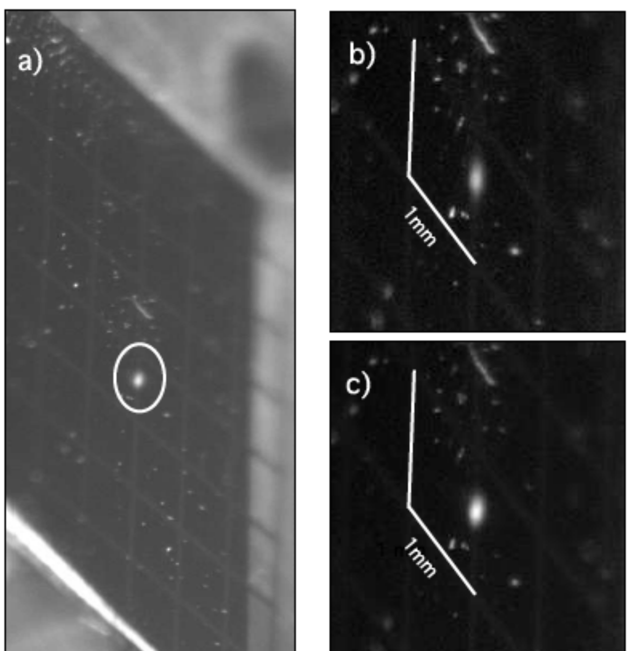


Figure 6
Spot at the APXPS end station sample position captured at a photon energy of 250 eV. The panel a) shows the Ce:YAG crystal mounted with adhesive carbon tape on a sample holder of the APXPS system. The beam spot is circled. Panels b) and c) show the beam spot at the photon energy of 250 eV and c_{ff}=2.25 for exit slit openings of 500 µm and 50 µm, respectively. The intensity of the photon beam was attenuated by a 200 nm thick Al window for recording the spot size with the larger slit opening in order to keep the saturation of the YAG crystal at minimum and be able to compare the spot sizes. The white lines in panels b) and c) show the dimensions of the image (1 mm).

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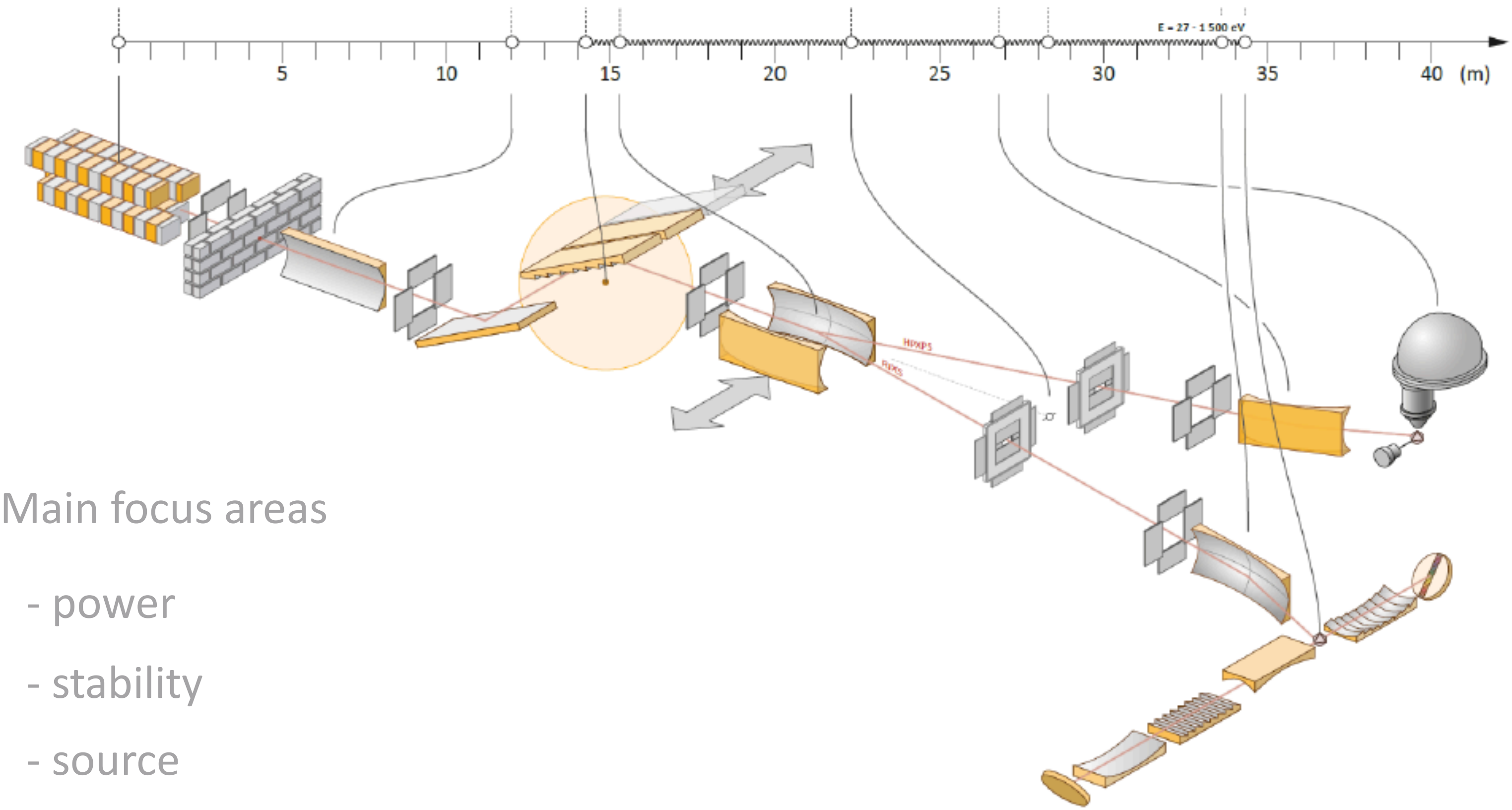
Design of the soft X-ray beamlines



Main focus areas

- power
- stability
- source
- coherence

Power from a soft X-ray undulator

Elliptically polarizing undulator at 3.0 GeV ring:

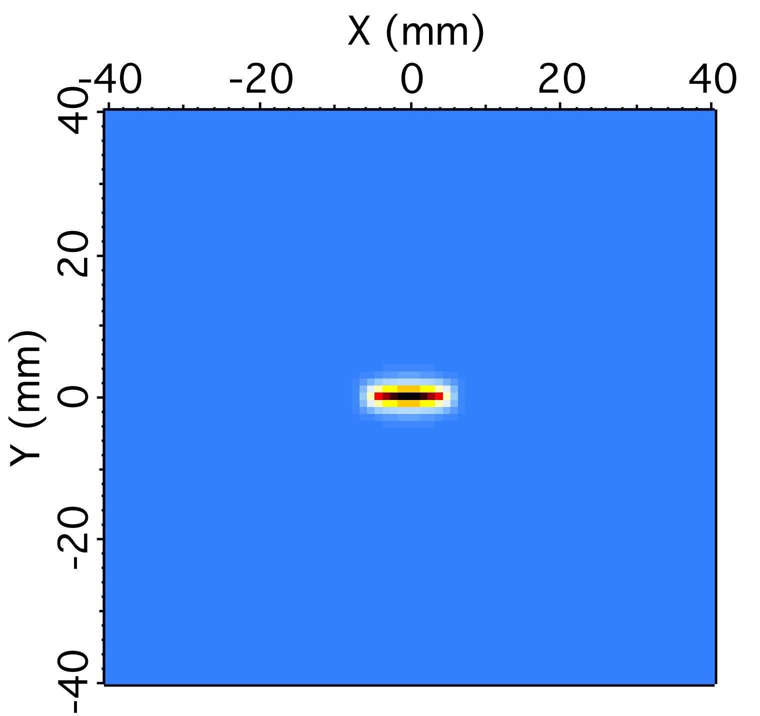
- EPU48
  - 48 mm period length, 81 periods, L = 3905.5 mm
  - K_{max} = 4.506, limited to K = 3.30 (6.2 kW)
  - 275 – 1500 (1^{st} harmonic)

