Imaging opportunities at 50-100 keV

Marco Stampanoni :: Head of SLS-TOMCAT
Other Science Opportunities @ FCCee – CERN, November 28th 2024

Medical... vs... synchrotron X-ray imaging

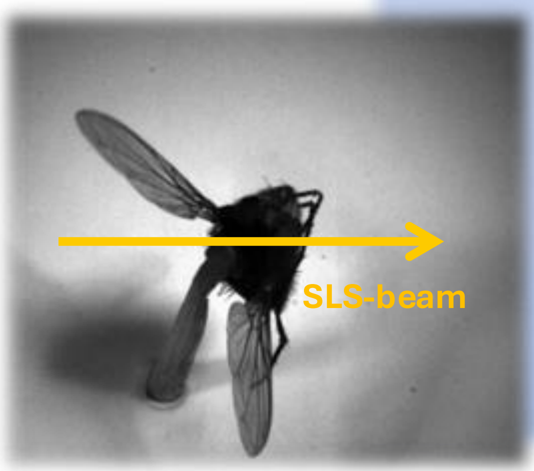
PSI

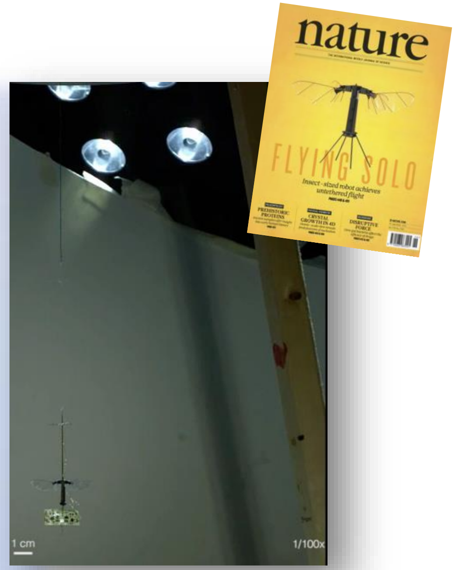
First X-ray (1896)

State-of-the-art X-ray imaging in hospitals

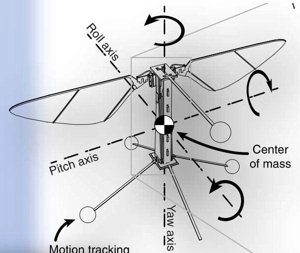
X-ray microradiography at SLS

Muscles and tracheal network *during* flight





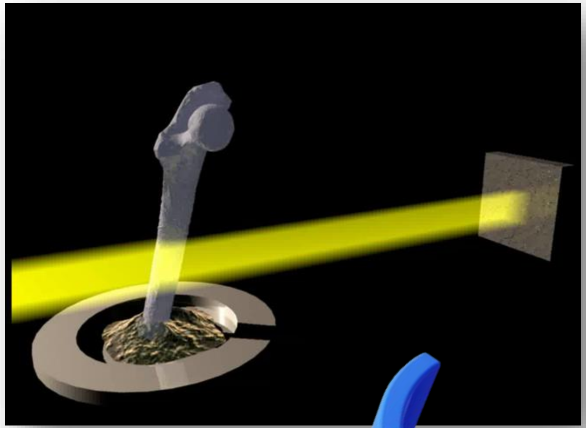
Jafferis et al., Nature 2019



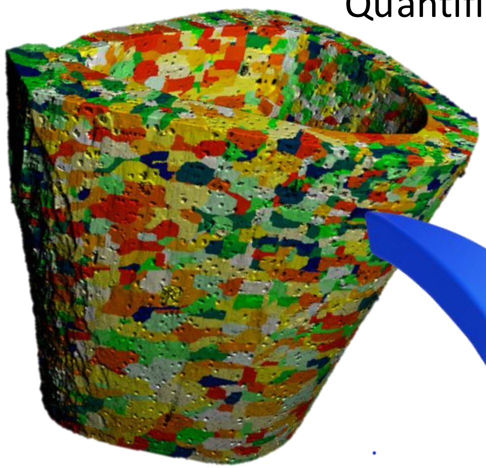
Walker et al., PloS Biology (2014) & Mokso et al., SciRep (2015)

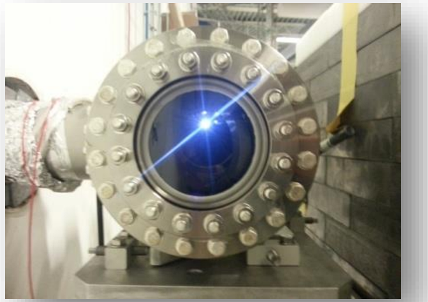
Computed tomography to gather 3D structural information from opaque samples

Measurement

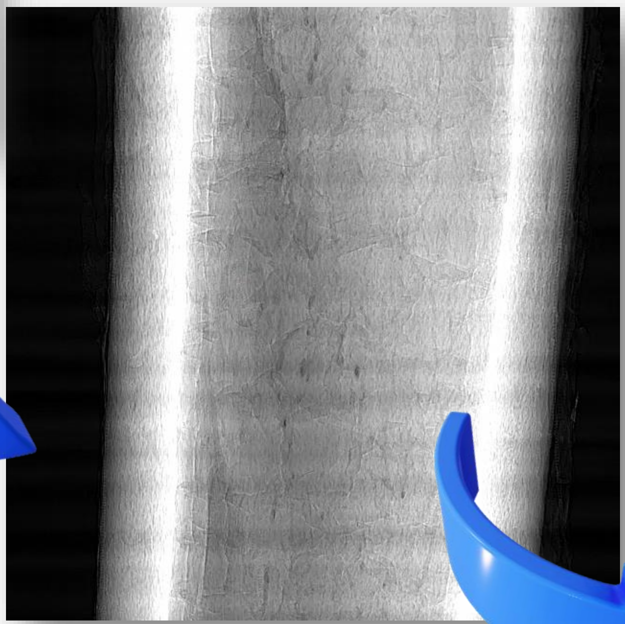


Quantification



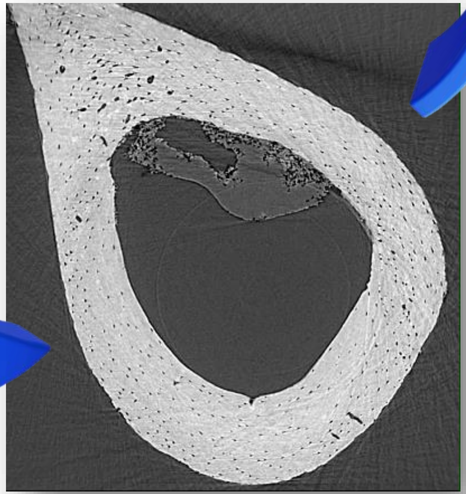


Bright beam from the synchrotron



Projections *[0,π]*

$$P = ln\frac{I_0}{I} = \int_0^d \mu(z)dz$$



Reconstructions

$$\mu(x,y) = \int_0^\pi \mathrm{d}\theta \int_{-\infty}^{+\infty} \tilde{P}(\omega,\theta)|\omega|e^{j2\pi\omega t}\mathrm{d}\omega$$

«Chasing the phase...»

PSI

General form of a wave in vacuum: $\psi_{vacuum}(\vec{r},t) = Ae^{i(\vec{k}\cdot\vec{r}-\omega t)}$

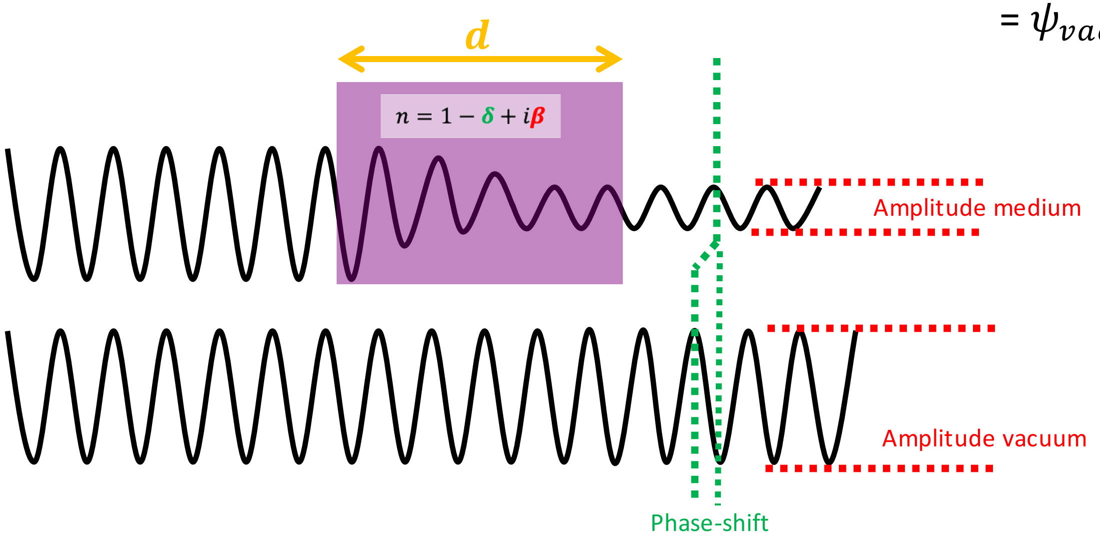
For a wave traveling in the z-direction: $\vec{k} = (0,0,k = \frac{2\pi}{\lambda})$

Plane wave propagating in z-direction: $\psi_{vacuum}(\vec{r},t) = Ae^{i(\vec{k}\cdot\vec{r}-\omega t)} = Ae^{i(kz-\omega t)}$

For a wave traveling in a medium: $n = 1 - \boldsymbol{\delta} + i\boldsymbol{\beta}$

Wave propagating in a medium: $\psi_{medium}(z,t) = Ae^{i(nkz-\omega t)} = Ae^{-i\omega t}e^{(1-\delta)ikz}e^{-\beta kz} =$

$$= \psi_{vacuum} \cdot \underbrace{e^{-i\delta kz}}_{\text{Phase-shift}} \cdot \underbrace{e^{-\beta kz}}_{\text{Attenuation}}$$



