Analysis and design of X-ray optical systems applying hierarchical models including partial coherence

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ESRF
(including work done in Berkeley)

High Precision X-ray measurements 8-10 June 2021

The European Synchrotron

BERKELEY LAB

Contents

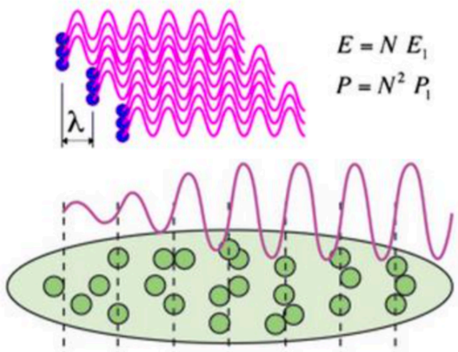
- Motivation: optics for 4th generation synchrotron sources
- Hierarchical approach for beamline simulation (with examples)
- Ray tracing
- Wave optics
- Partial coherence
- Crystal optics

4^{TH} GENERATION SYNCHROTRON SOURCES

X-FEL

Bunch length ~ wavelength emitted:

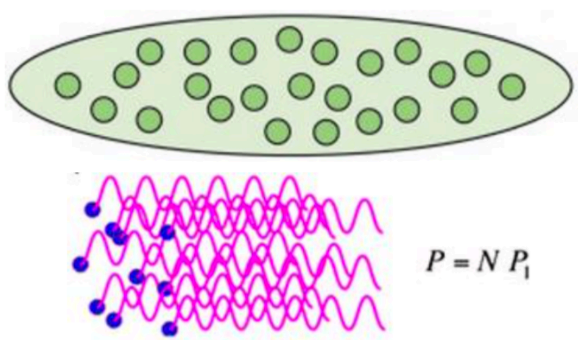
emission from different electrons add coherently:
almost full transversal (spatial) and longitudinal (time) coherence



STORAGE RINGS

Bunch length >> wavelength:

emission from electrons add incoherently:
low longitudinal (time) coherence (then improved with monochromators) and partial transversal (spatial) coherence



DLSR (diffraction limited storage ring) sources:
natural emission >> electron size.

At present diffraction limit (total coherence) can be attained at low photon energies only (< 1keV), but hard X-rays present partial coherence.

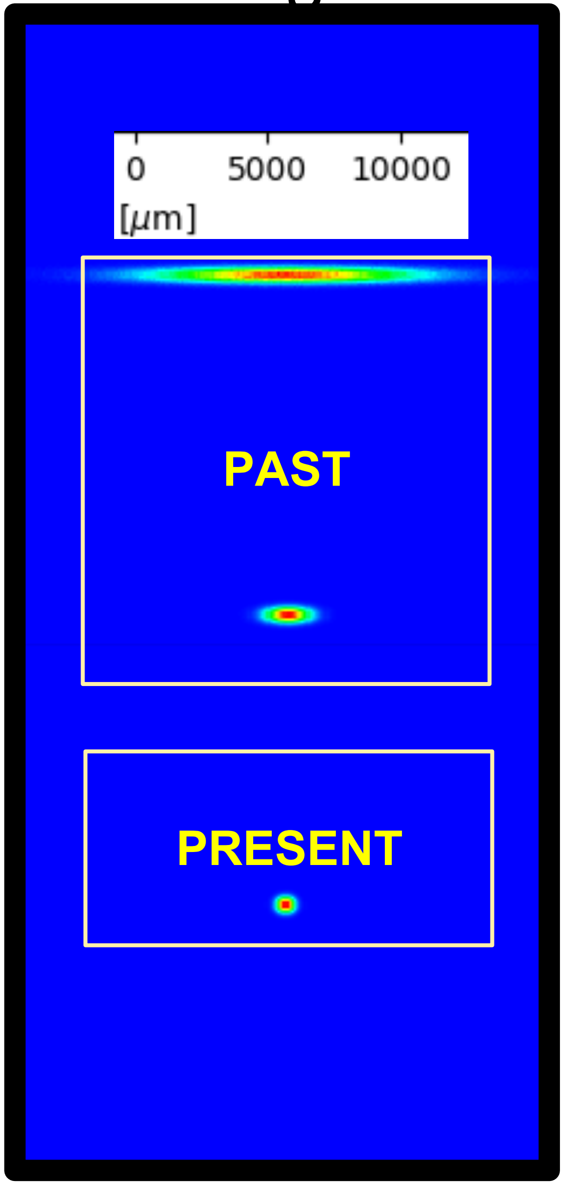
The beamline optics cam improve the coherence fraction (at the price of lowering intensity).

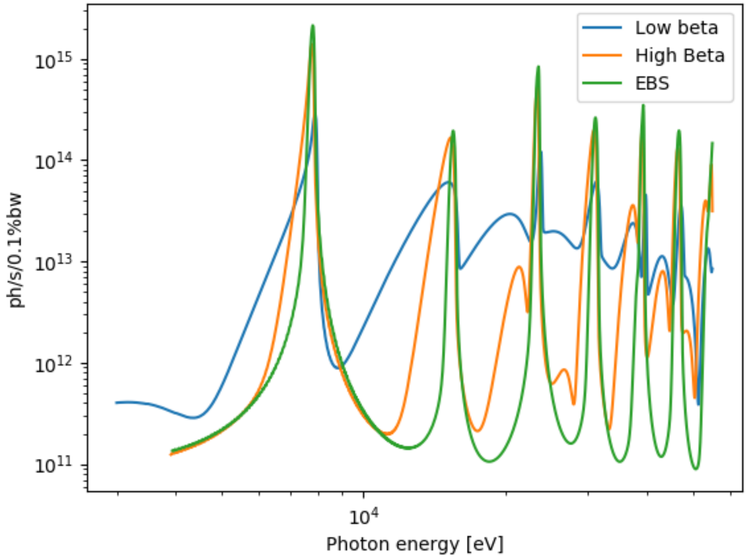
Big increase of brightness and transverse coherence