Elliptically polarizing undulator at 1.5 GeV ring:

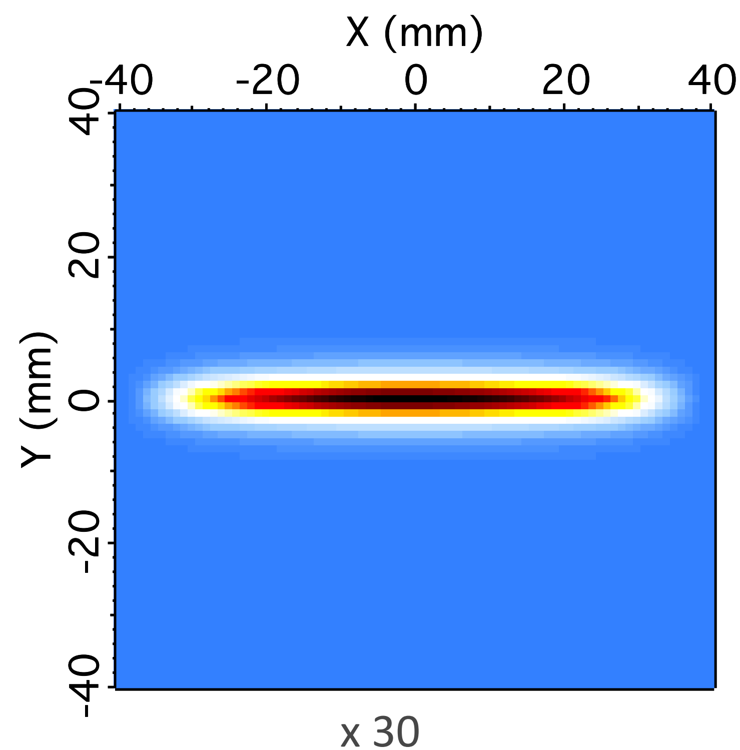
- EPU95p2
  - 95.2 mm period length, 25 periods, L = 2380 mm
  - K_{max} = 10.065 (2.6 kW)
  - 4 – 1000
  - Experiments up to 1486.295 eV (Al Kα)

Power from a soft X-ray undulator

EPU48



EPU95.2



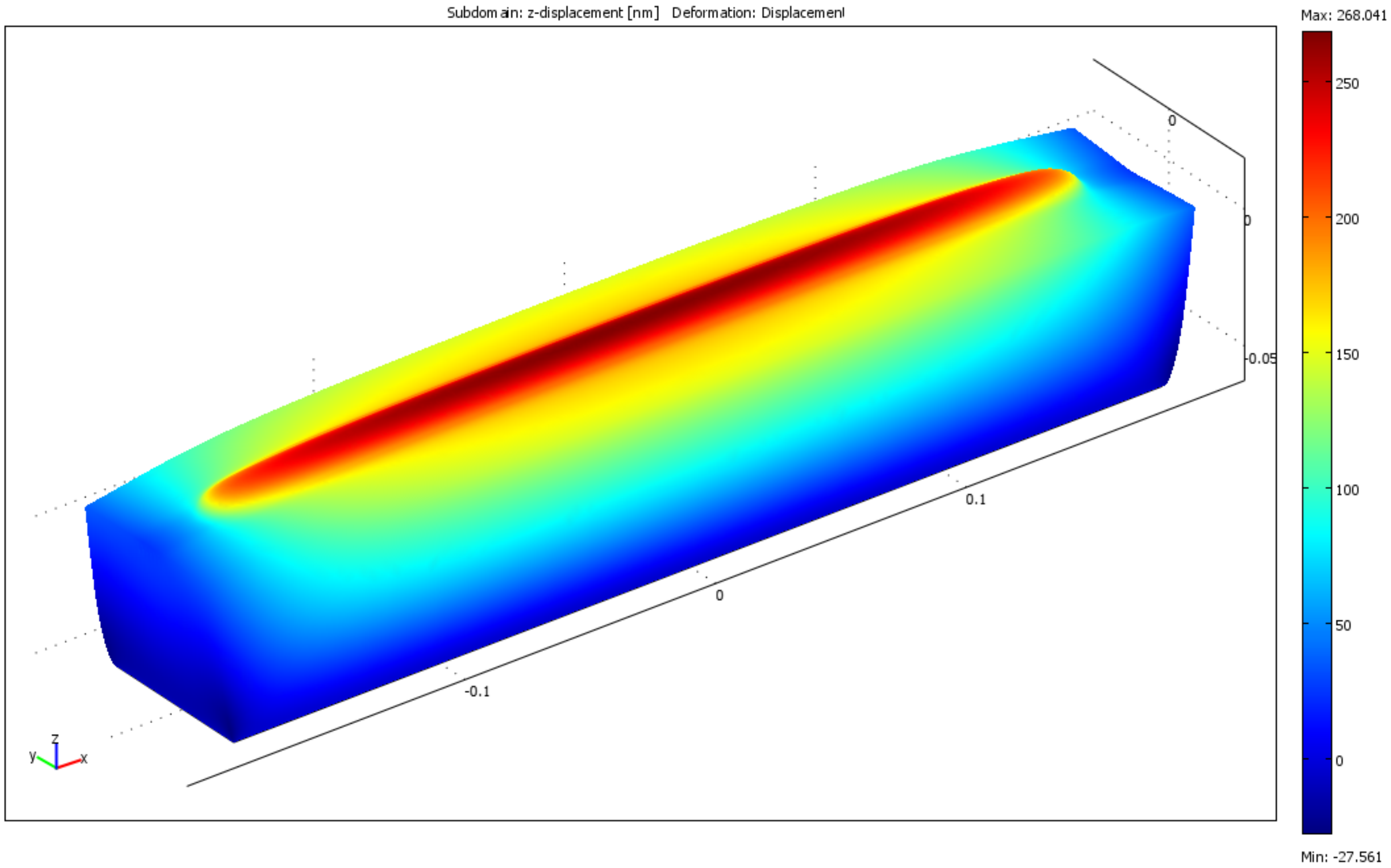
Max. power density at 10m: 26.6W/mm^2

Max. power density at 10m: 0.9W/mm^2

Calculations with SPECTRA v10.