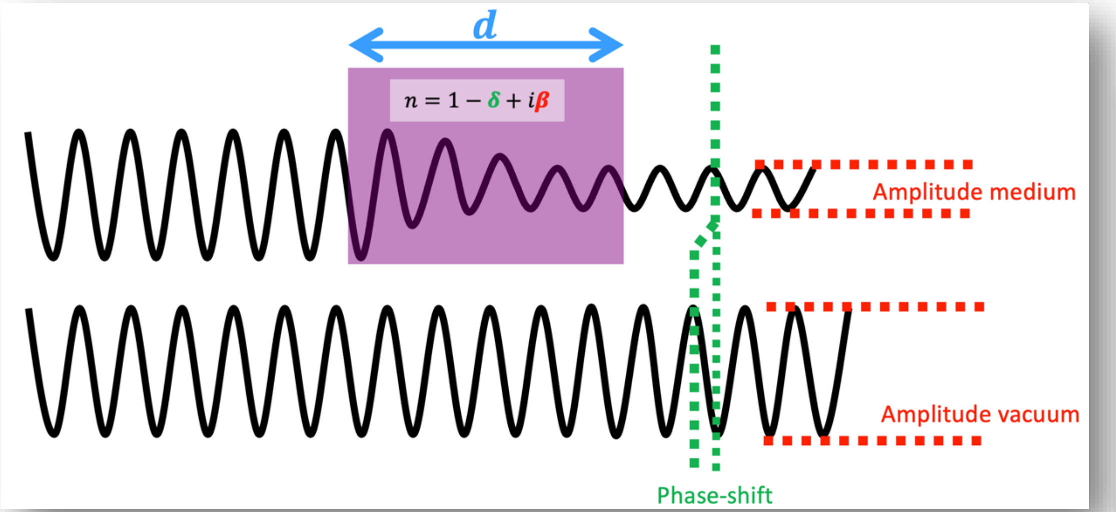
After medium of length d:

$$\boldsymbol{T(d)} = \frac{I_m(d)}{I_v(0)} = \frac{|\psi_m(d,t)|^2}{|\psi_v(0,t)|^2} = e^{-2k\beta d}$$

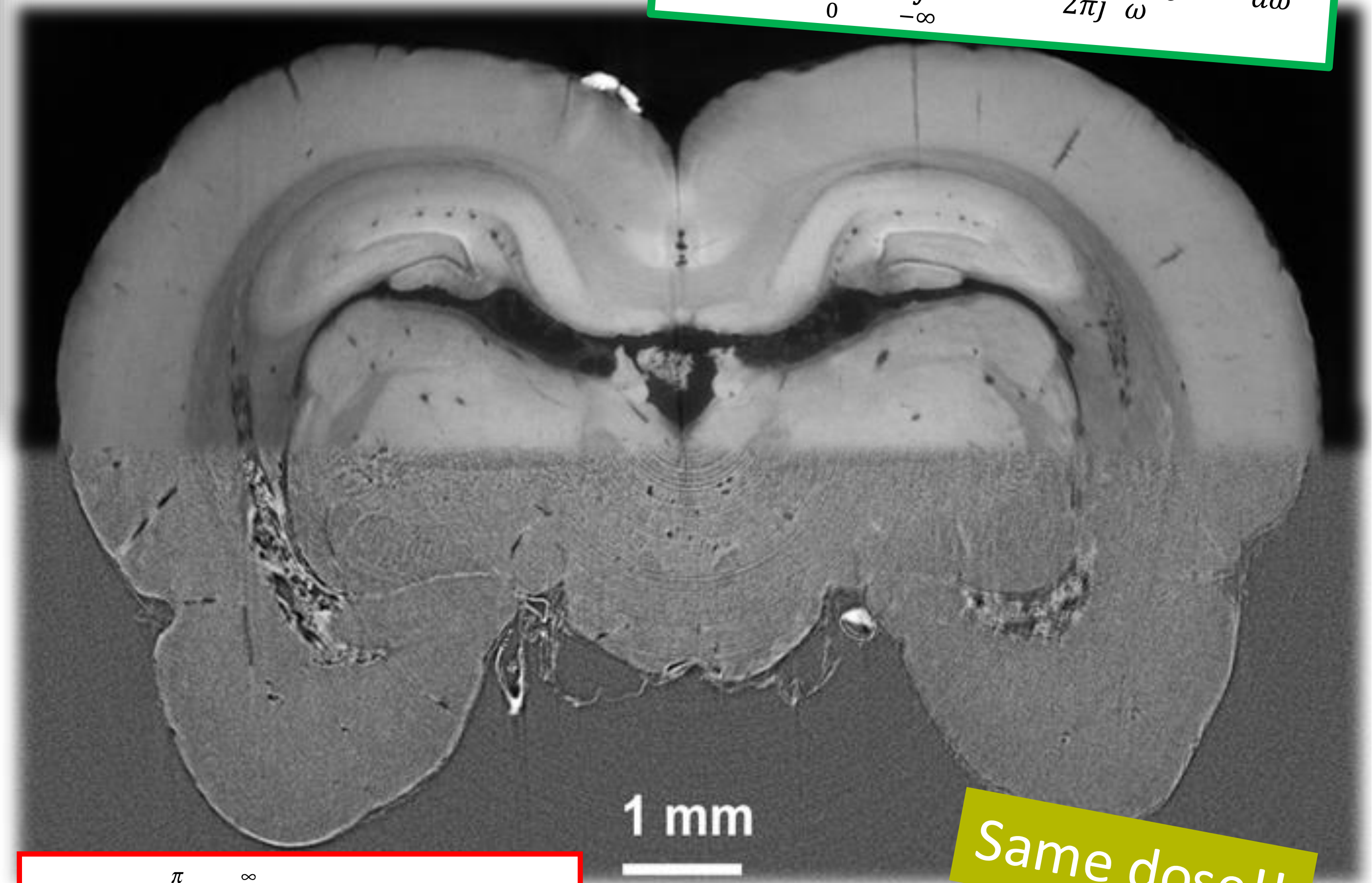
$$\boldsymbol{\Delta\phi(d)} = \delta kd$$

Why is phase interesting for imaging?

PSI



$$\delta(x,y) = \int_0^{\pi} d\theta \int_{-\infty}^{+\infty} \tilde{D}(\omega,\theta) \frac{1}{2\pi j} \frac{|\omega|}{\omega} e^{j2\pi\omega t} d\omega$$



$$\mu(x,y) = \int_0^{\pi} d\theta \int_{-\infty}^{\infty} \tilde{P}(\omega,\theta) |\omega| e^{j2\pi\omega t} \, d\omega$$

Same dose!!

«Gedankenexperiment»

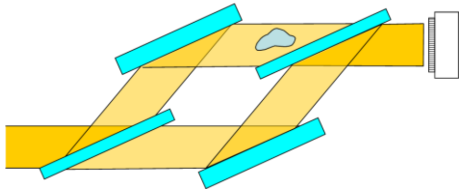
- 20 keV X-rays
- 50 µm thick organic sample

➔ **only 0.2 % absorption**
➔ **but π phase shift!**

} **Higher contrast @ same dose**

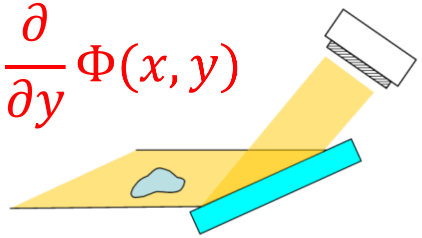
Accessing X-ray "phase-driven" contrast

$\Phi(x,y)$



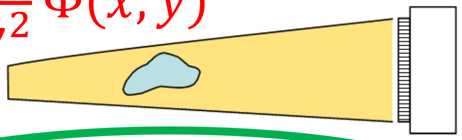
Crystal interferometry
Bonse et al. APL 6, 155 (1965)

$\frac{\partial}{\partial y}\Phi(x,y)$



Diffraction enhanced imaging
Chapman et al., *PMB,* 42, 2015 (1997)
Davis et al., JOSA A 13, 1193 (1996)

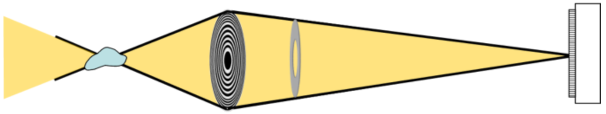
$\frac{\partial^2}{\partial y^2}\Phi(x,y)$



Free space propagation
Snigirev et al., RSI 66, 5486 (1995)
Cloetens et al., APL 75, 2912 (1999)

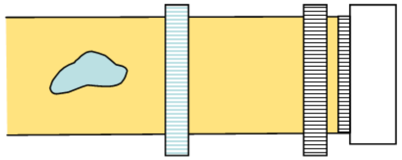
Enables ultrafast dynamic imaging!

$\Phi(x,y)$



Zernike phase contrast
Weiss et al., UM 84, 185 (2000)
Holzner et al., NatPhys 6 (2010)

$\frac{\partial}{\partial y}\Phi(x,y)$

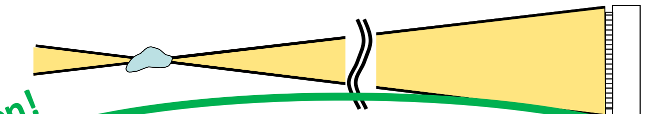


Talbot-(Lau) interferometry
Weitkamp et al., OptExp 13, 6296 (2005)
Pfeiffer et al., NatPhys 2, 258 (2006)

Coded apertures
Olivo et al., APL 91 (7) 2007

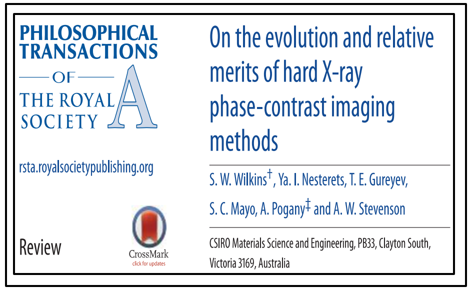
Speckles
Cerbino et al., NatPhy 4, 2008

$\Phi(x,y)$



Coherent diffractive imaging - Ptychography
Miao et al., Nature 400 (1999)
Thibault et al., Science, 321, 379 (2008).

Reaches nm resolution!