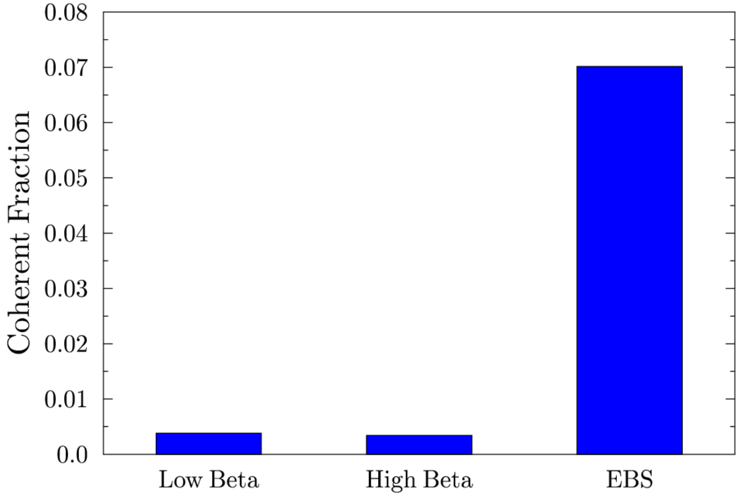
Low Beta U18

High Beta U18

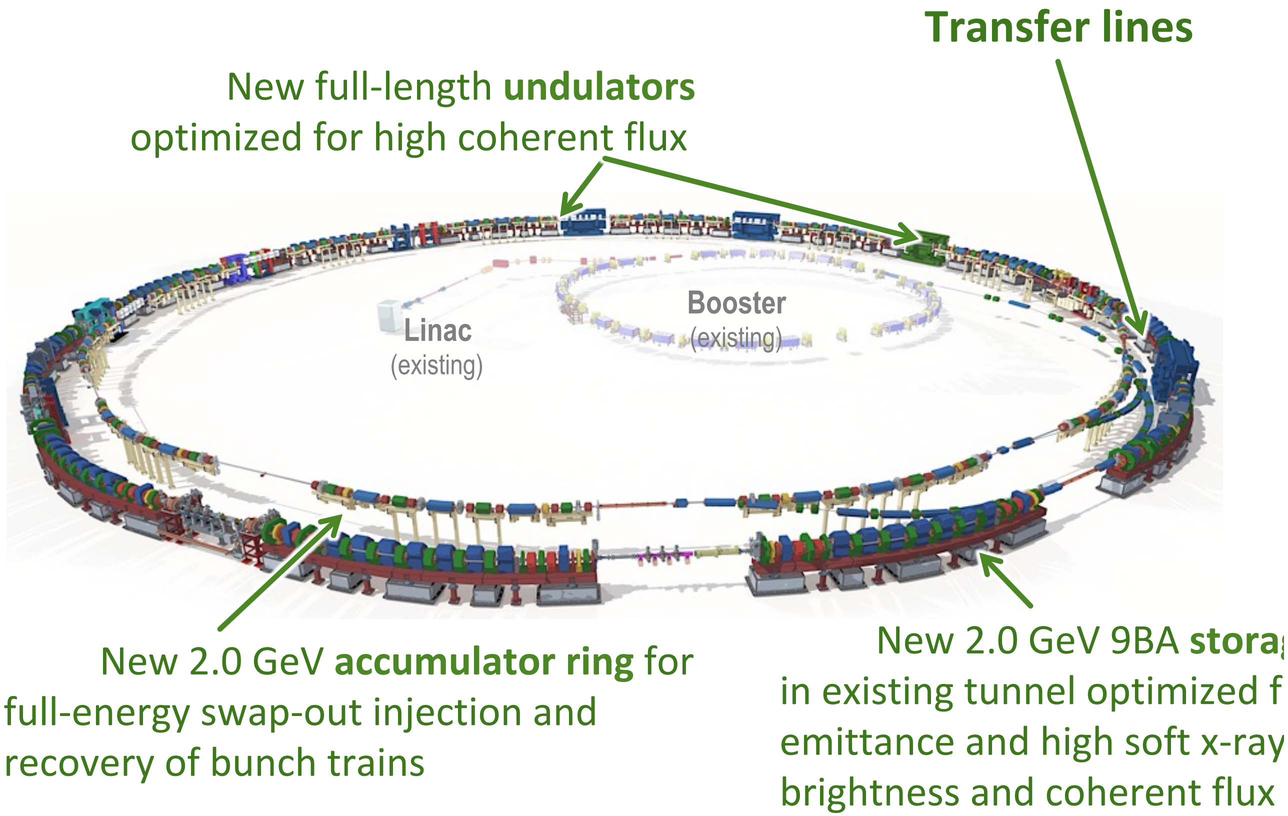
EBS U18



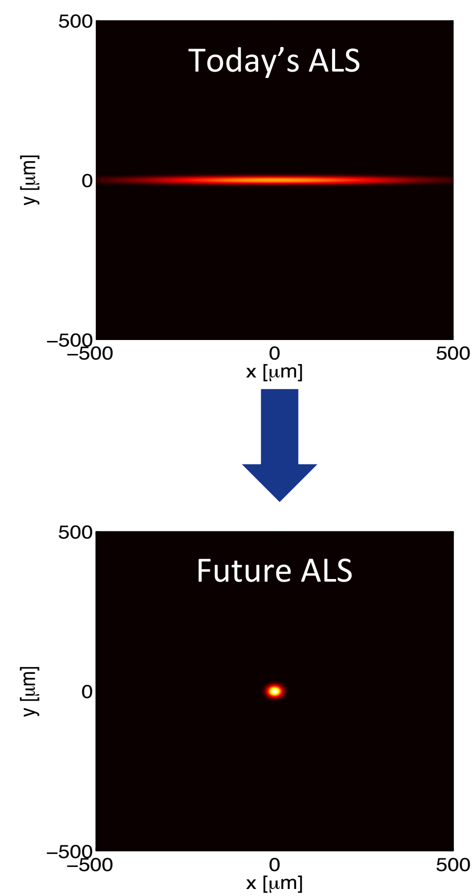




ALS-U



Electron Beam Profiles

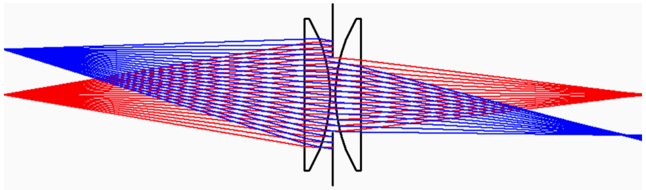


CF ~ 0.8 with a 4 m undulator at 230 eV

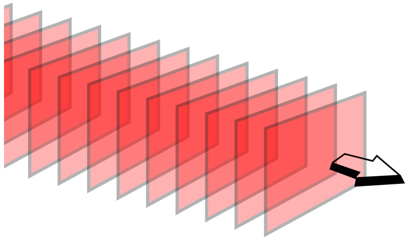
COMPLEXITY

Analytical model (by hand)

Ray tracing (ShadowOui)



Hybrid model (ShadowOui)



Simplified wave optics (WOFRY)

Monte Carlo (multi e$^-$) wave optics (SRW)

Coherent Mode Decomposition (COMSYL/WOFRY)

M. Sanchez del Rio et al, JSR 26 1887 (2019)
https://doi.org/10.1107/S160057751901213X

FROM THEORY TO SOFTWARE: ALL ABOUT LIGHT

SRW | WOFRY | COMSYL

$$\nabla \cdot \vec{D} = \rho_{\text{free}}$$

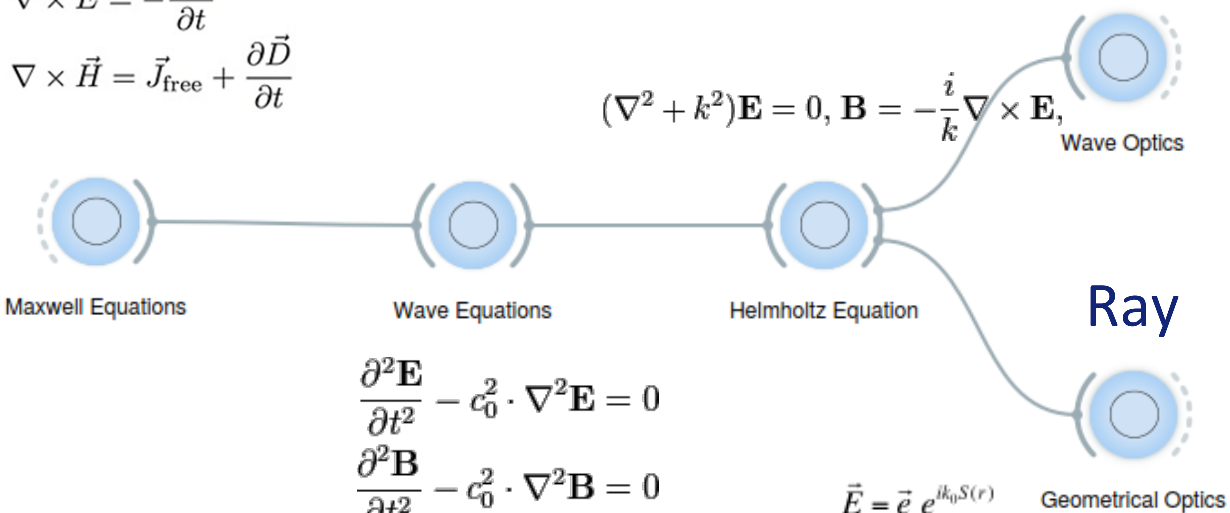
$$\nabla \cdot \vec{B} = 0$$

$$\nabla \times \vec{E} = -\frac{\partial \vec{B}}{\partial t}$$

$$\nabla \times \vec{H} = \vec{J}_{\text{free}} + \frac{\partial \vec{D}}{\partial t}$$

Wavefront

$$(\nabla^2 + k^2)\mathbf{E} = 0,\ \mathbf{B} = -\frac{i}{k}\nabla \times \mathbf{E},$$



Ray

$$\frac{\partial^2 \mathbf{E}}{\partial t^2} - c_0^2 \cdot \nabla^2 \mathbf{E} = 0$$

$$\frac{\partial^2 \mathbf{B}}{\partial t^2} - c_0^2 \cdot \nabla^2 \mathbf{B} = 0$$

$$\vec{E} = \vec{e}\ e^{ik_0 S(r)}$$

$$\vec{H} = \vec{h}\ e^{ik_0 S(r)}$$

$$(\nabla S)^2 = n^2$$

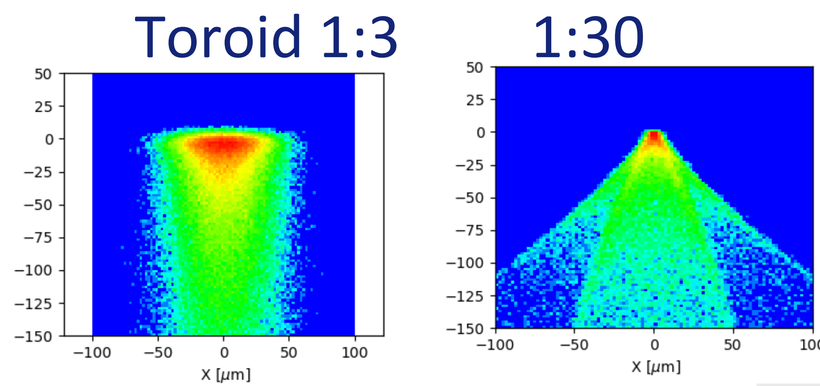
$$\nabla S = n\,\vec{s}$$

$$\frac{d}{ds}\left(n\frac{d\vec{r}}{ds}\right) = \nabla n$$

$$\nabla n = 0 \Rightarrow \frac{d\vec{r}}{ds} = 0 \Rightarrow \vec{r} = s\vec{a} + \vec{b}$$