Power from a soft X-ray undulator

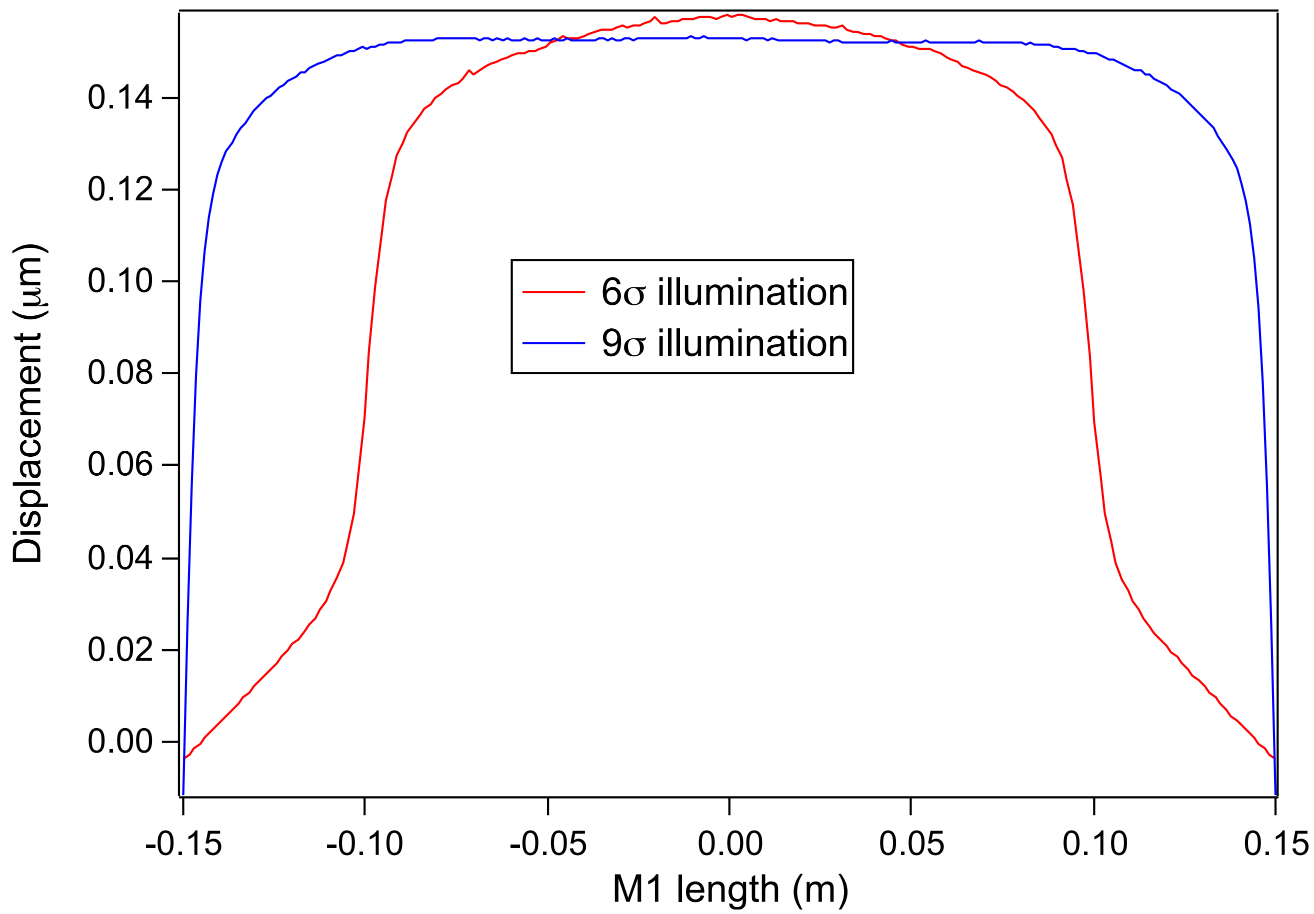
Heat load induced structural changes, M1



Calculations with COMSOL, v3.5, www.comsol.com

Power from a soft X-ray undulator

Heat load induced structural changes, aperture effect



Power from a soft X-ray undulator

Heat bump profiles can be inserted into ray tracing

- SHADOW[1], RAY[2], RAY-UI[3], XRT[4],…
- Most heat bumps can be regarded as additional convex mirrors, radius defines imaging effect
- Dense mesh or interpolating important
- Looping automatized finite element analysis into ray tracing possible, and with present computers that is also feasible

POSTERS:
RAY-UI/Peter Baumgärtel/HZB
MASH/Peter Sondhaus/MAX IV

[1]M. Sanchez del Rio, N. Canestrari, F. Jiang
http://www.esrf.eu/Instrumentation/softw

[2] F. Schäfers in: Modern Developments in X

[3]https://www.helmholtz-berlin.de/forschu

[4]K. Klementiev and R. Chernikov, Proc. SPIE 9209, 92090A (2014); http://pythonhosted.org/xrt/

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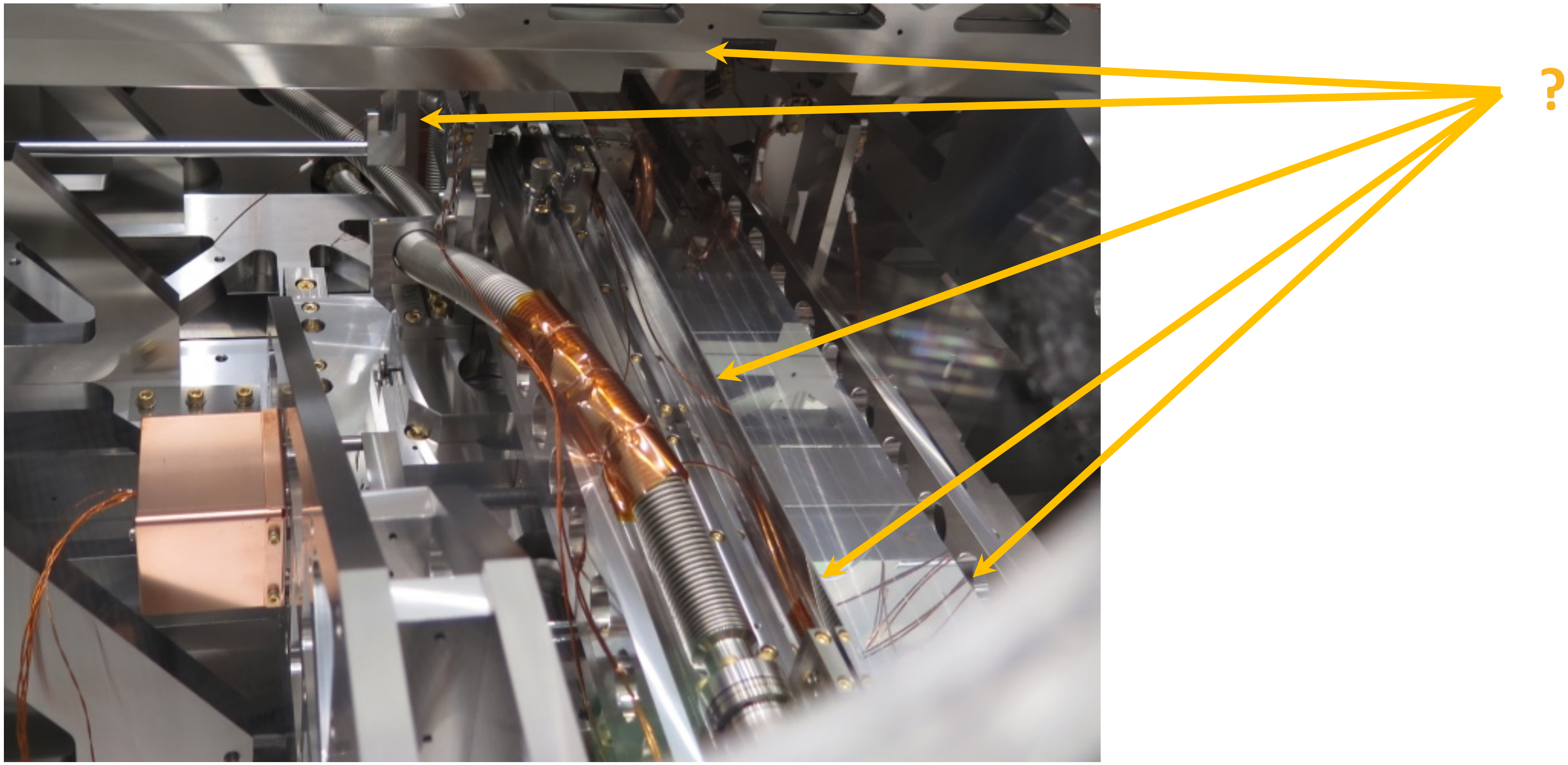
Stability

The cooling solution presented earlier relies on turbulent flow in the narrow cooling channels under surface of the mirror.