PHILOSOPHICAL TRANSACTIONS OF THE ROYAL SOCIETY A
rsta.royalsocietypublishing.org
Review

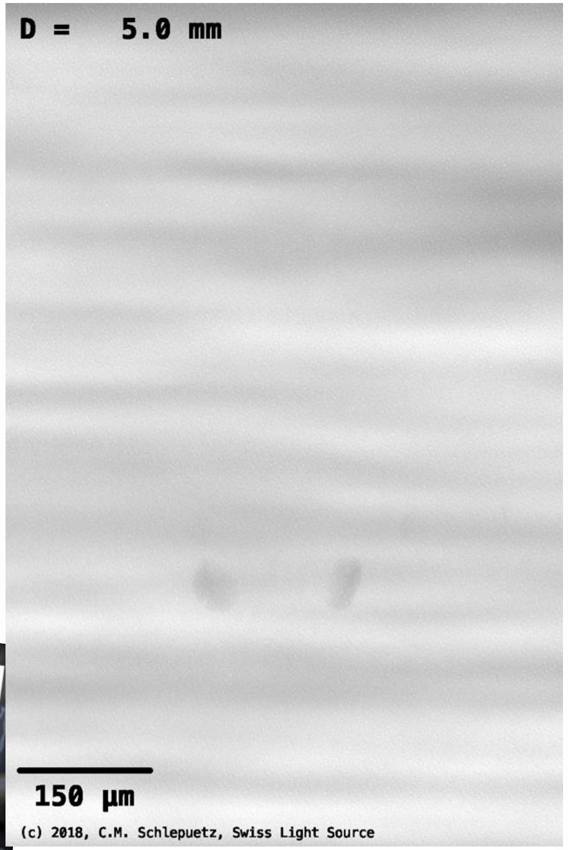
On the evolution and relative merits of hard X-ray phase-contrast imaging methods

S. W. Wilkins[†], Ya. I. Nesterets, T. E. Gureyev, S. C. Mayo, A. Pogany[‡] and A. W. Stevenson

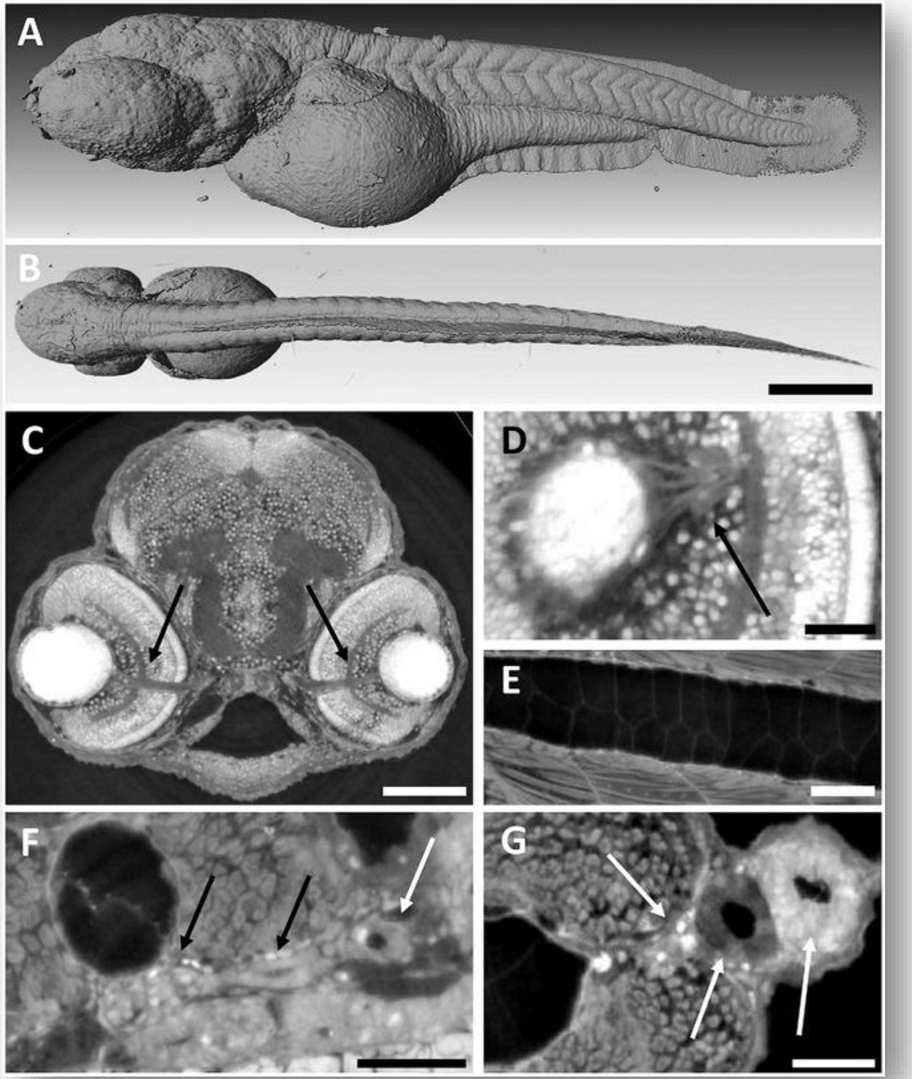
CSIRO Materials Science and Engineering, PB33, Clayton South, Victoria 3169, Australia

Free-space propagation to push contrast in low-absorbing materials

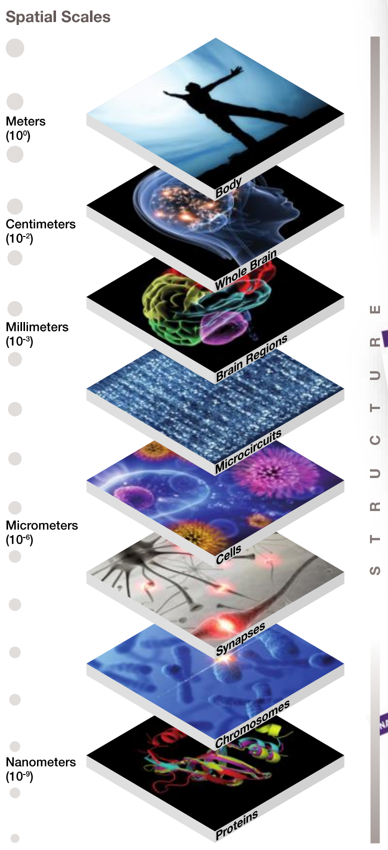
$$H(\nu_x, \nu_y) = \exp\left[-i2\pi\sqrt{\frac{1}{\lambda^2} - \nu_x^2 - \nu_y^2}\cdot d\right]$$

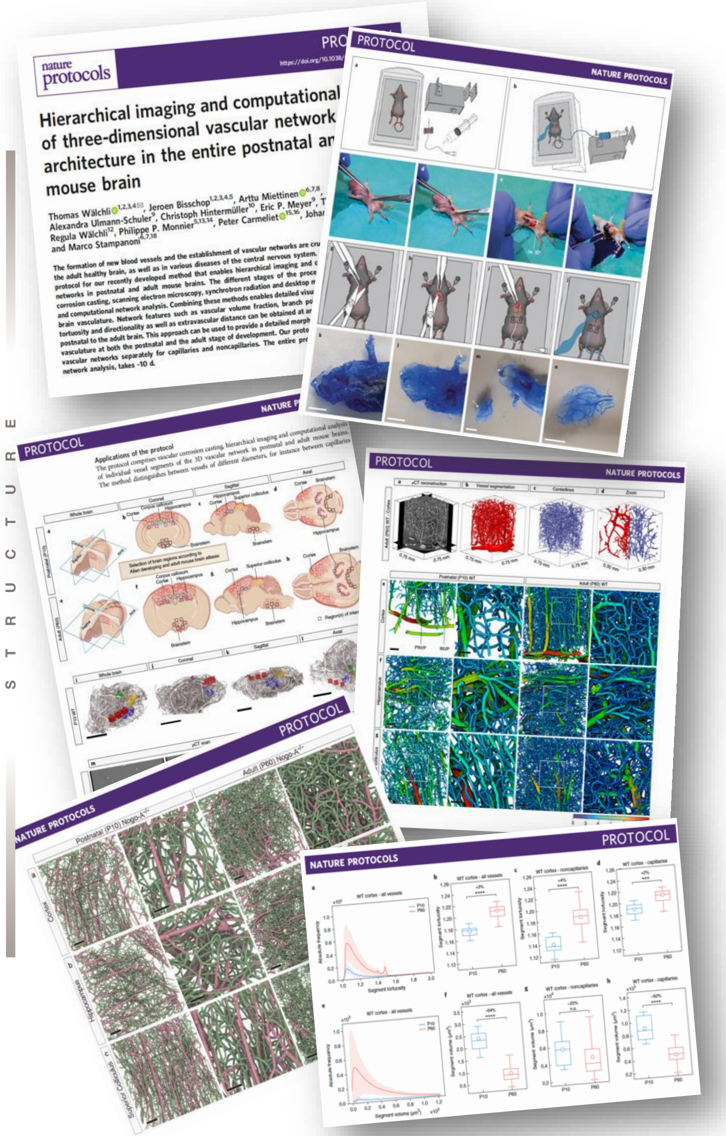


Cörek *et al.*, Small 16 (31) 2020 - 10.1002/smll.202000746



Whole mouse brain microvascular architecture



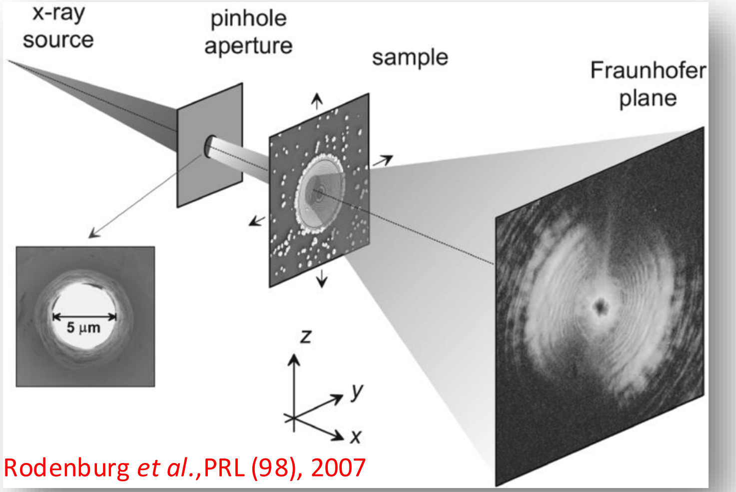


Miettinen *et al.,* BioInformatics 2019 - Wälchli et al., Nature Protocols 2022

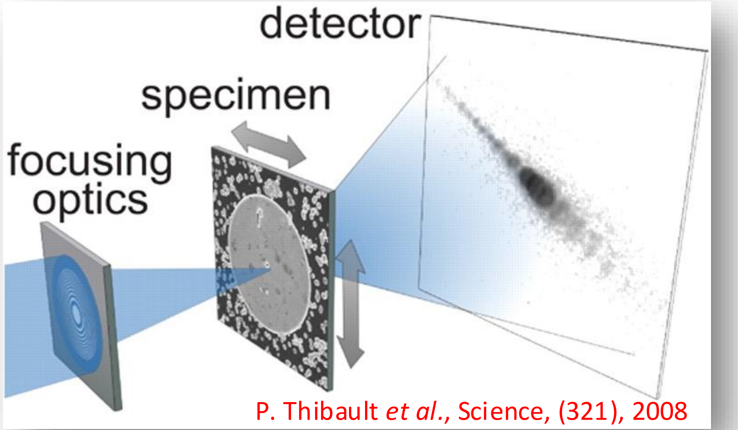
Stitched tomogram of more than 1000 single volumes, assembled non-rigidly.
Size of data shown: 12 TB