ShadowOui | XOPpy

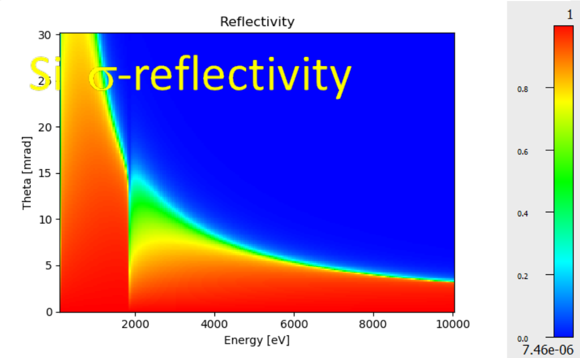
Evolved from SHADOW



Accurate values of

Beam sizes including cropping, and aberrations

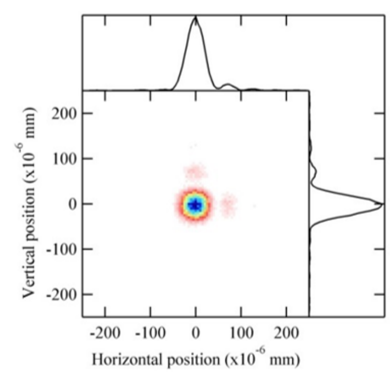
Flux including o.e. physical models (reflectivity transmittivity)



Monochromators/Analysers

Incoherent addition of rays (no interference/diffraction)

New features



Interoperability

Optical element deformation database DABAM (Sanchez del Rio *et al.* http://dx.doi.org/10.1107/S1600577516005014)

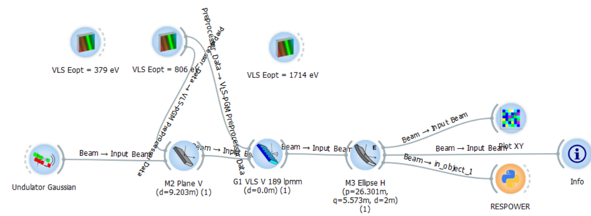
Corrections for coherence with Hybrid (Shi *et al.* http://dx.doi.org/10.1107/S160057751400650X)

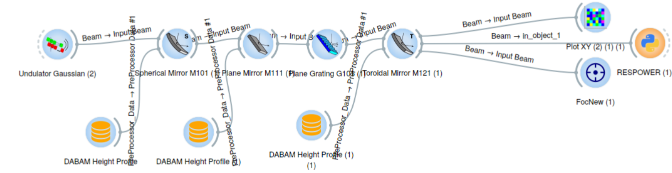
Power transport (Rebuffi *et al.* http://dx.doi.org/10.1107/S160057752000778X)

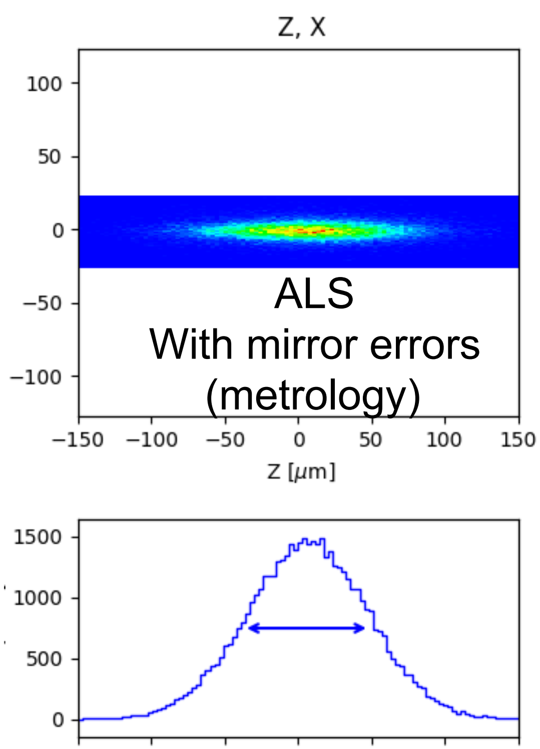
ALS->ALS-U WHAT HAPPENS IF WE USE THE NEW SOURCE WITH AN EXISTING BEAMLINE?

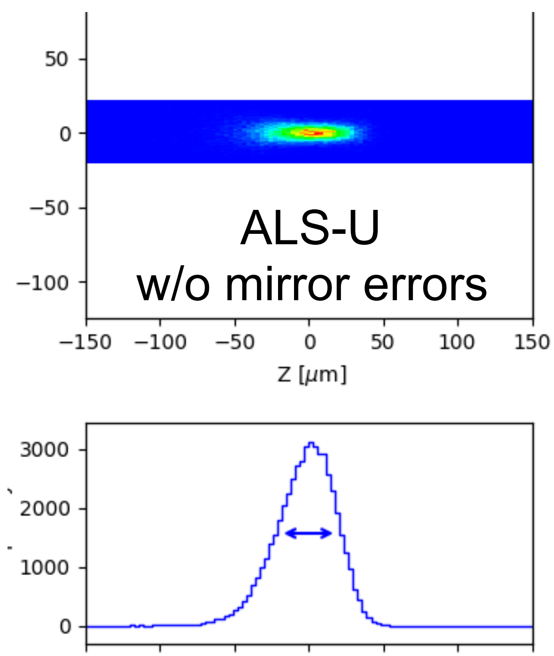
94 x 7 um (806eV)
RP~3000
source: 6.8e14 ph/s/0.1%bw

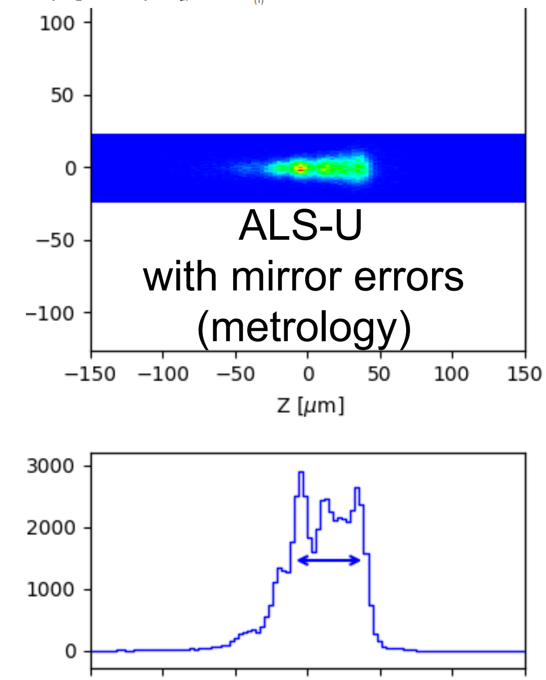
8.5 x 7 um (806eV)
RP~7000
source: 1.2e15 ph/s/0.1%bw