Total water flow will be several liters per minute → large diameter feeding line needed, with practical sizes the flow will not be laminar there either.

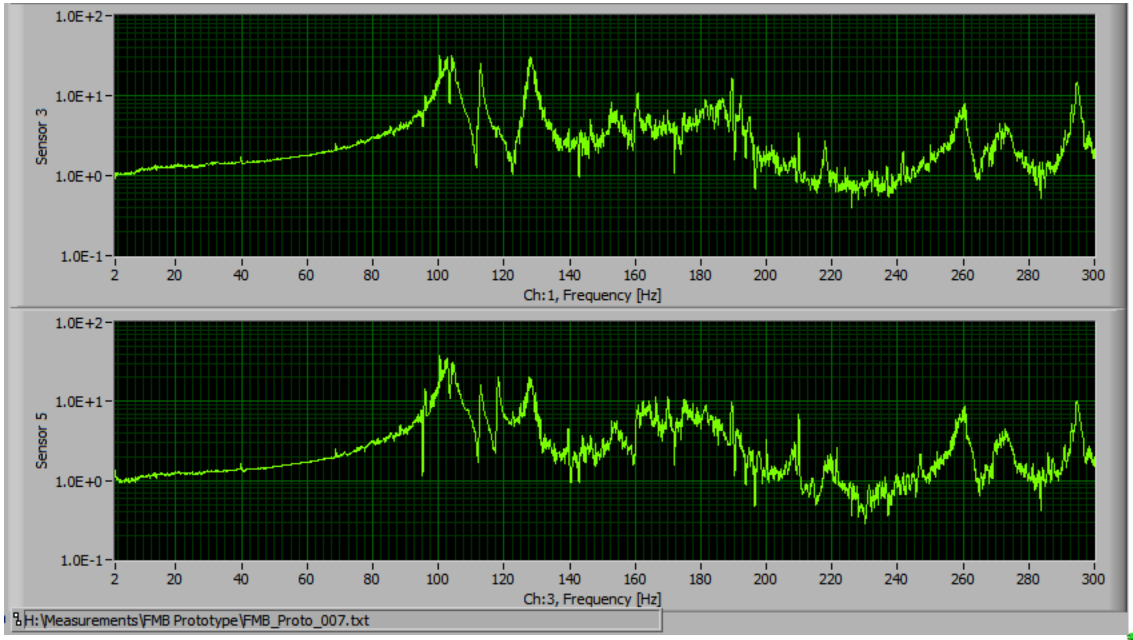
Turbulence induced vibrations by the cooling channels and lines is one of the future for the stability group.

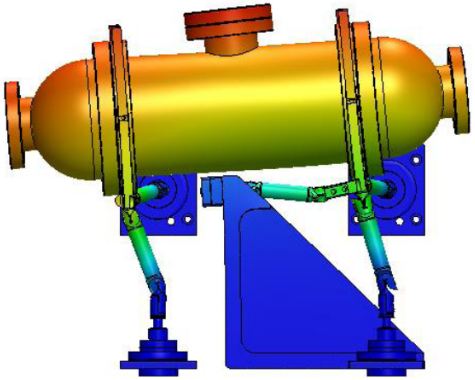
Stability

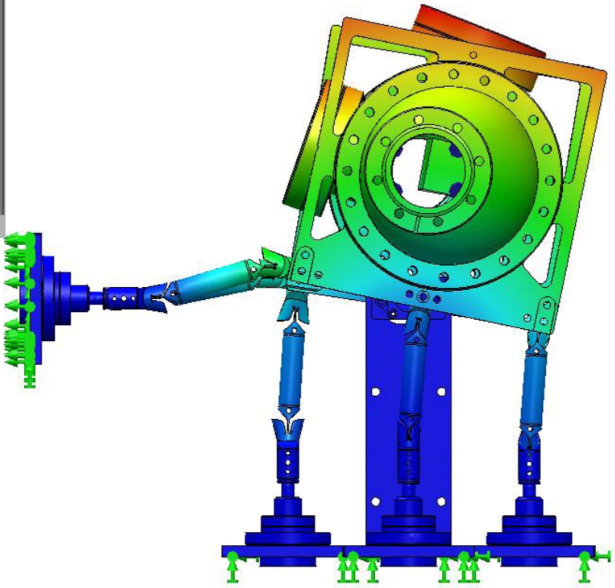


"For estimating vibrations, the transition points from laminar to turbulent flow needs to be known – measurements needed to fix those points."