Ptychography leverages on coherence to push resolution

PSI



Rodenburg *et al.*,PRL (98), 2007



P. Thibault *et al.*, Science, (321), 2008

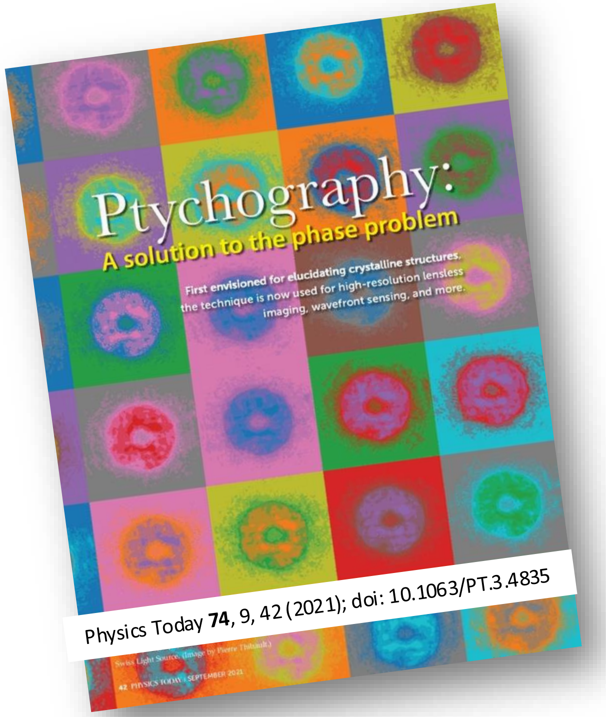
Coherence: allows the interpretation of observations based on modeling of propagation and interaction with matter

Ψ

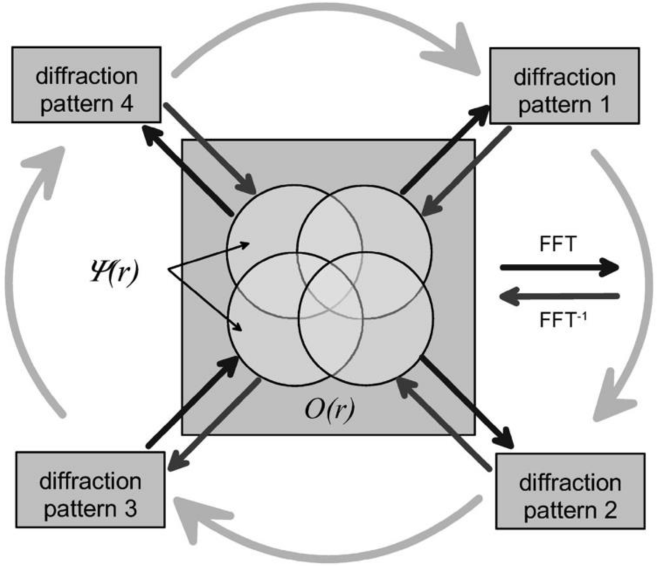
Measurement: leads to the loss of part of the information

$|\Psi|^2$

This is the phase problem!



Physics Today **74**, 9, 42 (2021); doi: 10.1063/PT.3.4835



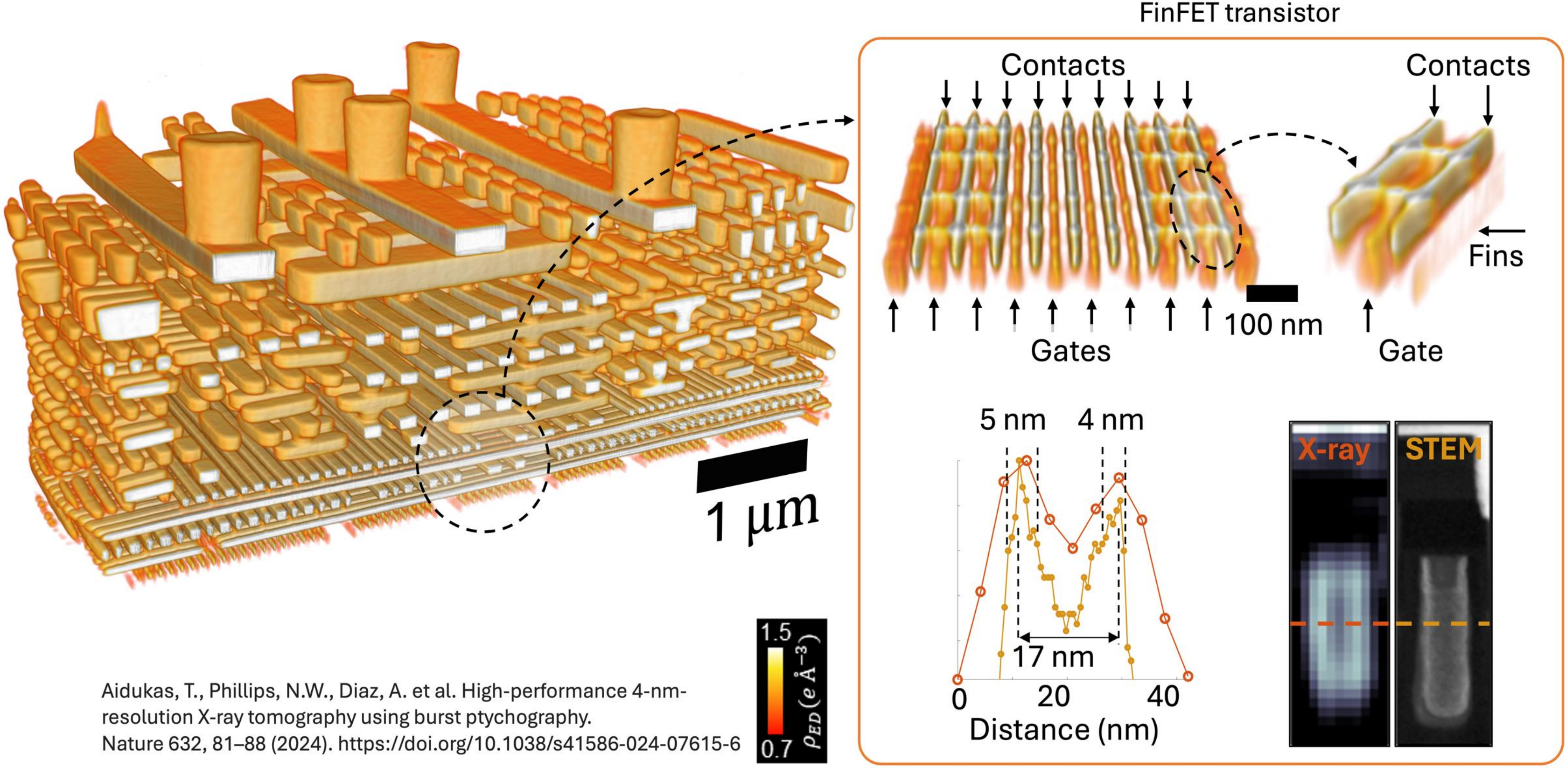
Ptychographic Iterative Engine (PIE)

- Initial exit wave calculation (based on current estimate)
- Propagation to the Fraunhofer plane
- Modulus replaced by recorded data while preserving phase (usual for iterative methods)
- Back-propagation
- Resulting difference used to update the estimate

Important note: subsequent data from adjoining areas are fed into the algorithm to speed up convergence!

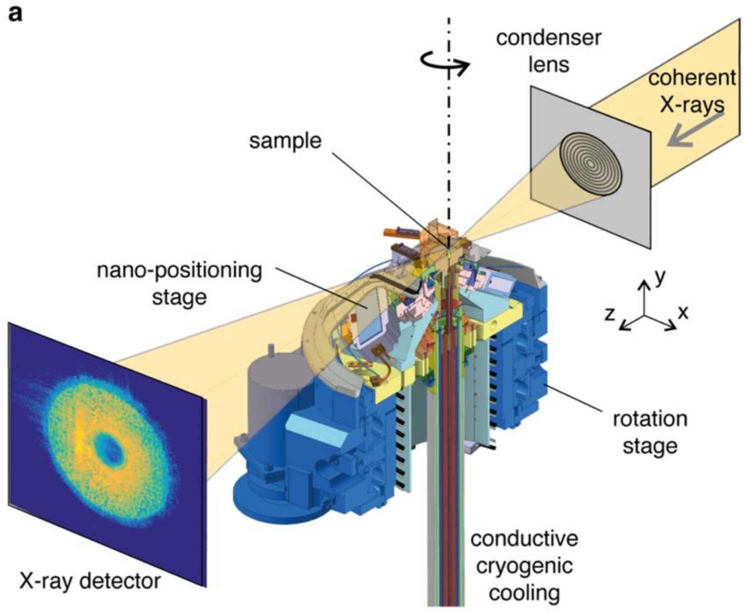
Burst ptychography yields to 4 nm resolution tomogram

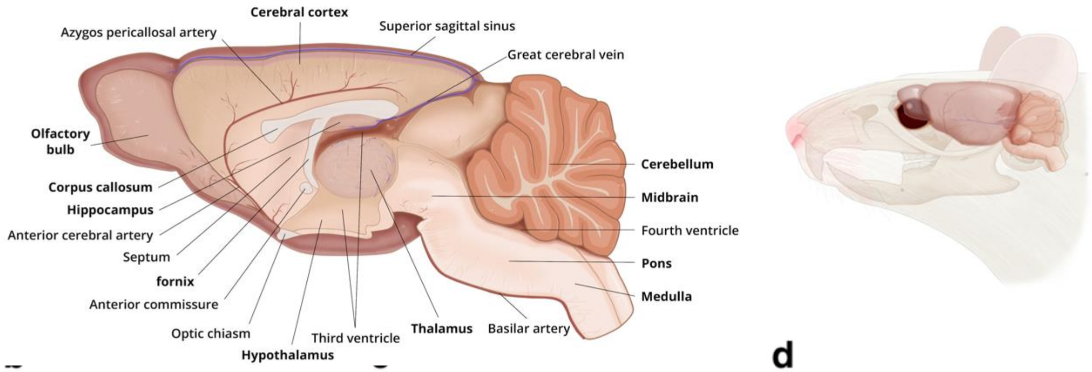
Highest X-ray tomography resolution to date!