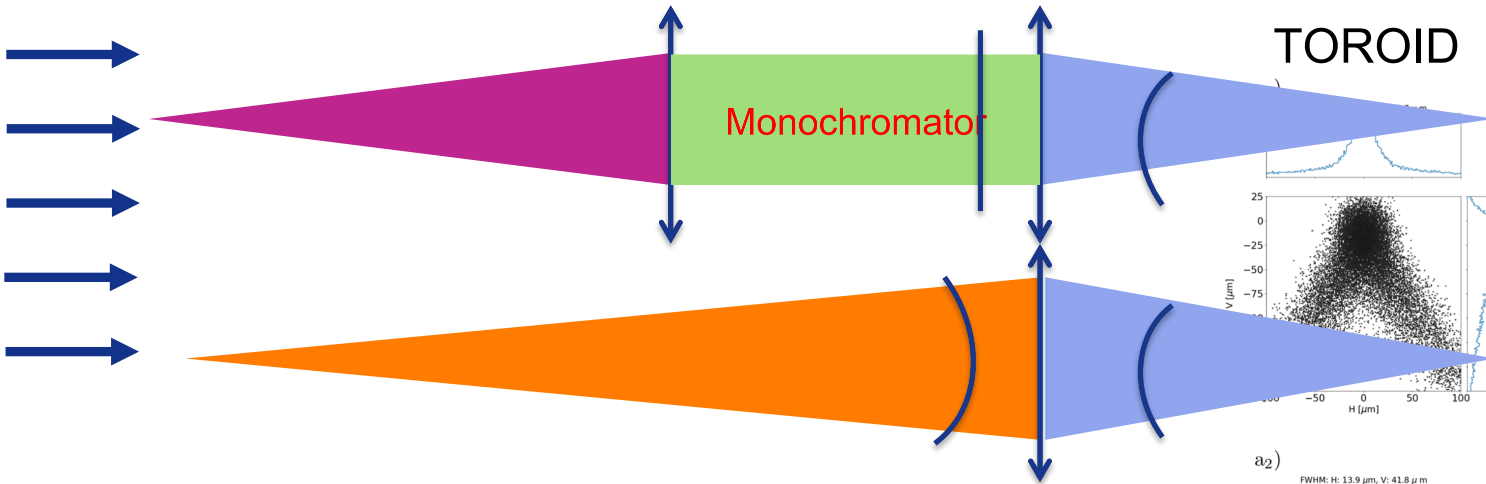
Current source w/slope

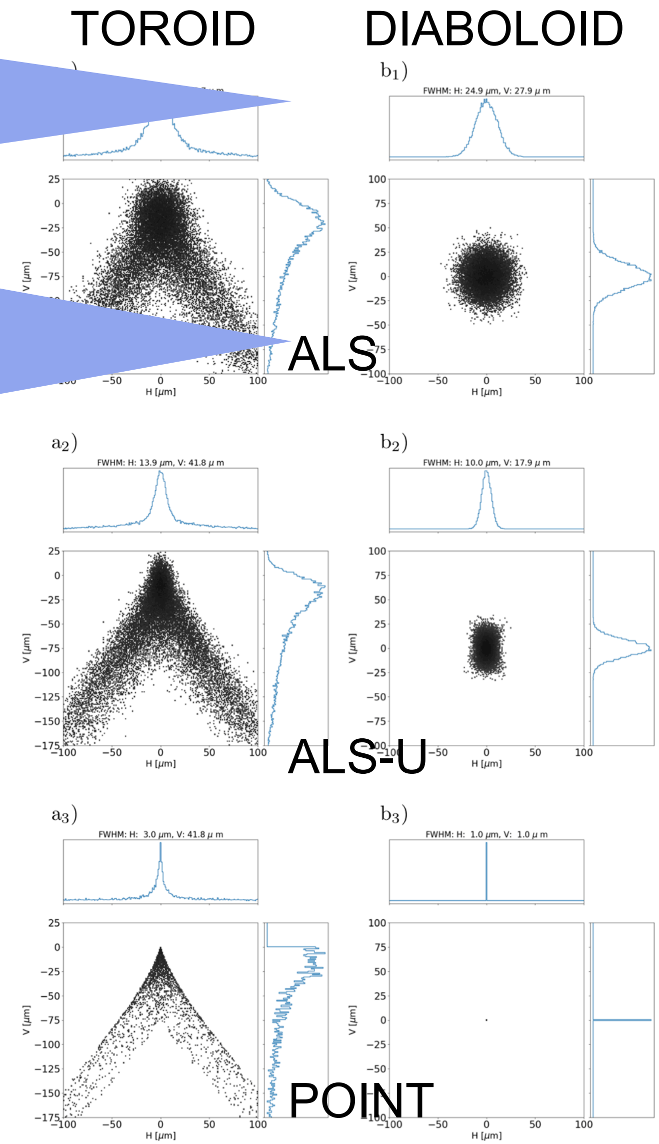
new source no/slope

new source w/slope

We need a new beamline!!

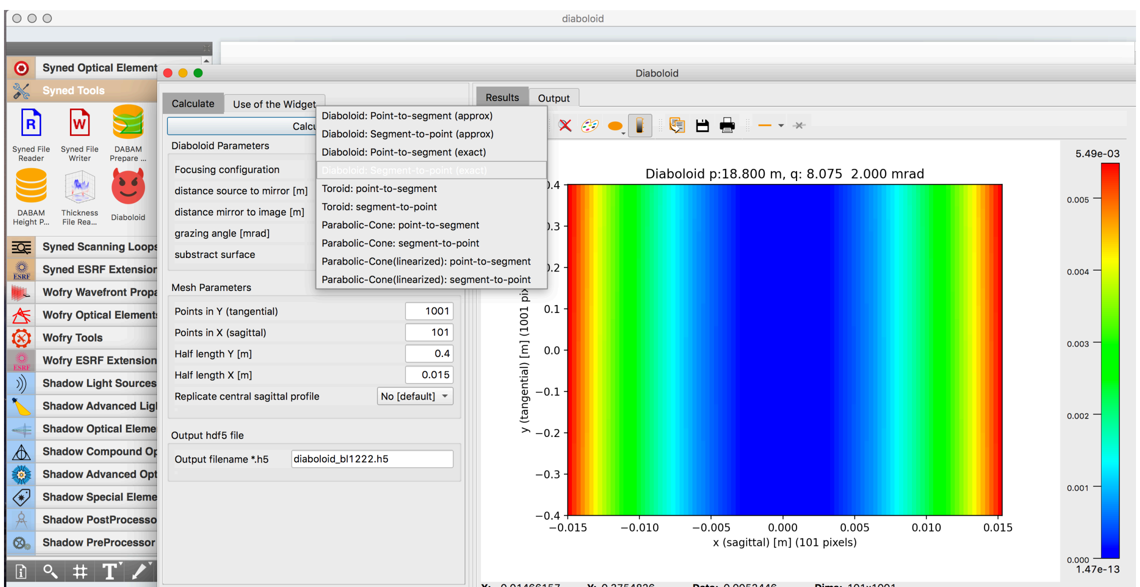
EXAMPLE OF RAY TRACING: DIABOLOID





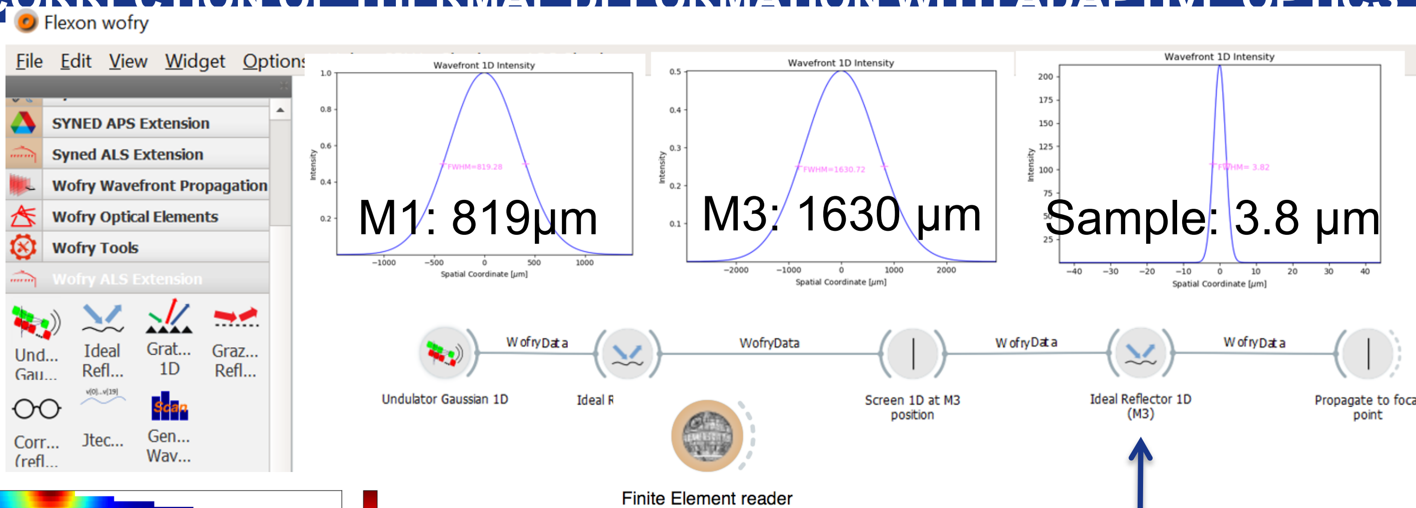
Approximated surface: Toroid (aberrations, good for 3rd SR, not for 4th)

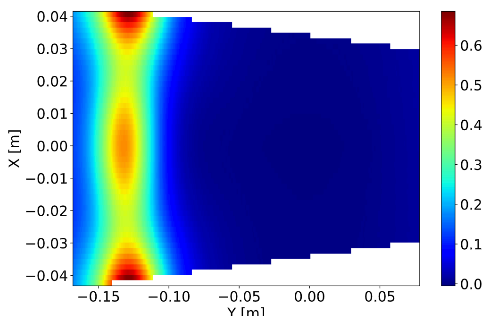
Exact surface: Diaboloid (converts a wavefront from cylindrical to spherical)

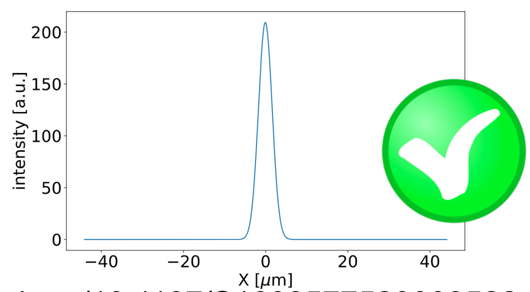


M. Sanchez del Rio et al, JSR 2021 https://doi.org/10.1107/S160057752100401X
V. Yashchuk et al. JSR 2021 https://doi.org/10.1107/S1600577521004860