Stability

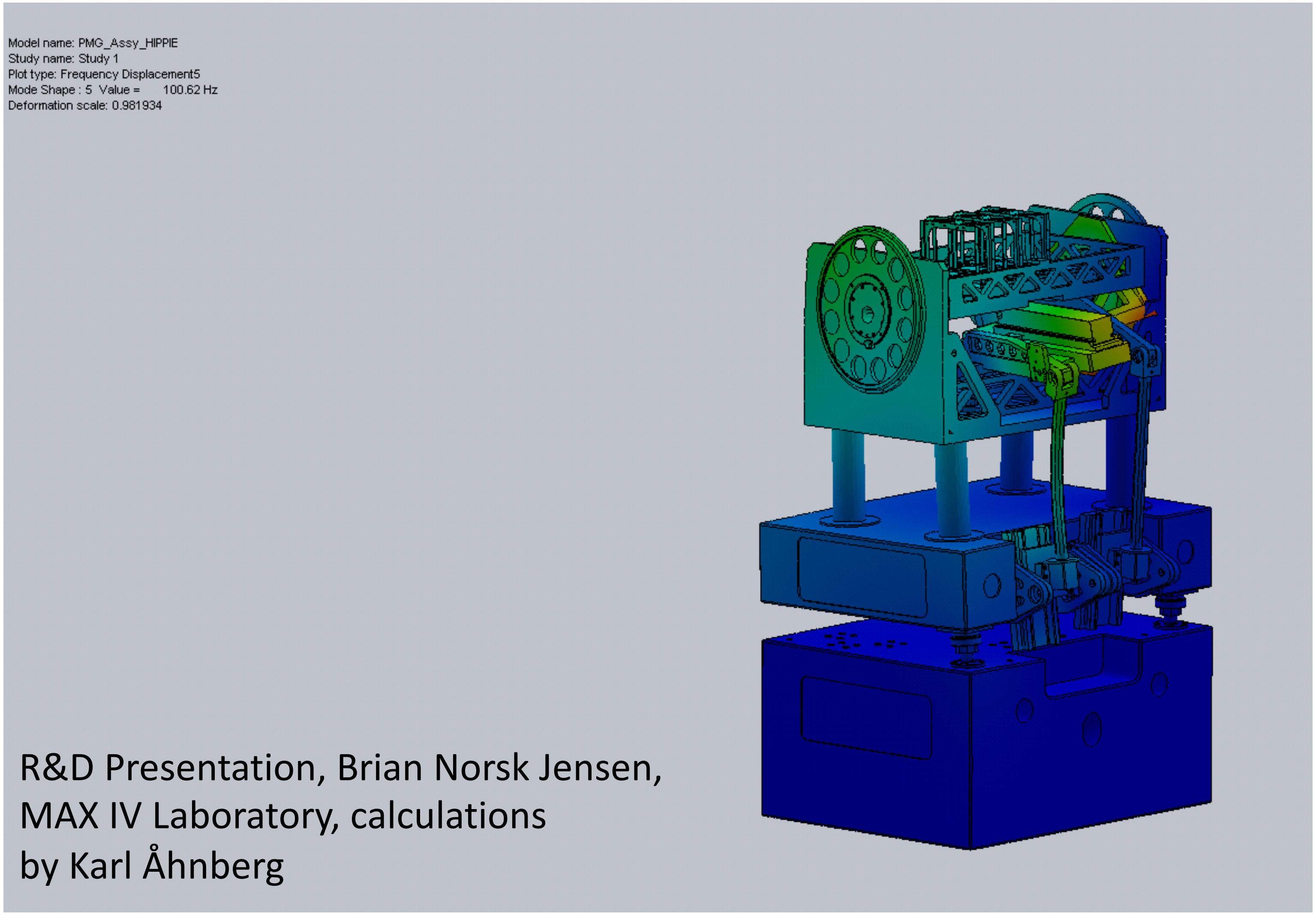






R&D Presentation, Brian Norsk Jensen,
MAX IV Laboratory, calculations
by Karl Åhnberg

Stability



R&D Presentation, Brian Norsk Jensen, MAX IV Laboratory, calculations by Karl Åhnberg

The source

Gaussian approximation is widely used in describing the undulator light source. However, precise calculations* predict clear deviation from it, resulting in

$$\sigma' = \sqrt{\frac{\lambda}{2L}} \; and \; \sigma = \frac{\sqrt{2\lambda L}}{2\pi}$$

i.e source size is about twice as large as the one given by Gaussian approximation. With low emittance storage rings this starts to dominate the source size and divergence.

Another question comes with using the undulator as wiggler for high photon energies.

*P. Elleaume in: Undulators, wigglers and their applications, eds. H. Onuki and P. Elleaume, Taylor& Francis, 69-108 (2003).

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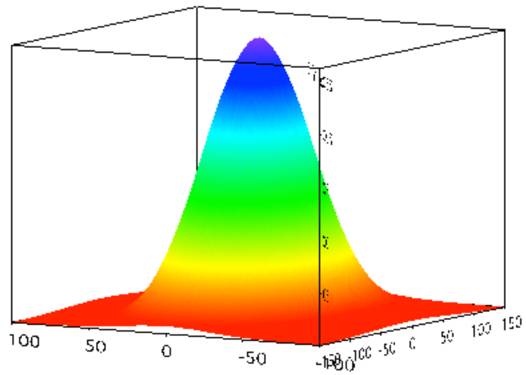
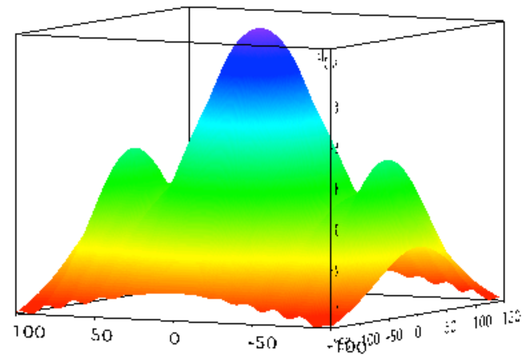
The source

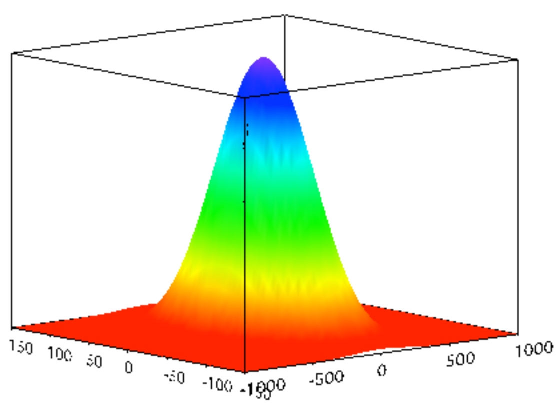
EPU48 on axis



EPU48 1/N detuning



EPU95.2 closed gap, 1000eV



These calculations with SPECTRA v10, SRW also used for these.

The source

For ray tracing the source characteristics were modeled in SPECTRA[1] and SRW[2] – those values were used as input parameters in e.g. RAY.

At present, the ray tracing/wave propagation program XRT is used. It includes also near field calculations for undulators, and can use electron trajectories calculated with RADIA[3]

[1]T. Tanaka and H. Kitamura, J. Synchrotron Rad. 8, 1221 (2001).
[2]O. Chubar and P. Elleaume, Proc. EPAC-98, 1177 (1998).
[3]O. Chubar, P. Elleaume, and J. Chavanne, J. Synchrotron Rad.,5, 481 (1998).

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Partial coherence

Low emittance synchrotrons provide light with high degree of transverse coherence, some tens of percent at few hundred eV

$$B_{\mathrm{avg}}(\lambda) = \frac{N_{\mathrm{ph}}(\lambda)/\mathrm{s}/\%\mathrm{BW}}{(2\pi)^2 \cdot (\varepsilon_r(\lambda) \oplus \varepsilon_x(\mathrm{e}-)) \cdot (\varepsilon_r(\lambda) \oplus \varepsilon_y(\mathrm{e}^-))} \qquad \mathcal{D}_{photon} = \frac{\mathcal{B}\lambda^3}{4c}$$

For applications utilizing coherence, like coherent X-ray imaging, preserving and refining coherence for the experiment is crucial – this applies also to diffraction limited imaging with zone plates

Partial coherence

Chose to be made between two philosophies: using secondary source, or undisturbed expansion until final, acceptance limited, refocusing mirror?

Looking at properties at focus (and around)

- Size, divergence, flux
- Coherence length
- Degree of coherence
- flexibility

Partial coherence

- where to put FZP?
- what is the result if finite beam emittance?
- what are the coherence properties?
- how to isolate the coherent part?

M1	cylindrical	vertical collimation
M2	plane	deflecting
M3-STXM	toroidal (STXM)	hor and vert focusing
M3-CXI	cylindrical (CXI)	vert focusing
M4	plane elliptical	hor refocusing
M5	plane elliptical	vert refocusing
cPGM	collimated plane grating monochromator	
PG	plane grating	
ES	exit slits	
ZP	zone plate	