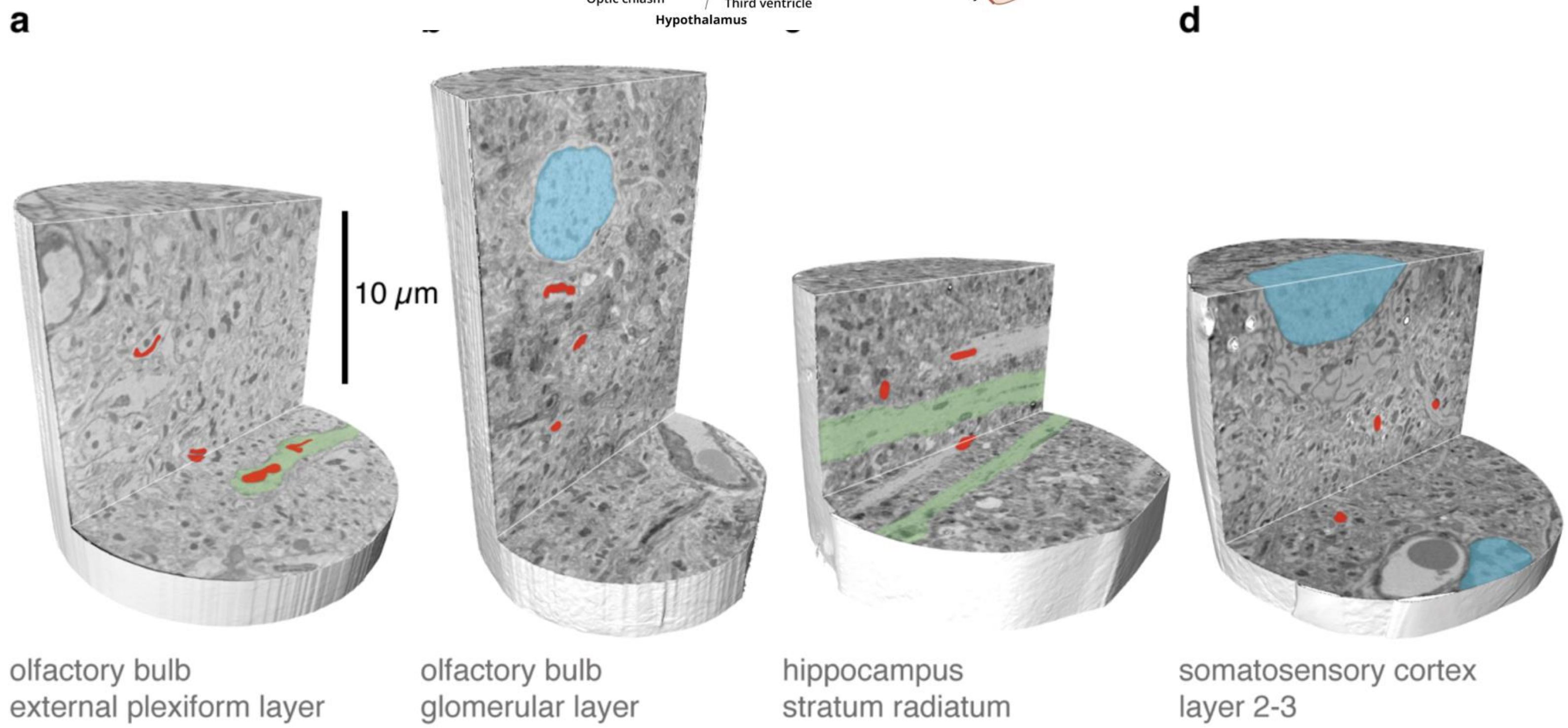


Aidukas, T., Phillips, N.W., Diaz, A. et al. High-performance 4-nm-resolution X-ray tomography using burst ptychography. Nature 632, 81–88 (2024). https://doi.org/10.1038/s41586-024-07615-6

Towards synaptic mapping (connectome)

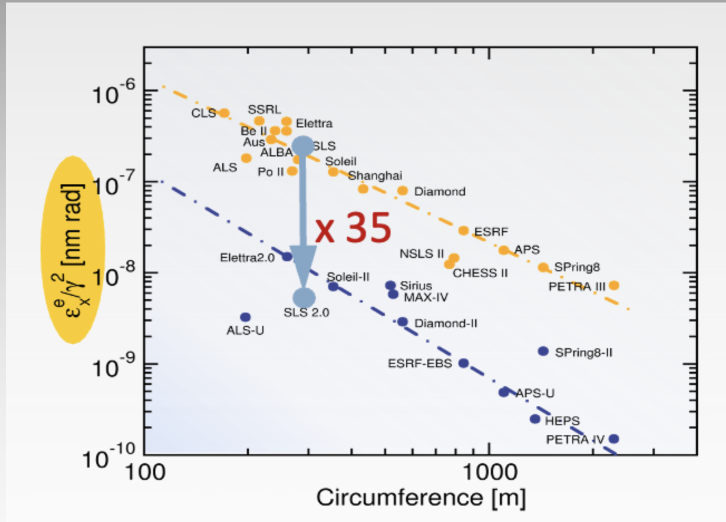


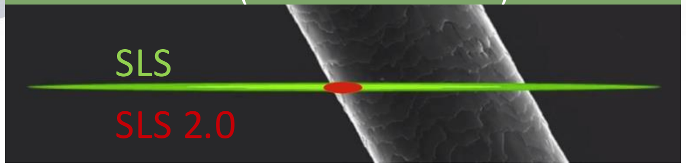




Bosch et al. https://doi.org/10.1101/2023.11.16.567403 (bioRxiv)

SLS 2.0: sharper and faster imaging





2021 · 2022 · 2023 · 2024 · 2025 · 2026

DECEMBER 2020
Swiss Parliament agrees on the Swiss Dispatch on Promotion of ERI

OCTOBER 2023
Start of construction. Dark period 15 months

JULY 2025
Restart of User Operation

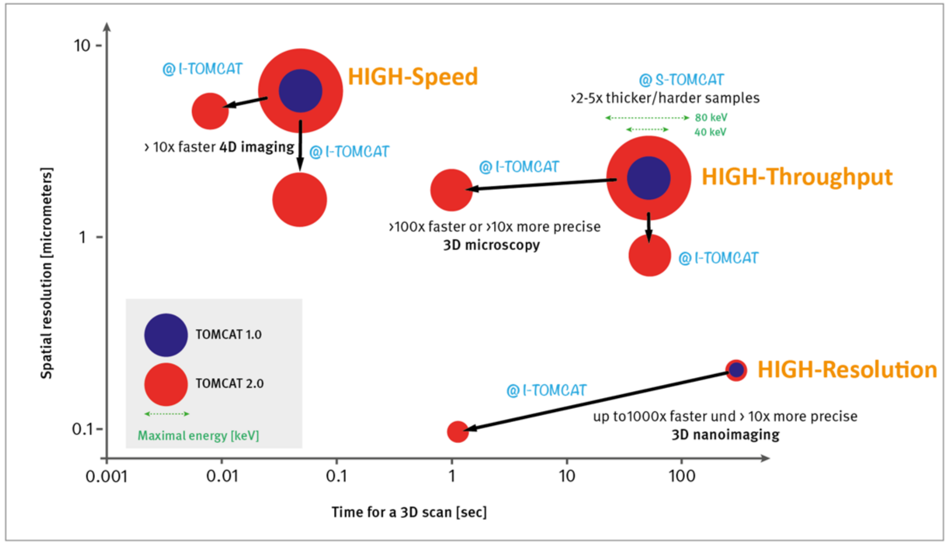
SWISSLOS Kanton Aargau

Push imaging on SLS2.0

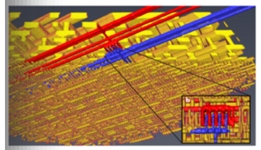
TOMCAT2.0 and cSAXS upgrade programs

TOMCAT2.0 → I-TOMCAT and S-TOMCAT

In a nutshell: Multiscale – Multimodal – Dynamic



X-ray ptychography at cSAXS at SLS 2.0



M. Holler *et al.*, Nature **543**, 402 (2017)

Calculations from one of our measurements in 2017 at 6.2 keV, called here “state of the art”

DEVELOPMENT	RESOLUTION (nm)	VOLUME (μm^3)	TIME
State of the art	**14.6**	**15x15x8**	**22 h**
SLS-2 (x30)	6.4	82x82x8	44 min
+ new undulator(x2)	5.5	116x116x8	22 min

Numbers indicate the gain in one parameter with respect to the ***state of the art*** *(M. Holler et al., 2017) when keeping the other two parameters constant*

On SLS2.0 we can expect

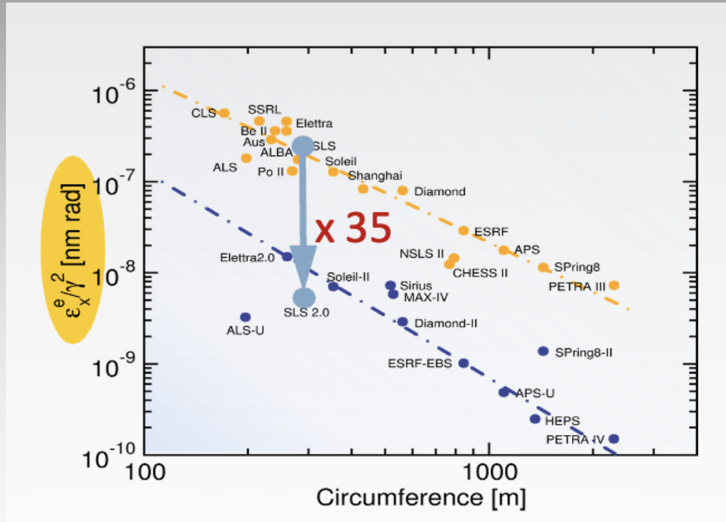
- 2.5x better resolution at same volume and acquisition time compared to SLS1.
- 60x larger volume at same resolution and acquisition time compared to SLS1
- 60x faster for same resolution and volume compared to SLS1