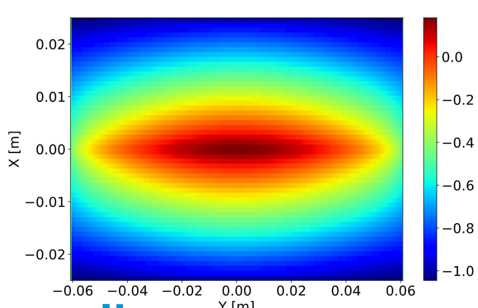
EXAMPLE OF WAVE OPTICS:
CORRECTION OF THERMAL DEFORMATION WITH ADAPTIVE OPTICS

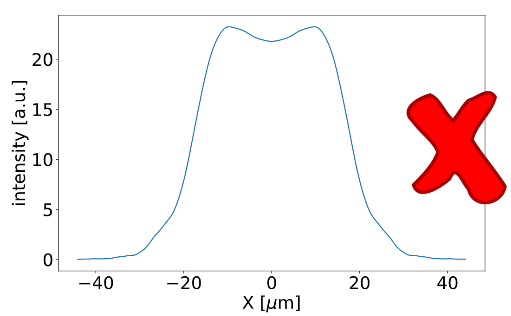


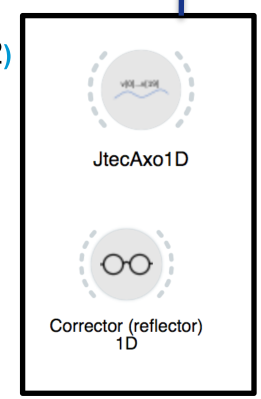


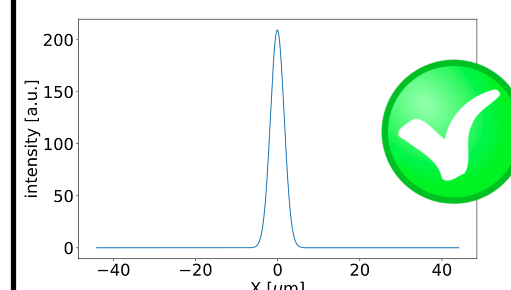


LN cooling Cutler *et al.* http://dx.doi.org/10.1107/S1600577520009522)









Water cooling

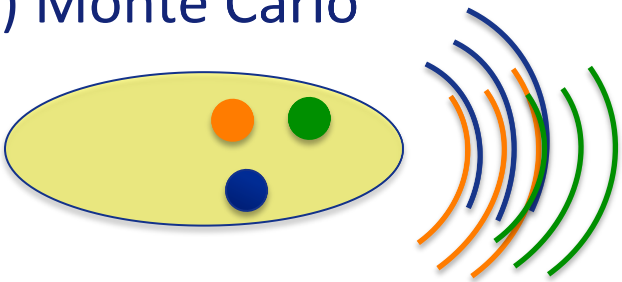
(CF ~ 0.8 with a 4 m undulator at 230 eV)

M. Sanchez del Rio et al, JSR 2020
http://dx.doi.org/10.1107/S1600577520009522

Partial coherence (work with several wavefronts)

$$< E^*(x_1,y_1)E(x_2,y_2) >= W(x_1,y_1,x_2,y_2)$$

1) Monte Carlo

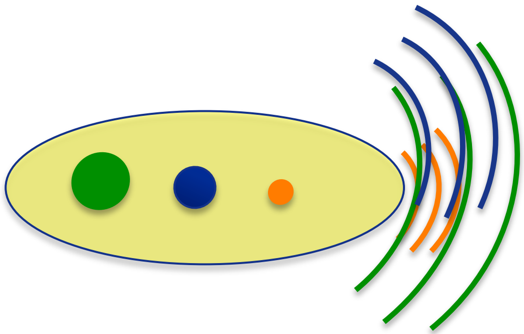


$N_x, N_y \in [100,1000]$.

W ~ $10^8 - 10^{12}$ (Gb-Tb)

- 4D W too big to calculate/store
- Not possible to calculate Coherent Fraction

2) Coherent Mode Decomposition



COMSYL (COherent Modes for SYnchrotron Light)
https://github.com/oasys-kit/comsyl

4D function — 2D functions

$$< E^*(x_1,y_1)E(x_2,y_2) >= W(x_1,y_1,x_2,y_2) = \sum_{i=0}^{\infty} \varphi_i \, \Phi_i^*(x_1,y_1)\, \Phi_i(x_2,y_2)$$

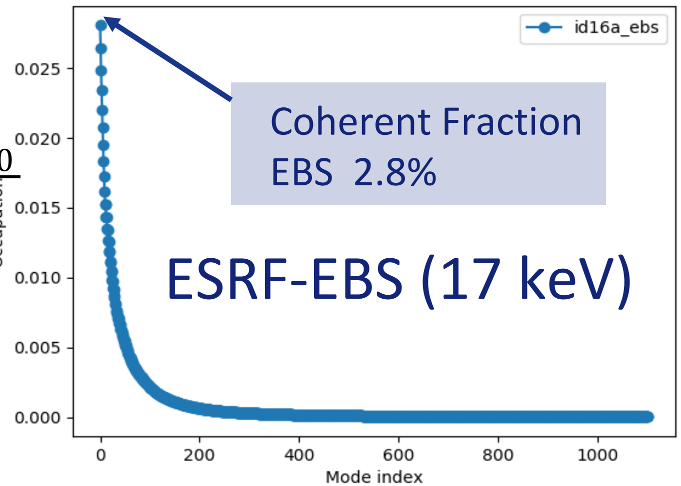
Store: m x N x N; Propagate: 2D integrals

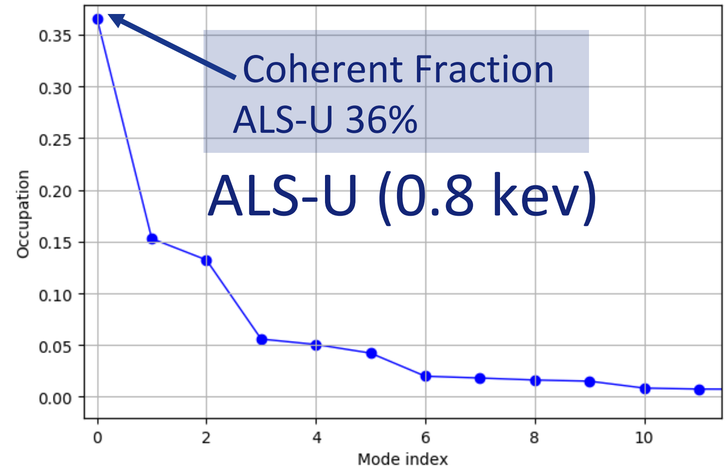
M Glass, M Sanchez del Rio, EPL Europhysics letters (2017)
http://dx.doi.org/10.1209/0295-5075/119/34004

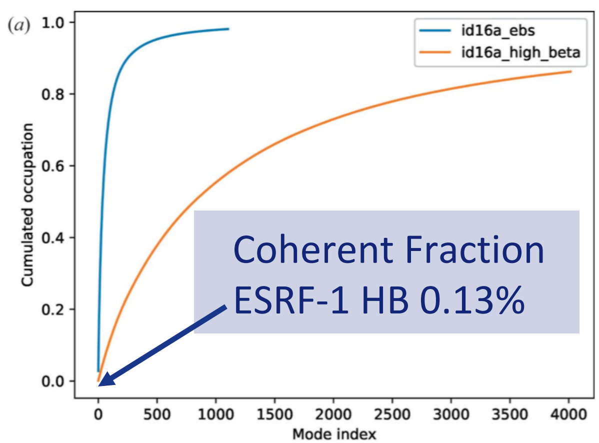
COHERENT MODE DECOMPOSITION: SPECTRUM OF MODES (OCCUPANCY)