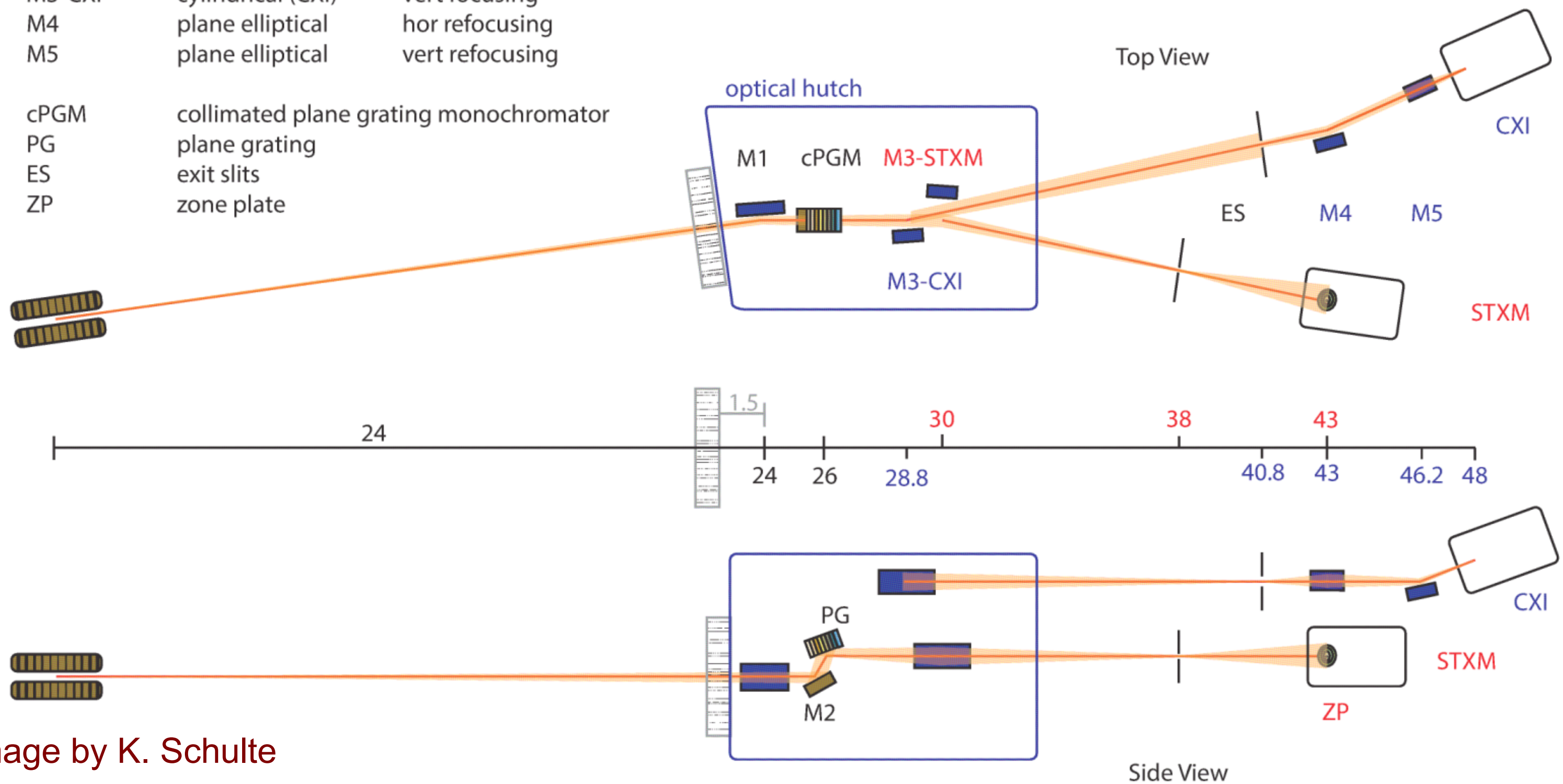
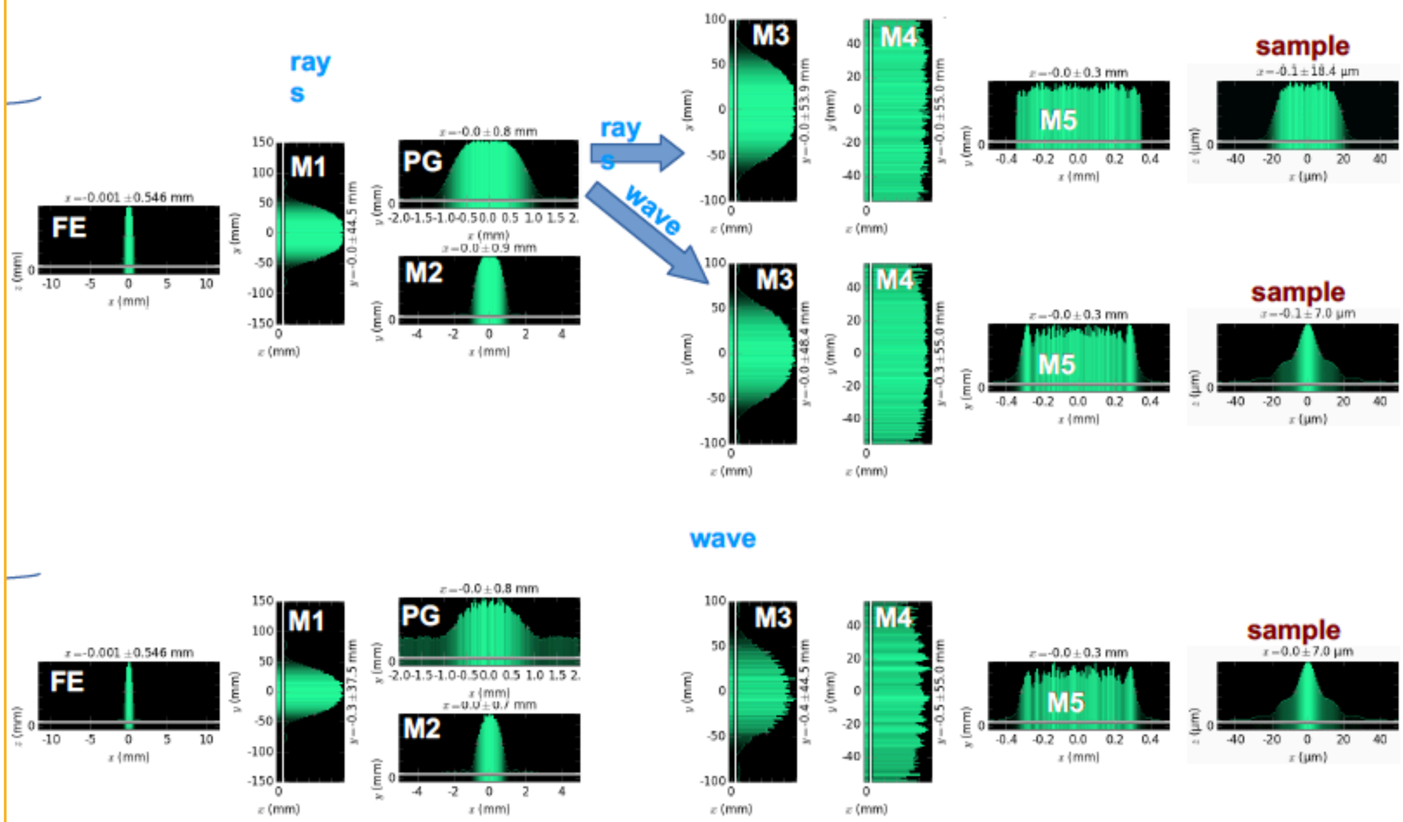


image by K. Schulte

Partial coherence

SoftiMAX/CXI: rays, waves and hybrid (rays+waves)



Partial coherence

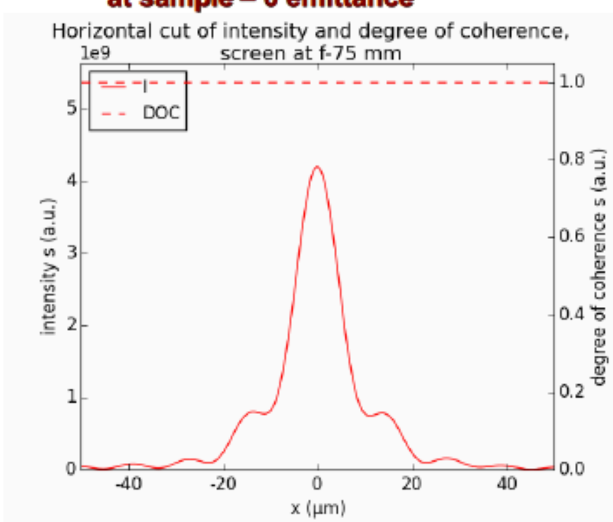
Degree of coherence

$$j(x,y,x',y') = \frac{\langle E^*(x,y)E(x',y')\rangle}{\langle I^*(x,y)I(x',y')\rangle^{1/2}}$$ – complex DOC