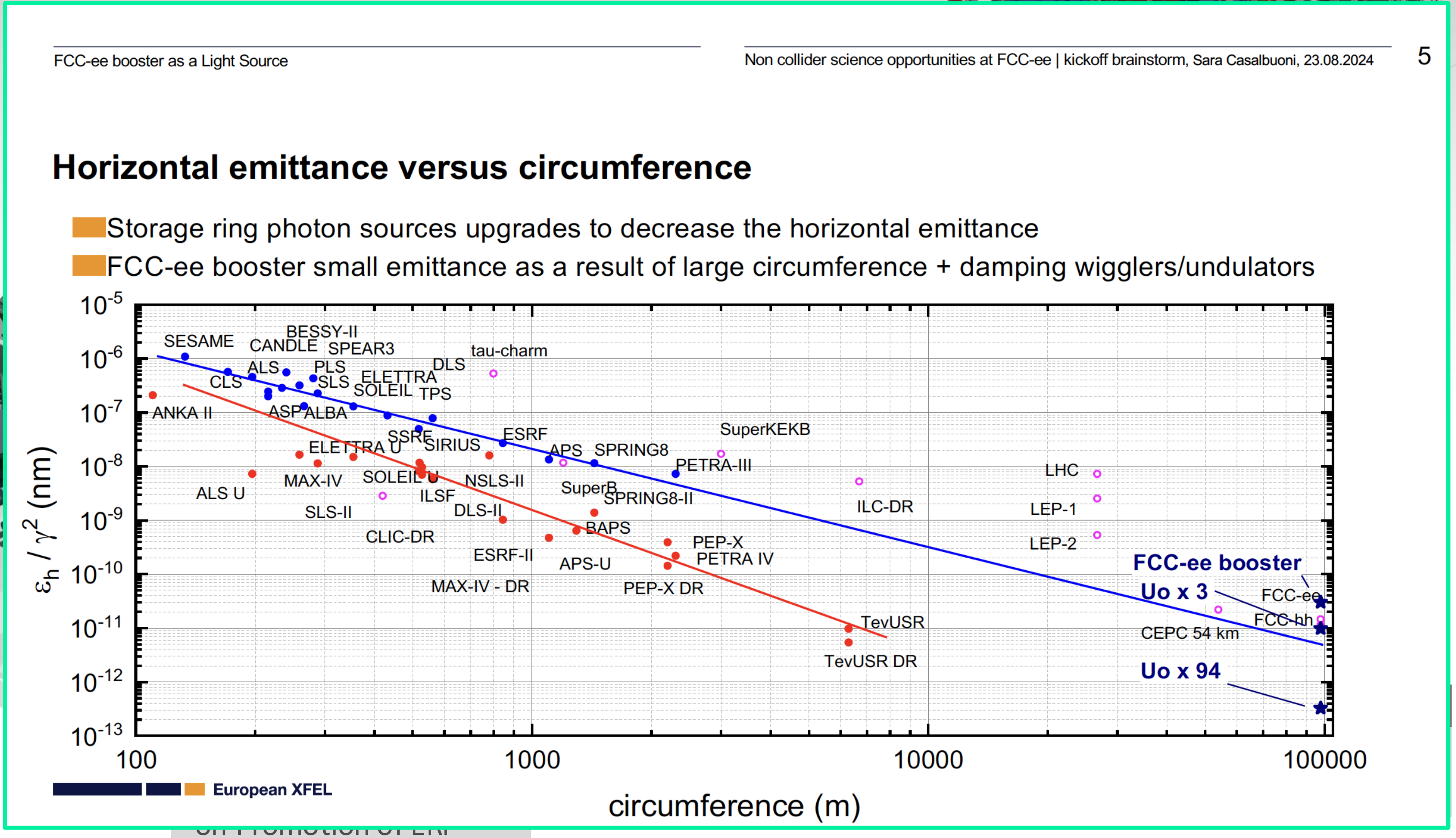
“Caveat”: how much dose/flux will a sample at the end tolerate?

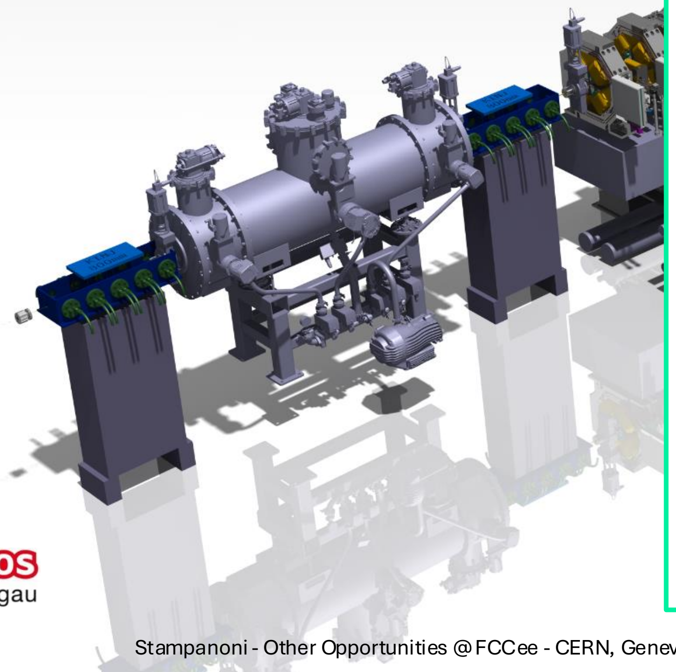
This might be efficiently mitigated if dose can be traded in with measurement at high-energies!

SLS 2.0: sharper and faster imaging

PSI

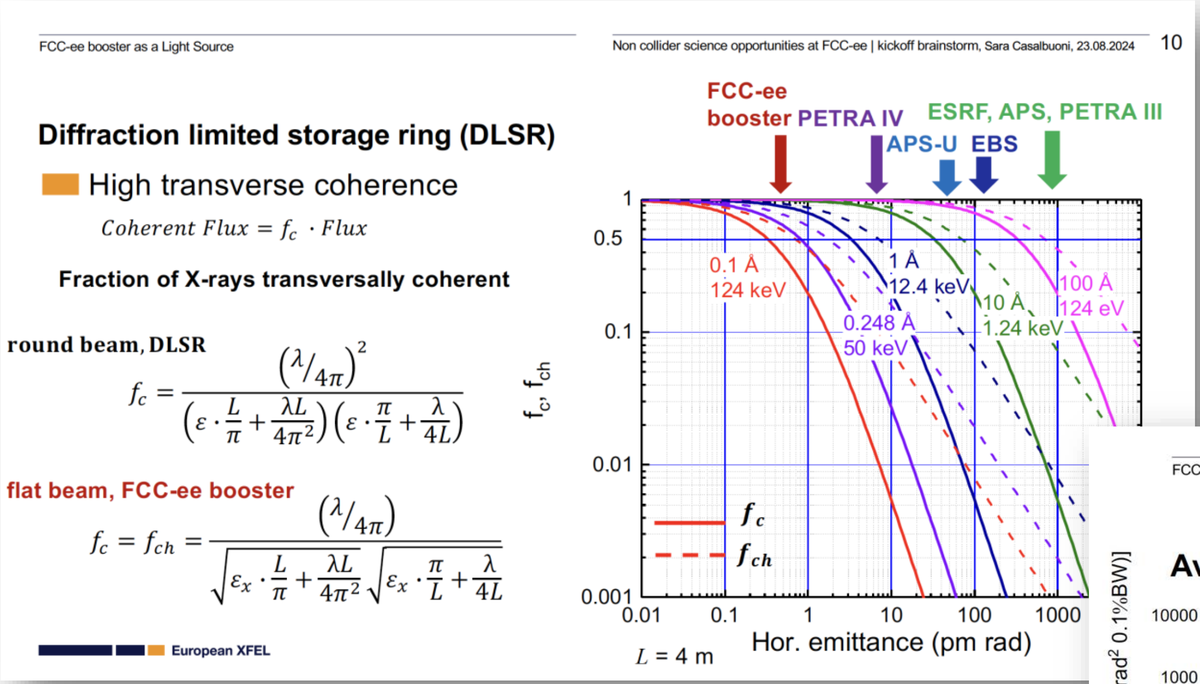






Imaging on FCC-ee?

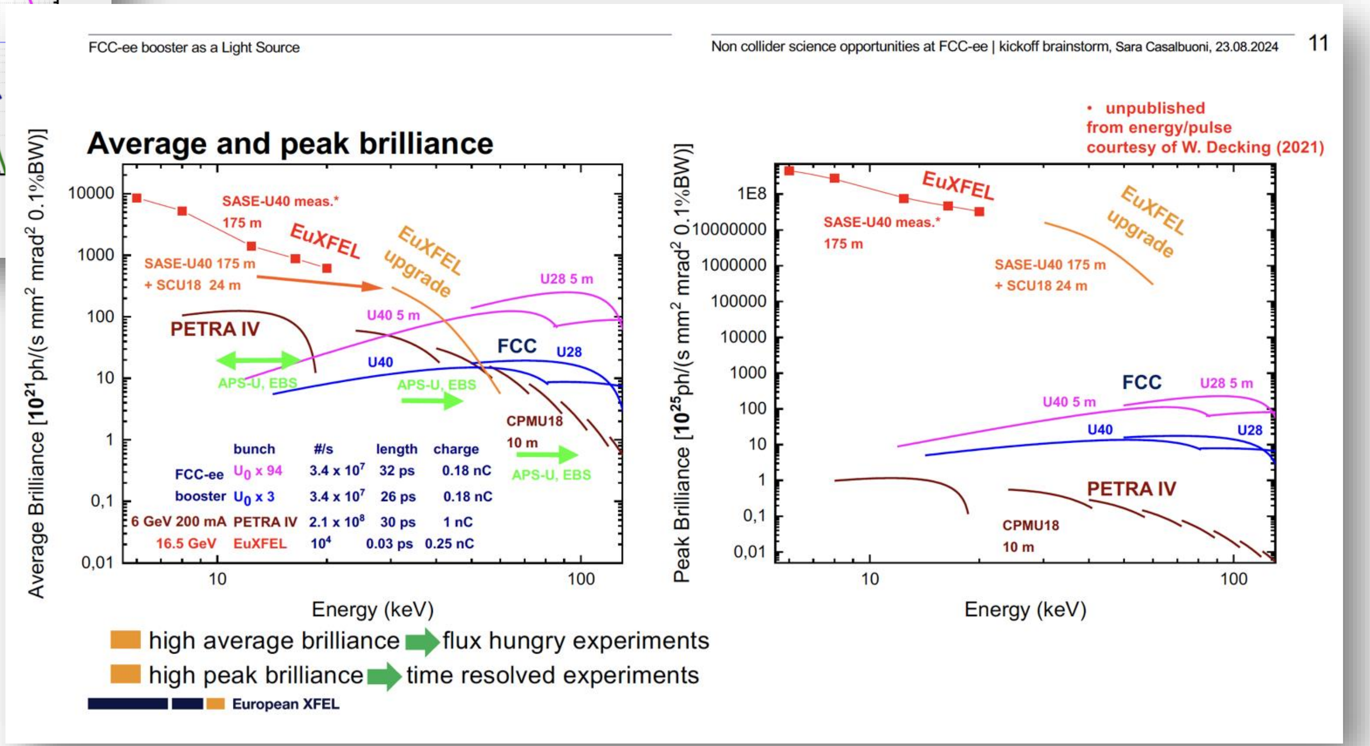
PSI



From August 2024 "Kick-off brainstorm" in Hamburg…

Compared to PETRA IV, at 50-100 keV the FCC-ee booster could produce:

- a fraction of coherent X-rays larger by one order of magnitude
- an average brilliance larger by up to two orders of magnitude
- a peak brilliance larger by up to four orders of magnitudes

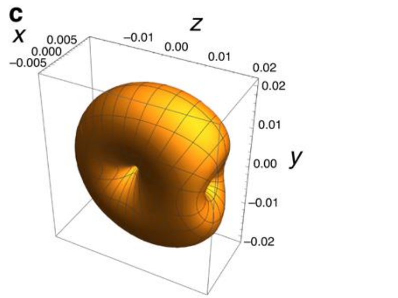


FCC-ee might boost imaging to unprecedented levels:

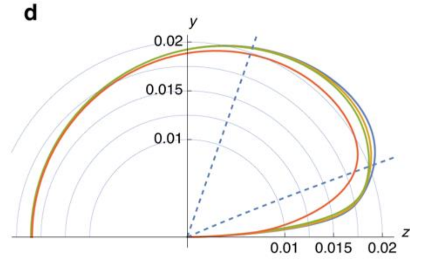
- Exceptional peak-brilliance and coherent fraction will enable high-energy time-resolved ptychographic imaging (larger samples, heavier materials, *in-situ/operando)*
- Exceptional average brilliance will push dynamic imaging beyond all currently achievable capabilities and eventually make scanning Compton X-ray Microscopy a valuable tool

Scanning Compton X-ray microscopy (SCXM)

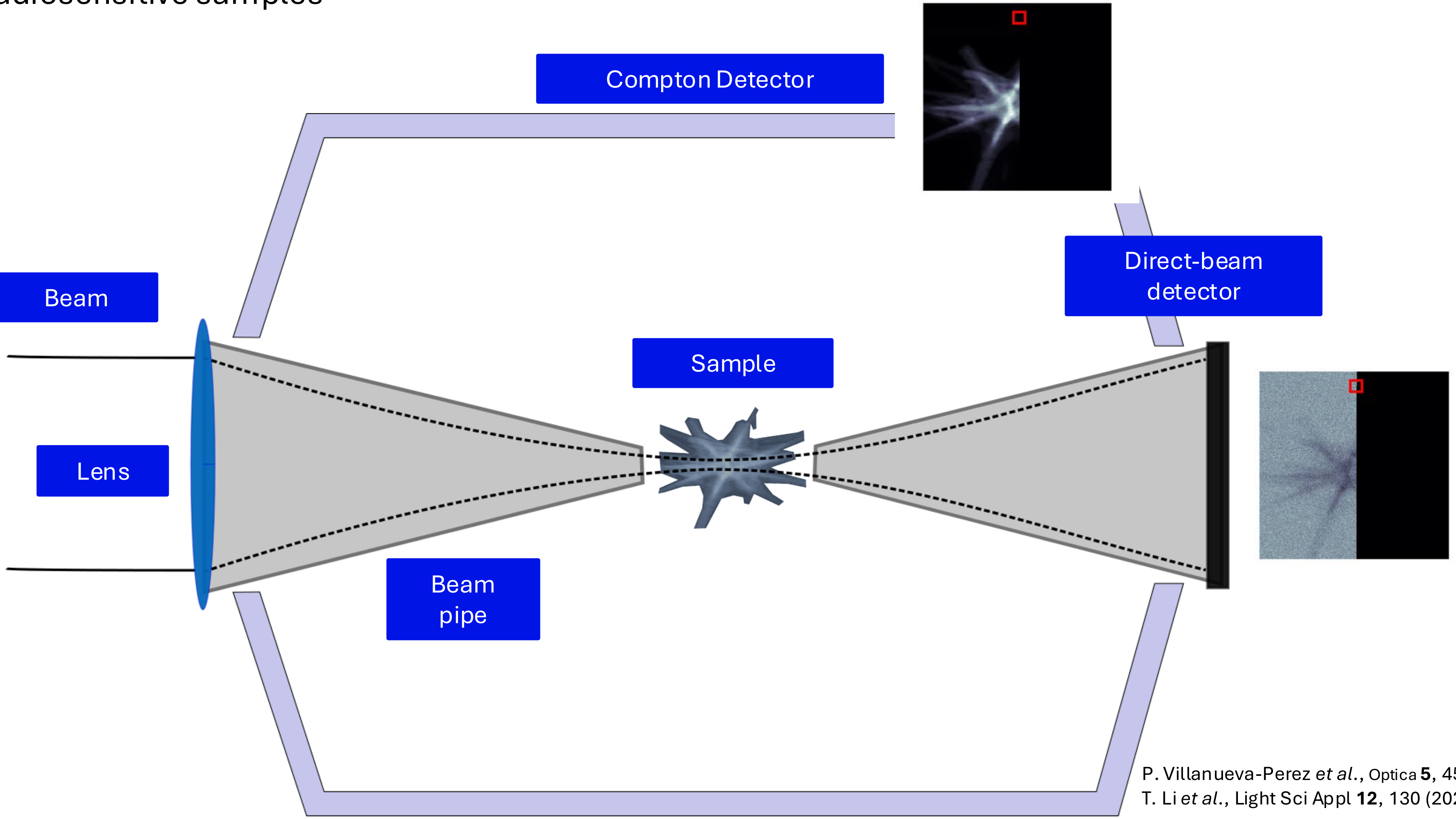
Currently neglected Compton interactions can lead to the highest achievable resolution when imaging biomedical and radiosensitive samples



Differential cross section of carbon in units of cm^2/g/solid angle at 60 keV photon energy