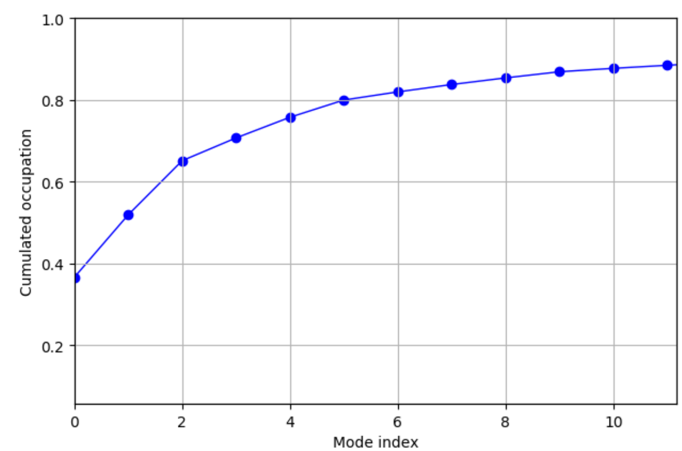
$$< E^*(x_1, y_1) E(x_2, y_2) > = W(x_1, y_1, x_2, y_2) = \sum^{\infty} \varphi_i \Phi_i^*(x_1, y_1) \Phi_i(x_2, y_2)$$

$$CF = \frac{\varphi_0}{\sum_{j=0}^{\infty} \varphi_j} = \frac{\varphi_0}{I}$$



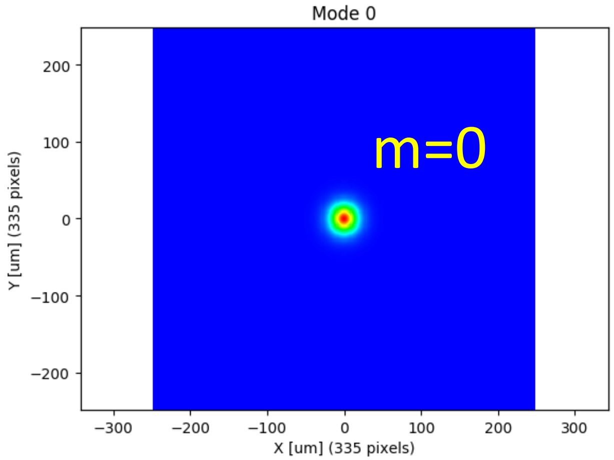


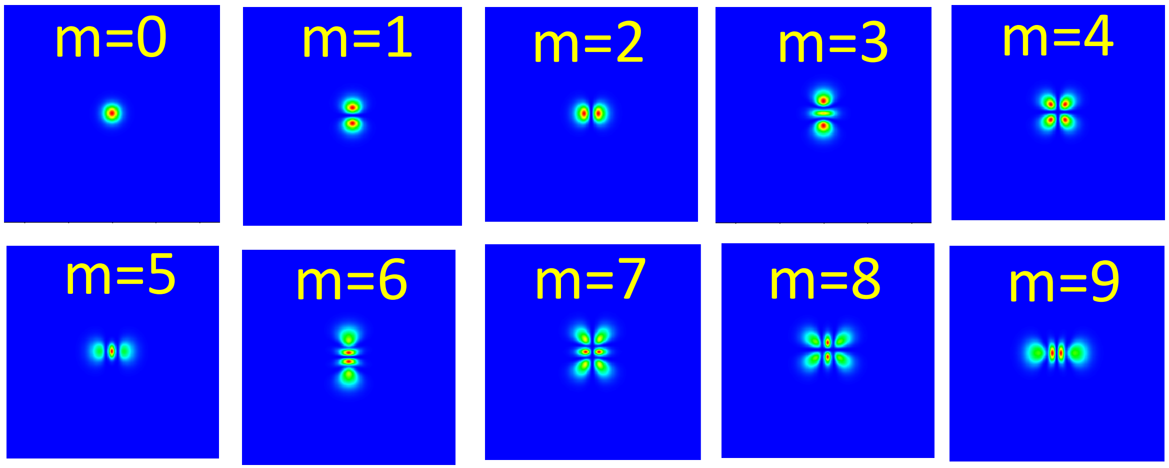




ALS-U U38 SOURCE 806 EV

$$< E^*(x_1,y_1)E(x_2,y_2) >= W(x_1,y_1,x_2,y_2) = \sum_{i=0}^{\infty} \varphi_i \Phi_i^*(x_1,y_1)\Phi_i(x_2,y_2)$$

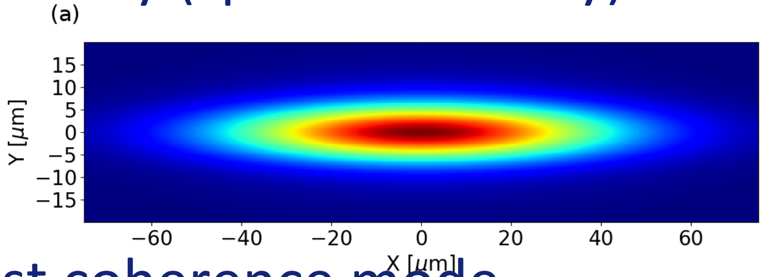




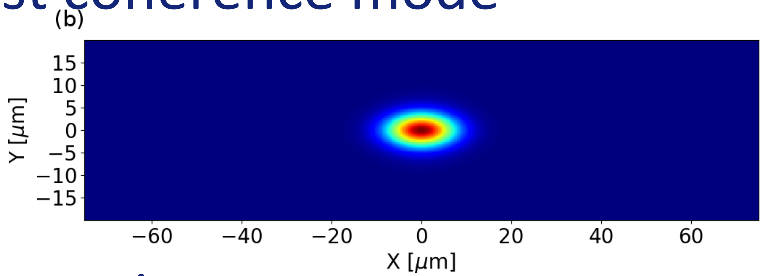
SINGULARITIES IN THE PHASE OF THE CROSS SPECTRAL DENSITY

COMSYL 1.4-m-long U18 EBS (6 GeV, 147 pm rad emittance)
Eo = 17.226keV (K =0.411)

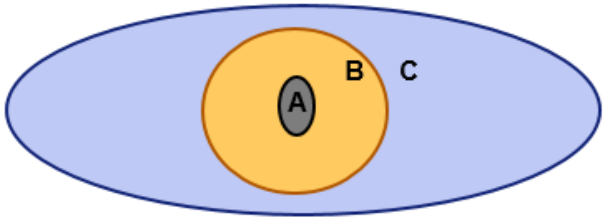
Intensity (spectral density)