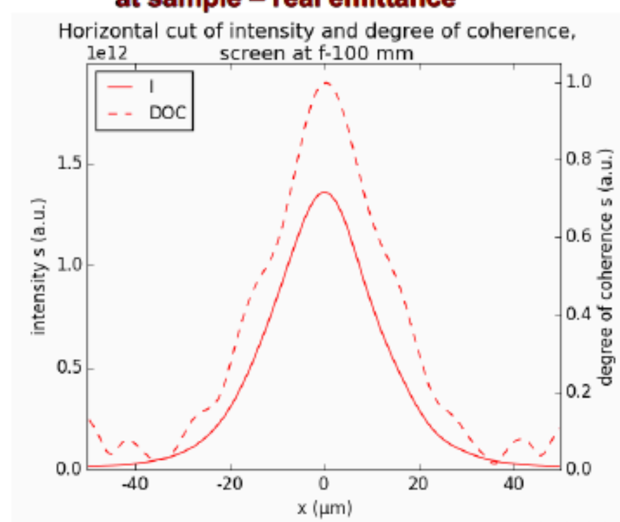
$$0 \leq |j(x,y,x',y')| \leq 1$$

- relative to the center: $j_0(x,y,0,0)$
- horizontal or vertical cuts: $j_x(x,Y,x',Y)$ or $j_y(X,y,X,y')$

at sample – 0 emittance



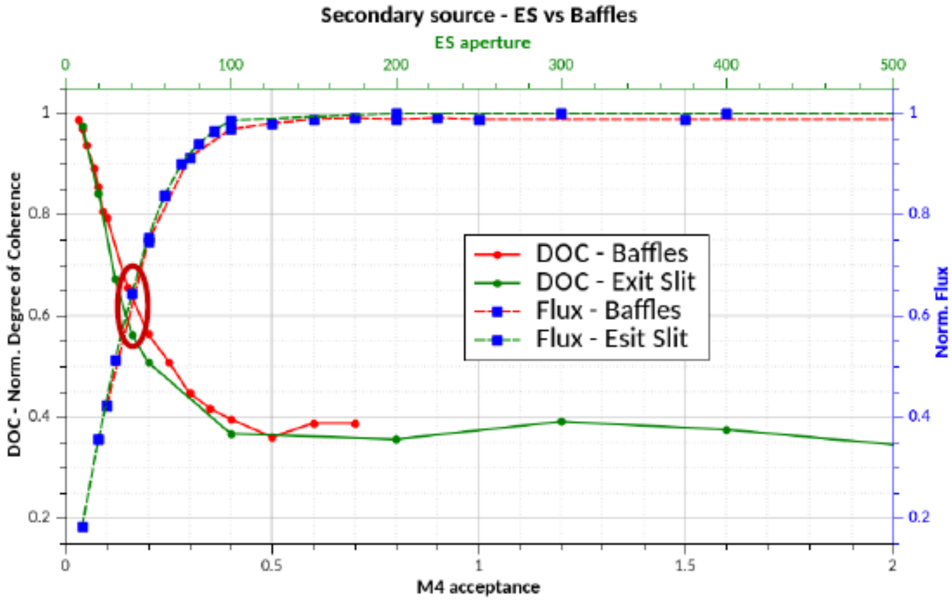
at sample – real emittance



Partial coherence

Results

→ Secondary Source: Baffles vs Exit Slit

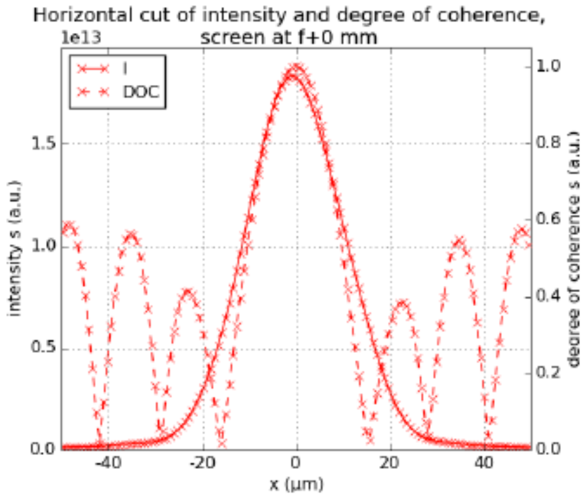


Partial coherence

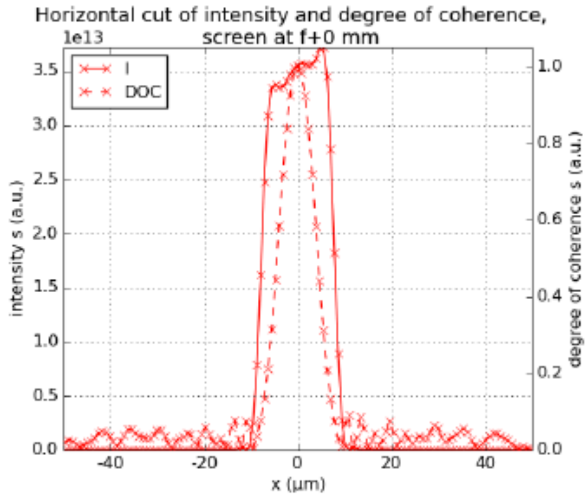
Results

- Secondary Source: Baffles vs Exit Slit

Baffles 0.15



ES 40µm



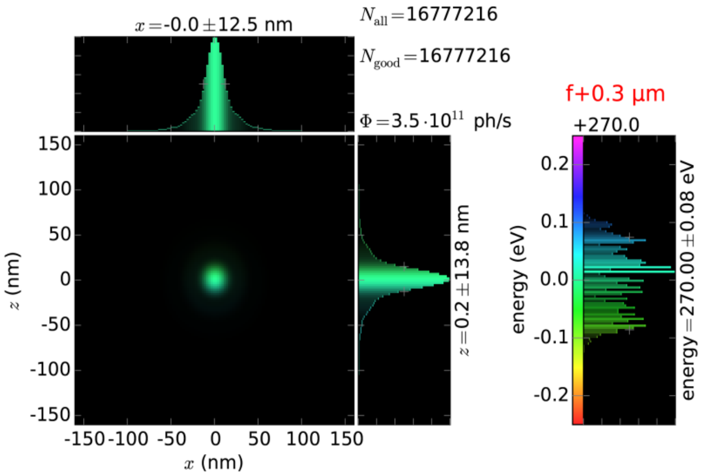
Partial coherence

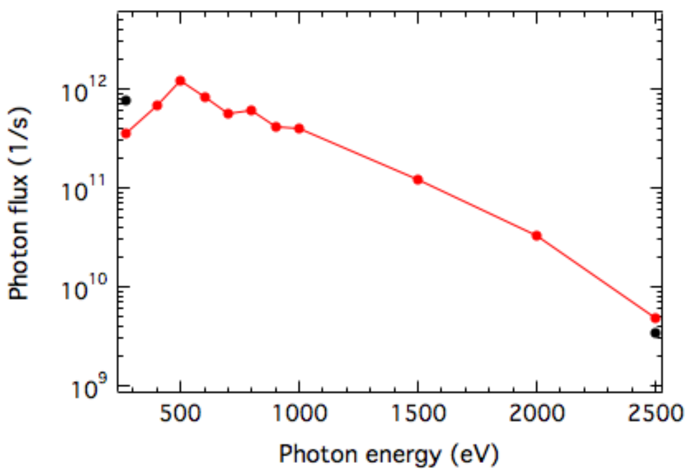
Results

- ➔ Secondary Source: Baffles vs Exit Slit:
  - ↳ Baffles:
    - Increase of DOC;
    - No change of spot size;
      - For very small apertures, beam increases due to diffraction;
    - Increase of Coh Length;
  - ↳ ES
    - Increase of DOC;
    - Change of spot size;
      - Ugly beam;
    - No change of Coh Length;