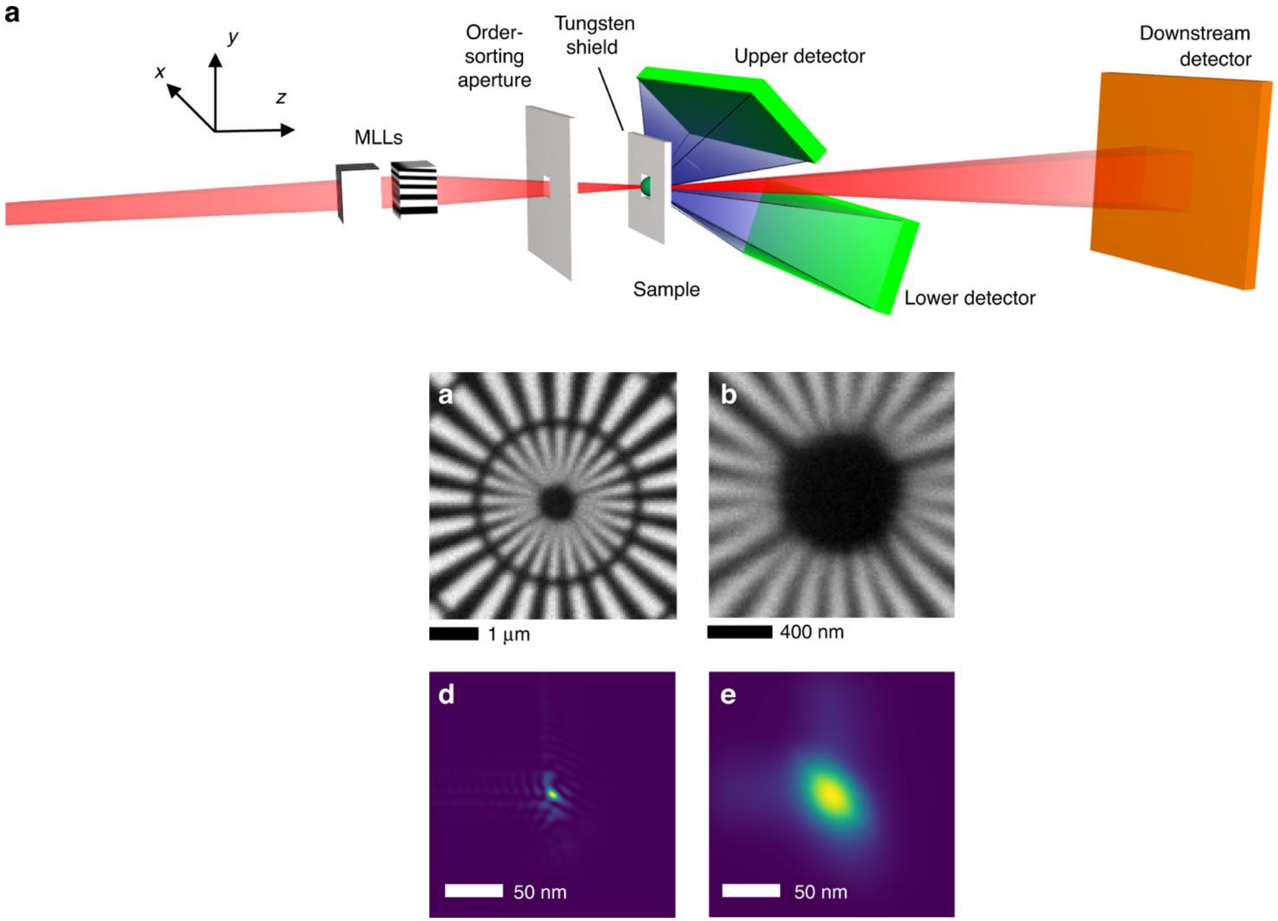


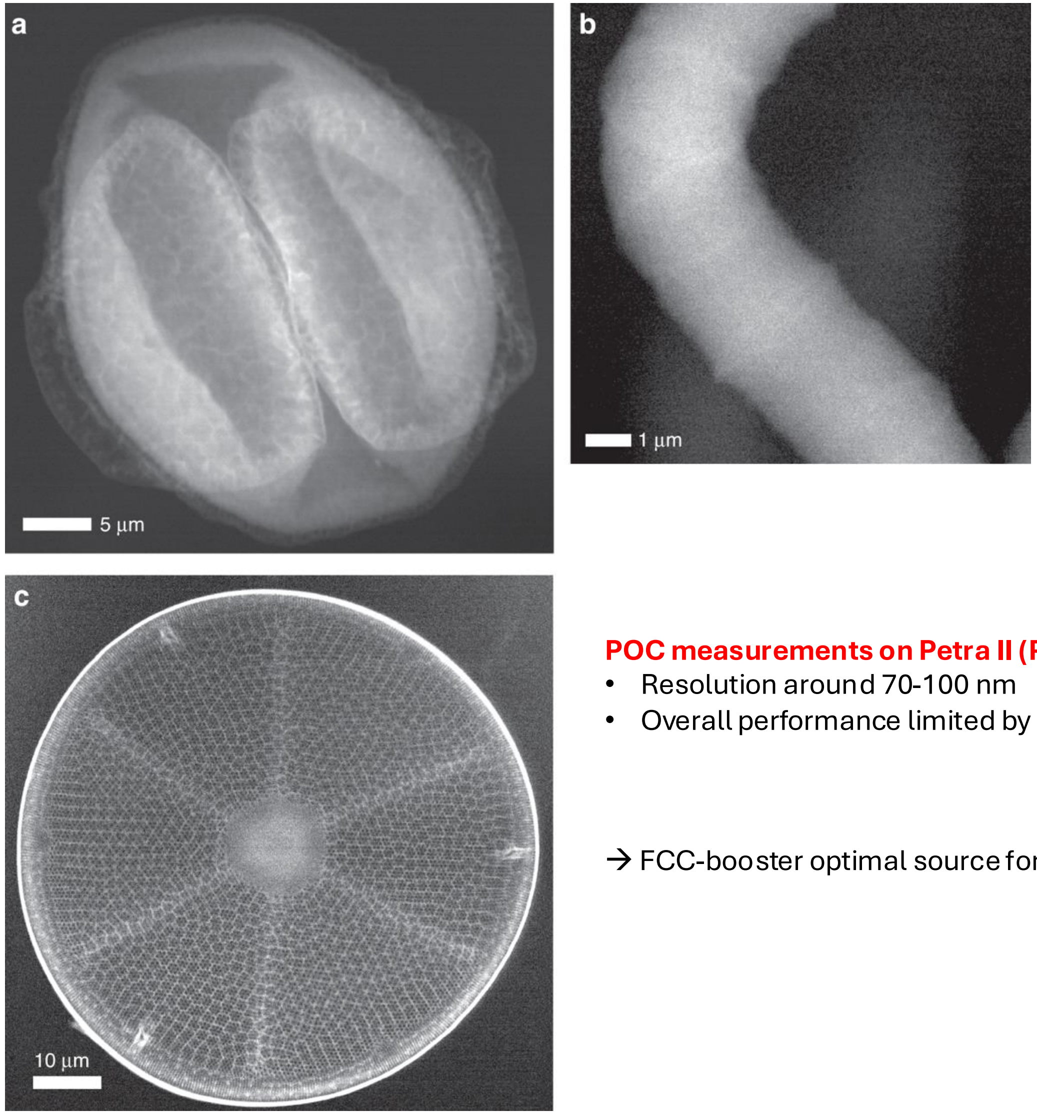
Slices of the differential cross sections in the same units of C (blue), N (yellow), O (green), and Si (orange).



P. Villanueva-Perez *et al.*, Optica **5**, 450-457 (2018)
T. Li *et al.*, Light Sci Appl **12**, 130 (2023)

Scanning Compton X-ray microscopy (SCXM)





POC measurements on Petra II (P07)

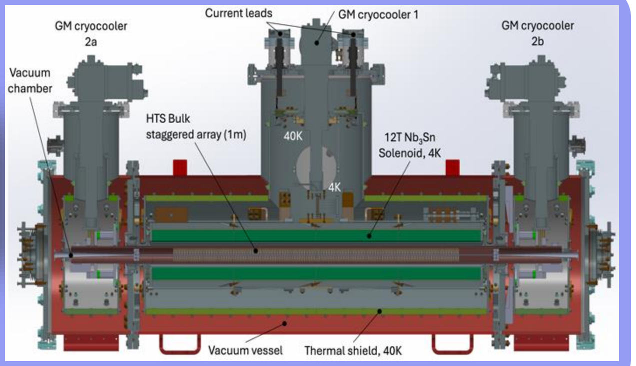
- Resolution around 70-100 nm
- Overall performance limited by brilliance…

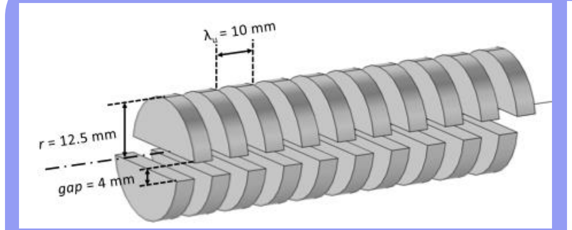
→ FCC-booster optimal source for SCXM

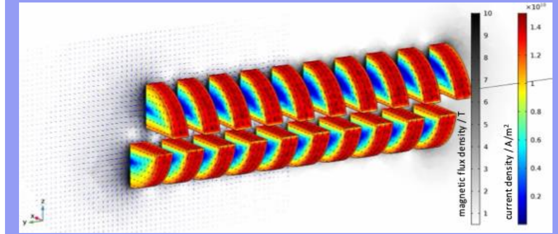
P. Villanueva-Perez, et al. ,Opt. Lett. **46**, 1920-1923 (2021)
T. Li *et al.*, Light Sci Appl **12**, 130 (2023)

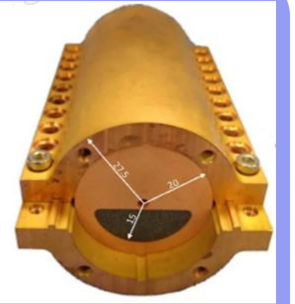
I-TOMCAT source: HTSU10 undulator

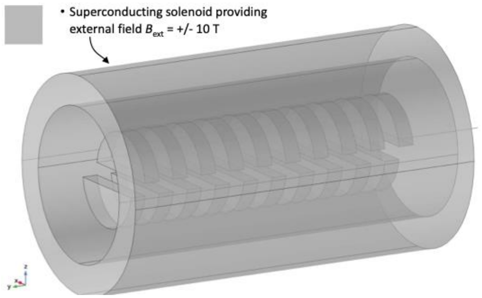
GdBCO by Nippon Steel – Design for 4.5 mm fix gap and 1.8T

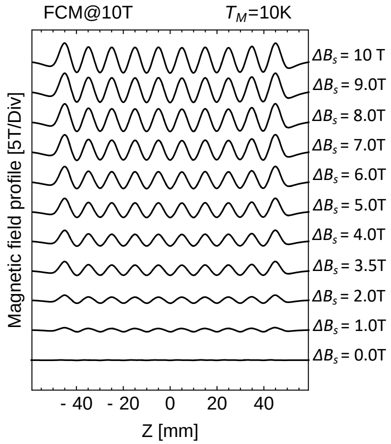


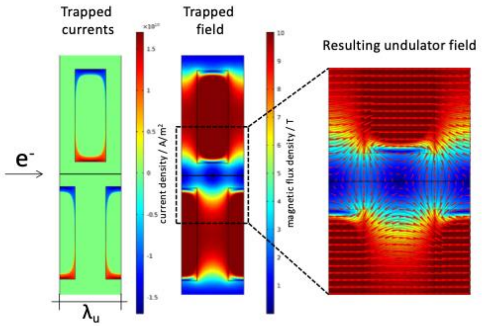




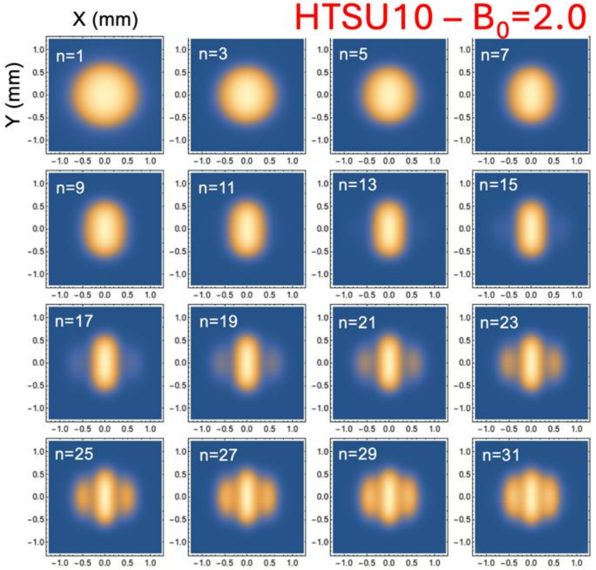


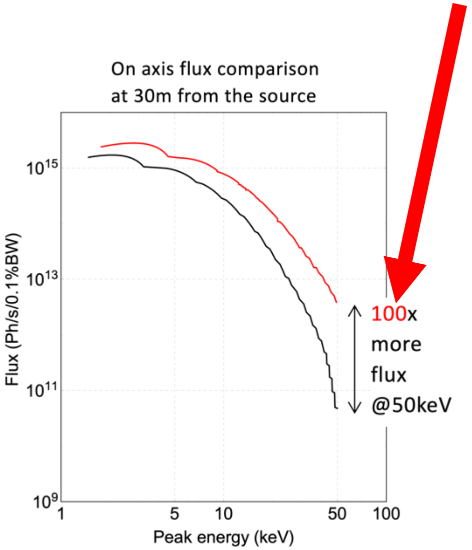




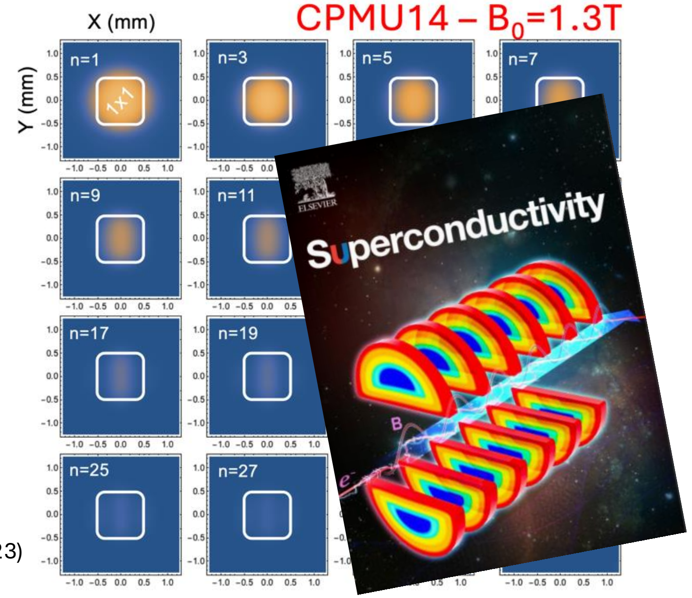


K. Zhang, M. Calvi et al.,
Superconductor Science and Technology **36** (2023)





In-house development by M. Calvi



THE METER LONG PROTOTYPE

- Active length : 1.0 m
- Total length : < 2m
- period length : **10.5** mm
- magnetic gap : **4.5** mm
- B_0 ~ **1.8** T
- Cryocoolers
- HTS Mag-temp 10K
- LTS temp 4.0K