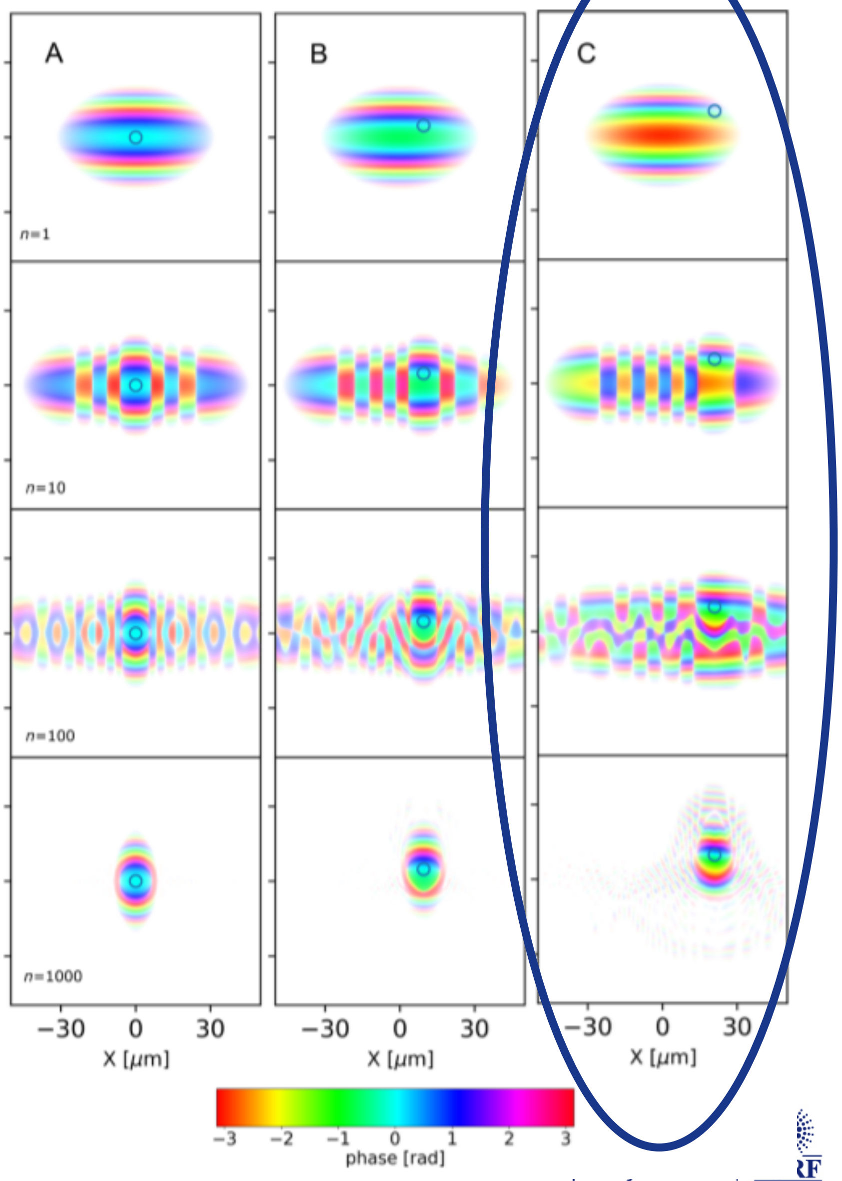
First coherence mode



Fix a point

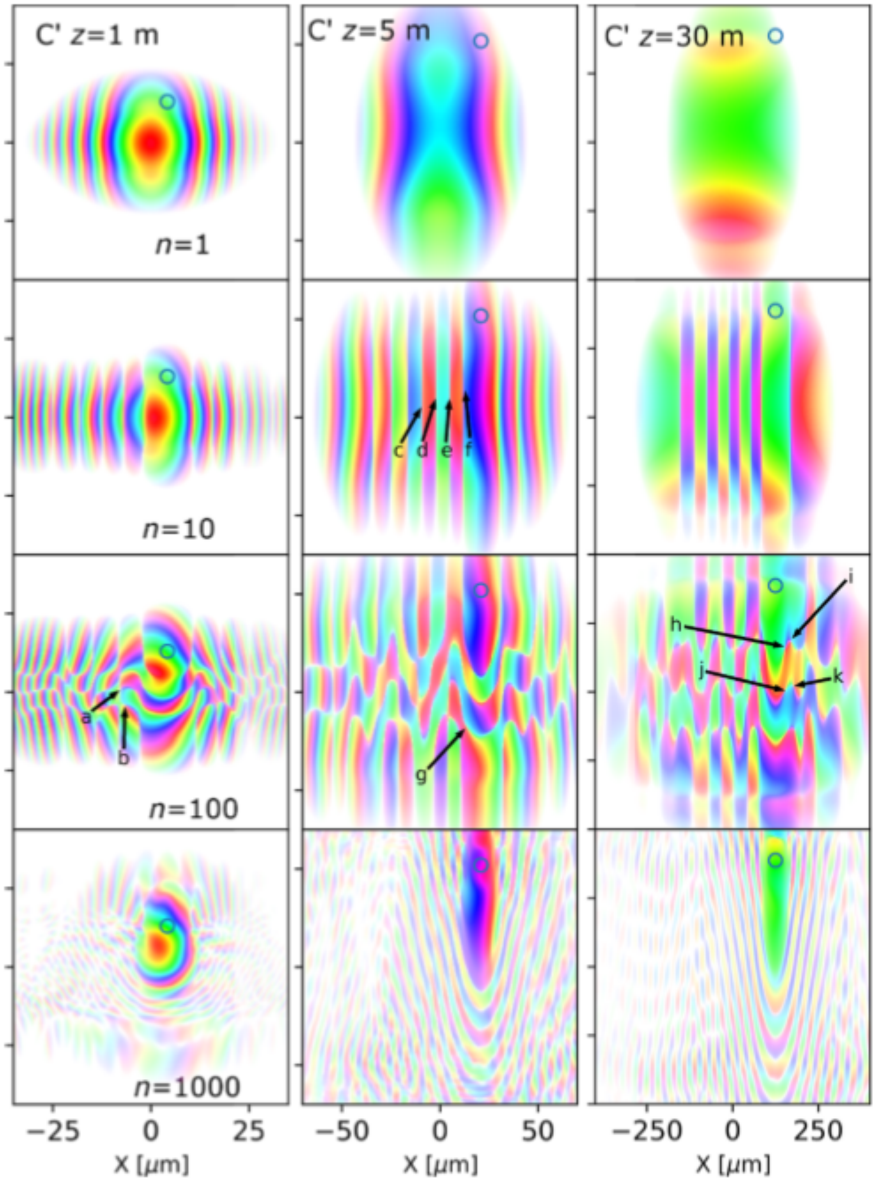


$arg[W(x,y,x_P,y_P)]$



D Paganin, M Sanchez del Rio, Phys Rev A (2019)
http://dx.doi.org/10.1103/PhysRevA.100.043813

PROPAGATED BEAM: DIFFERENT TYPES OF SINGULARITIES APPEAR



$$arg[W(x, y, x_P, y_P)]$$

Domain walls

Coherence vortices a,b, g

Vortex-antivortex hi,jk

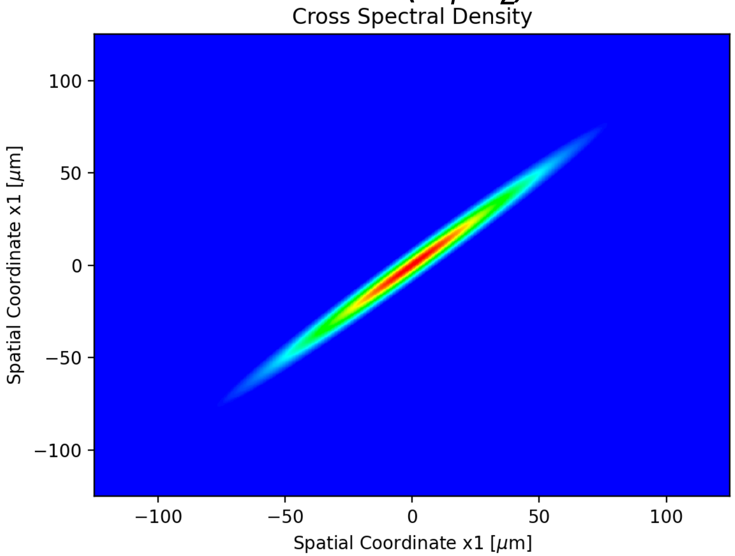
Halo of CSD speckle

D Paganin, M Sanchez del Rio, Phys Rev A (2019)
http://dx.doi.org/10.1103/PhysRevA.100.043813

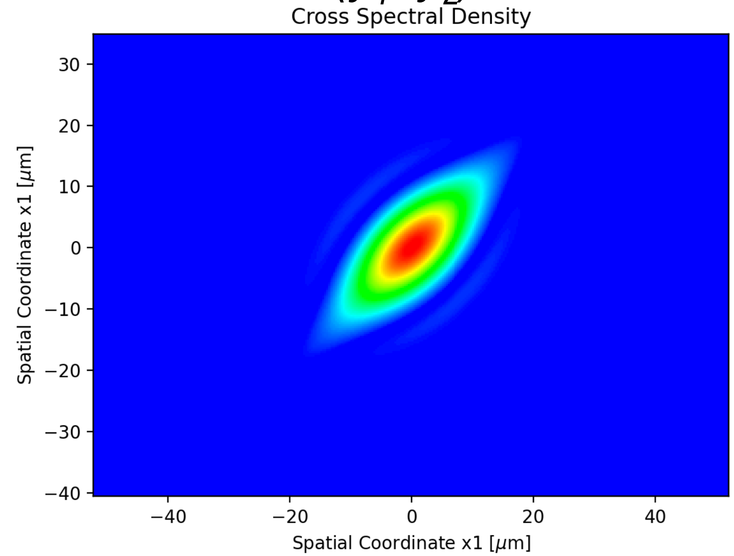
SIMPLER 1D CMD WITH WOFRY (EBS U18 2.5M 7 KEV)

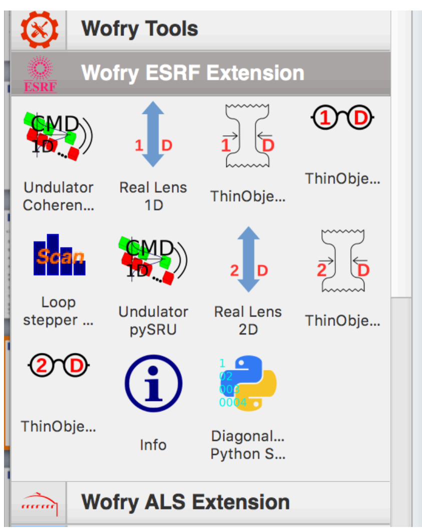
$$<E^*(x_1)E(x_2)> = W(x_1,x_2) = \sum_{i=0}^{\infty} \varphi_i \, \Phi_i^*(x_1)\, \Phi_i(x_2)$$