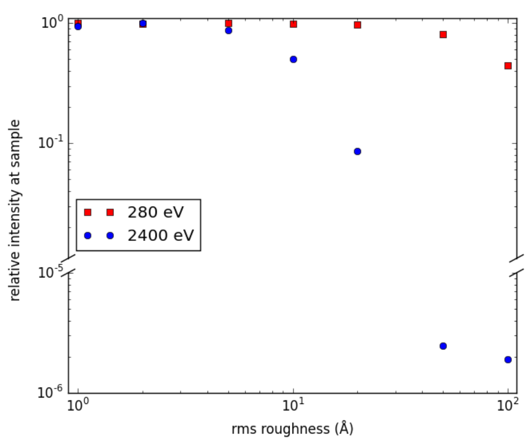
Partial coherence

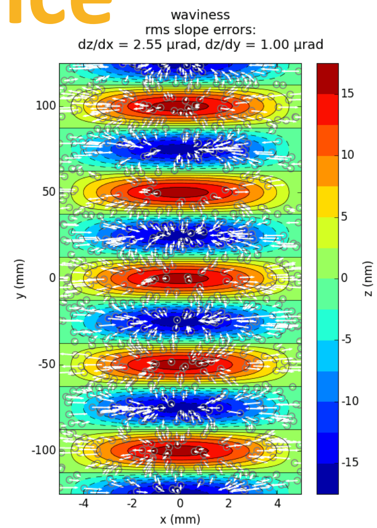
Performance estimation for the STXM branch; ray tracing until grating, wavefront propagation until sample

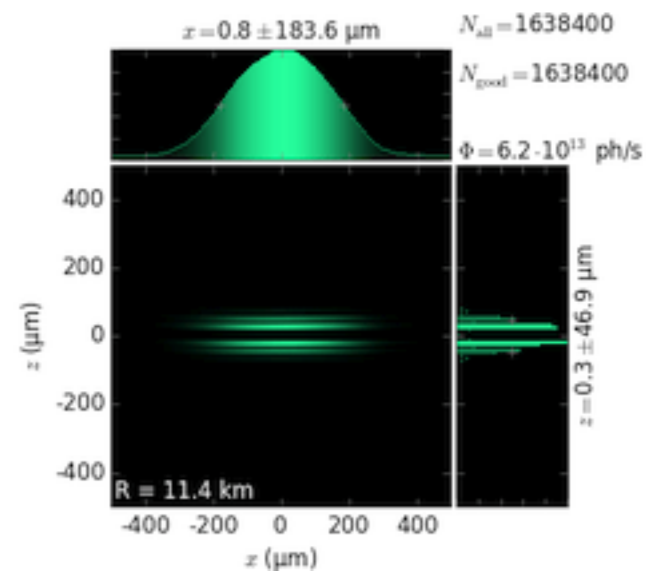


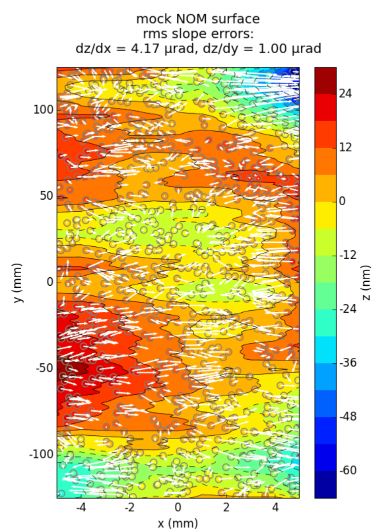


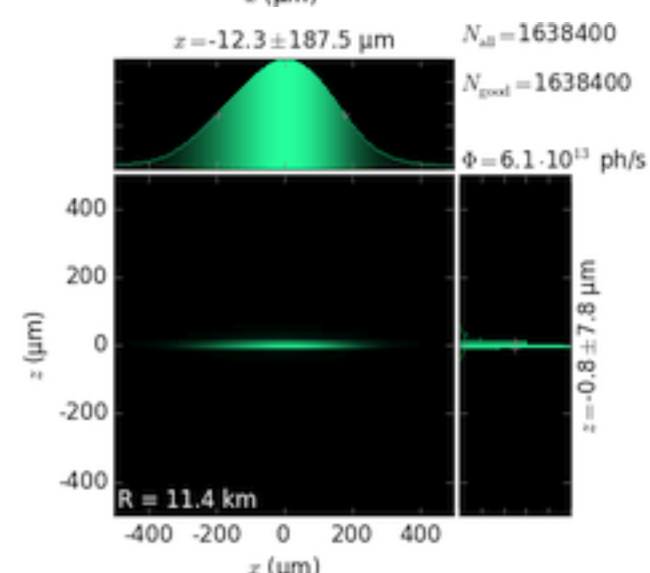
Partial coherence









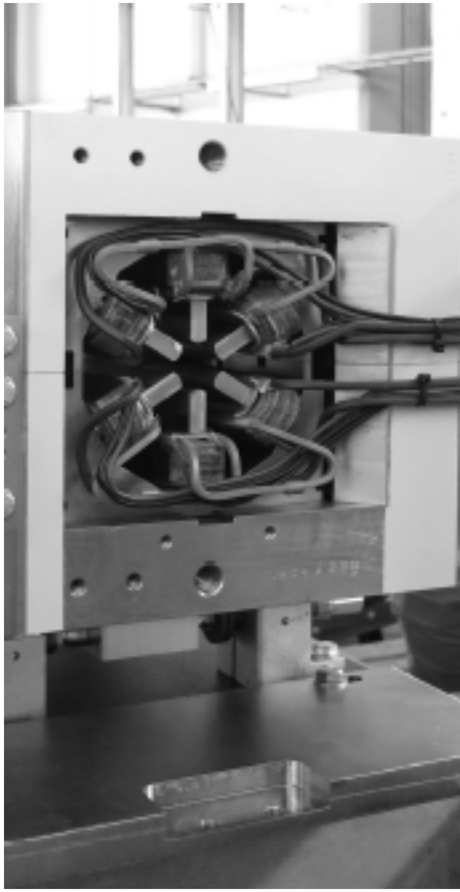


Final simulations, soft X-ray beamlines

- Include real optics into simulations when delivered
- Possible effect of shape outside tolerances
- Slope error maps instead of statistical slope error distributions (collaboration with HZB)
- Analysis of final performance
    - Real-time modelling assisted tuning within reach

Results and conclusions

- Classical ray tracing still the main tool for general design work
- Precise modeling of the source more important for low emittance rings
- Stability is vital part of transporting the beam – vibrations need to be included into simulation
- Partial coherence requires wavefront-based approach
- Tools need to be easy to use but most tools exist



Acknowledgements to colleagues at

ESRF

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PAUL SCHERRER INSTITUT PSI

SOLEIL SYNCHROTRON

Elettra Sincrotrone Trieste

BROOKHAVEN NATIONAL LABORATORY

SOLARIS NATIONAL SYNCHROTRON RADIATION CENTRE

DESY

ALBA

CERN

European XFEL

diamond

LCLS

Argonne NATIONAL LABORATORY

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