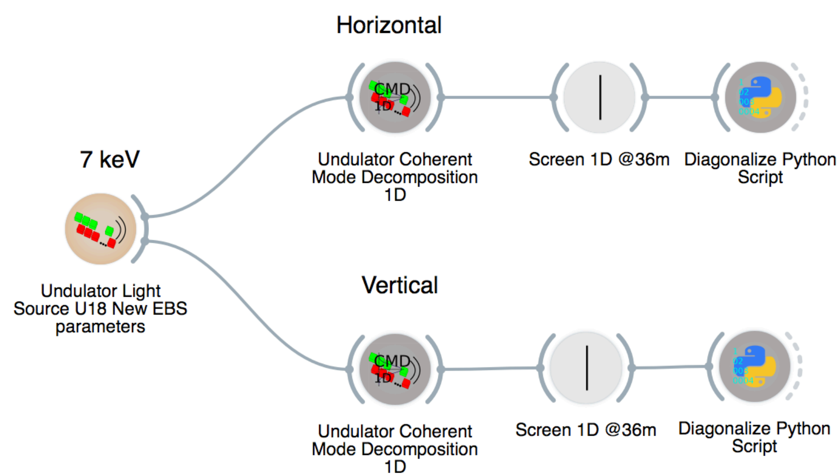
Horizontal $W(x_1,x_2)$



Vertical $W(y_1, y_2)$

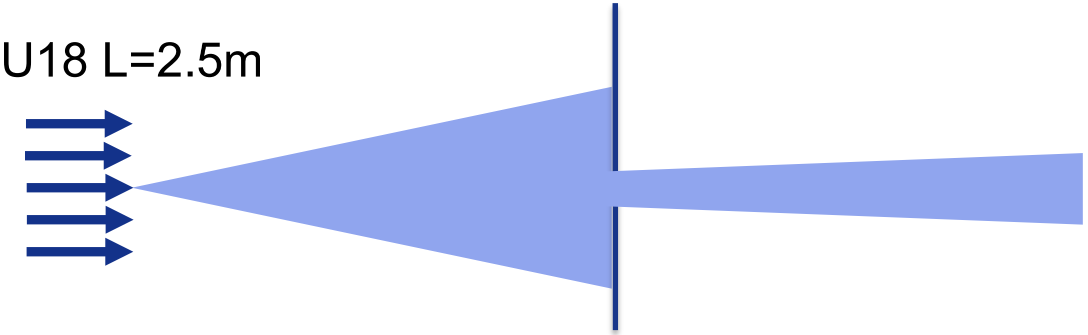


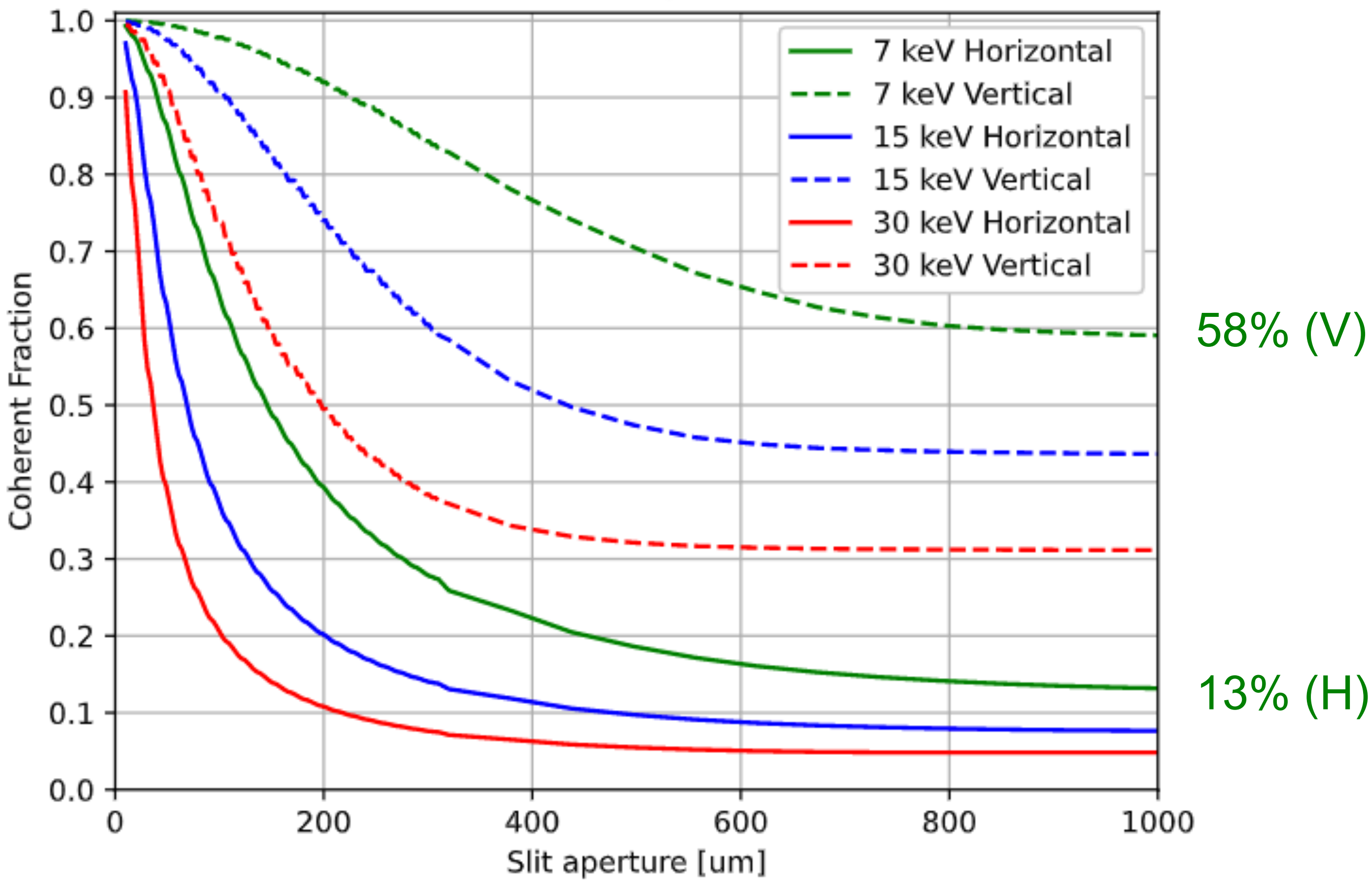




COHERENCE FRACTION MODIFICATION BY SLITS

EBS U18 L=2.5m





CRYSTAL OPTICS

PERFECTNESS

Dynamical theory of diffraction

Perfect plane crystals (Si, Ge, Diamond) 3-30 keV

Darwin/ Laue/Ewald/ James/ Zachariasen

Laue (transmission) > 30 keV

Bent (focusing)

Takagi- Taupin

High d-space (Quartz, etc) 2-5 keV

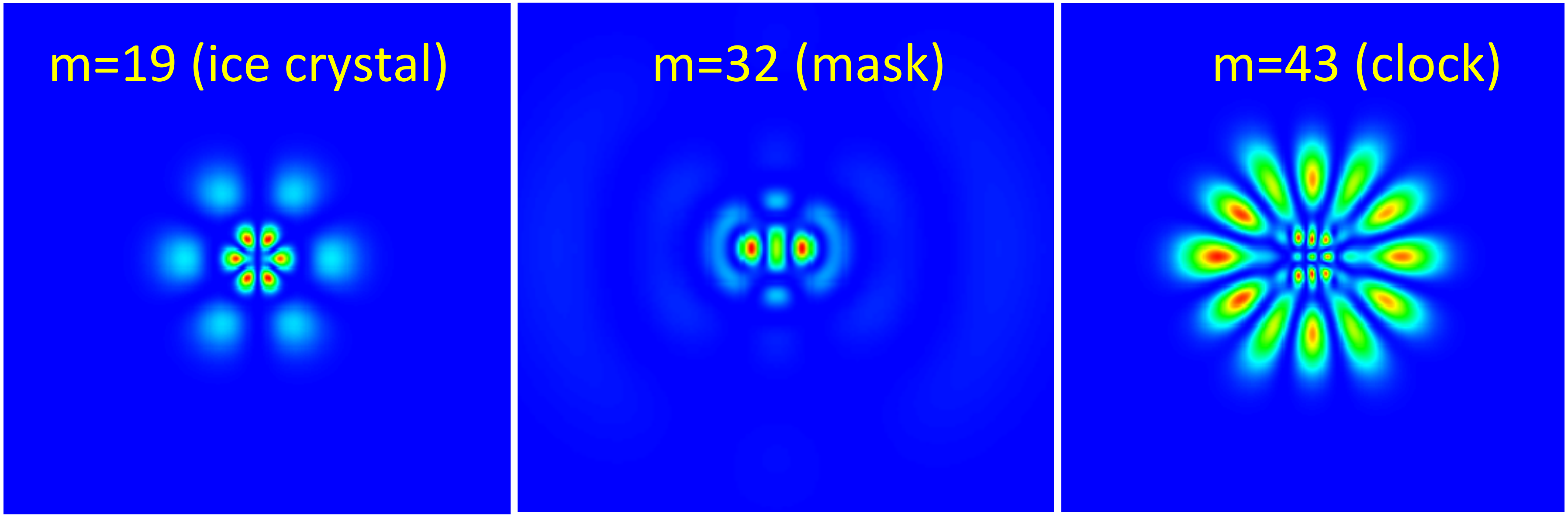
Zachariasen/ Sears

Ideally imperfect crystals (mosaic)

Mosaic crystals

THANK YOU!

Thank you very much



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ANL/APS: L Rebuffi, X Shi, R. Reininger, Y Shvyd'ko
Monash Univ.: D Paganin