Introduction to COMSYL

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U.S. DEPARTMENT OF ENERGY | Office of Science

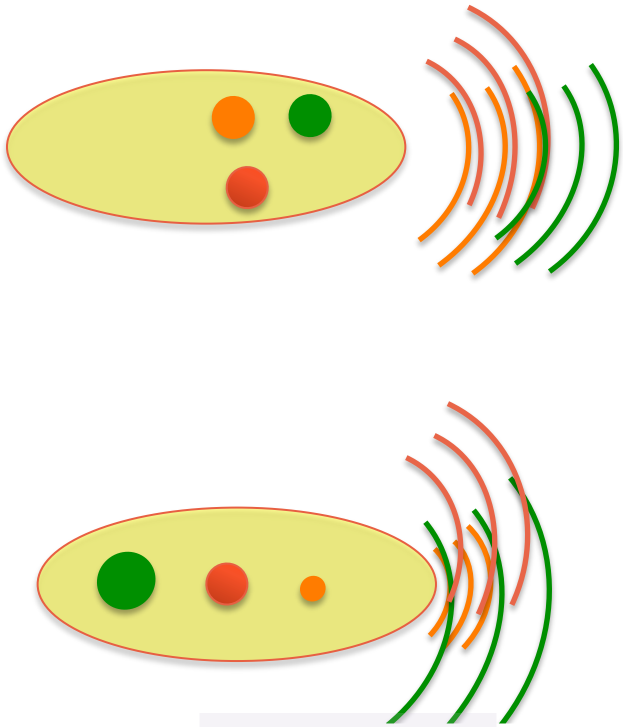
ALS ADVANCED LIGHT SOURCE

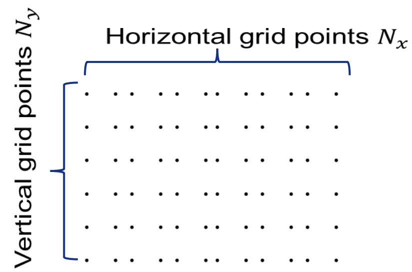
COMSYL

Coherent Modes of Synchrotron Light

(calculates the coherent modes for undulators in storage rings)

$$W(x_1, y_1, x_2, y_2, z, \omega) = \langle E^*(x_1, y_1, z, \omega) E(x_2, y_2, z, \omega) \rangle$$





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

W ~ 10^8 – 10^{12} (Gb-Tb)
Propagate: 4D integrals

4D function

2D functions

$$W(x_1, y_1, x_2, y_2, \omega) = \sum_m \lambda_m(\omega) \phi_m^*(x_1, y_1, \omega) \phi_m(x_2, y_2, \omega)$$

Store m x N x N Propagate: 2D integrals

Cross Spectral Density

- *Mutual* Coherent Function (t-dependency) or Cross *Spectral* Density (w-dependency)

- 8D function that propagates using a double wave equation

- Wide sense stationary: *W*≠0 if w_1=w_2=w
  Long bunch length, *high* w , *not to small* Dw
  Geloni et al. NIM A 588 463 (2008)

- Decoupling z: 4D function (for given z and w)

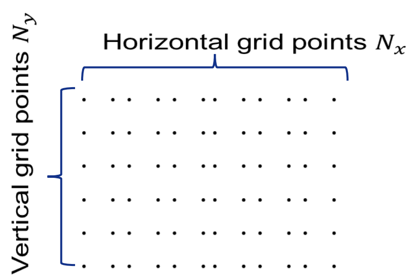
$$W(x_1, y_1, x_2, y_2, z, \omega) =$$
$$= \langle E^*(x_1, y_1, z, \omega) E(x_2, y_2, z, \omega) \rangle$$

- Spectral Density "intensity"

$$S(x, y, z, \omega) = W(x, y, x, y, z, \omega)$$

- Spectral Degree of Coherence

$$\mu(x_1, y_1, x_2, y_2, z, \omega) = \frac{W(x_1, y_1, x_2, y_2, z, \omega)}{\sqrt{S(x_1, y_1, z, \omega)}\sqrt{S(x_2, y_2, z, \omega)}}$$



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COMSYL (Coherent Modes for Synchrotron Light)

SRW

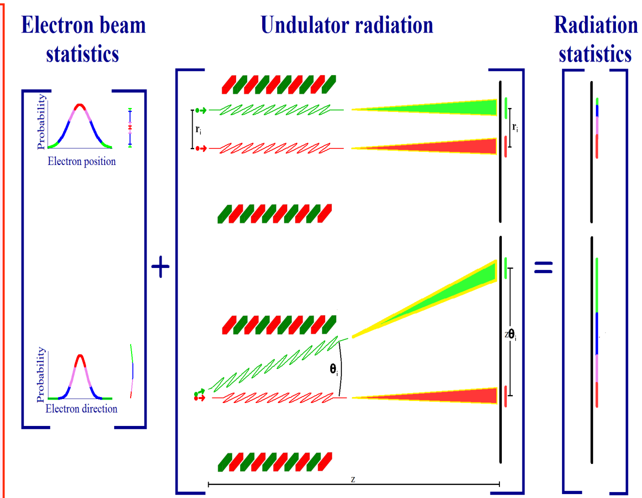
Undulator radiation

Calculate CSD

Coherent mode decomposition

COMSYL https://github.com/mark-glass/comsyl

Glass & Sanchez del Rio (2017) EPL 119 p 34004



K.-J. Kim Proc. SPIE 0582 (1986)

Propagate CSD along the beamline

Rediagonalize CSD

OASYS

Friedholm equation:

$$A_W[\phi_n] = \lambda_n \phi_n$$

$$A_W[f](\mathbf{r}_2) = \int W(\mathbf{r}_1, \mathbf{r}_2, \omega) f(\mathbf{r}_1) d\mathbf{r}_1$$

$$\mathrm{M}_{ij} = \langle b_i | A_W | b_j \rangle$$

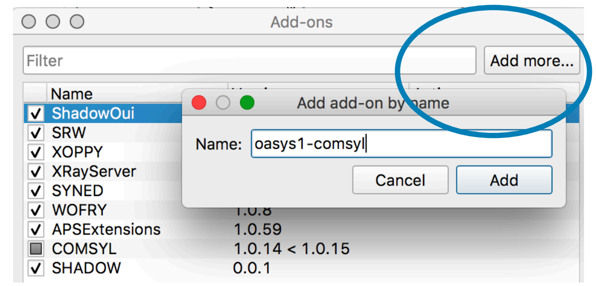
Diagonalize M with iterative solver slepc

- Large memory.
- Parallel computers using MPI.
- Large clusters (ESRF). Cloud computing (AWS, etc.)

Info COMSYL

- Repository: https://github.com/mark-glass/comsyl
- Installation: https://github.com/mark-glass/comsyl/wiki
- Paper: http://dx.doi.org/10.1209/0295-5075/119/34004
  Mark Glass, Manuel Sanchez del Rio (2017) Coherent modes of X-ray beams emitted by undulators in new storage rings EPL (Europhysics Letters) 119

Install Comsyl-Oasys (not for COMSYL calculations, only for displaying and propagating results)



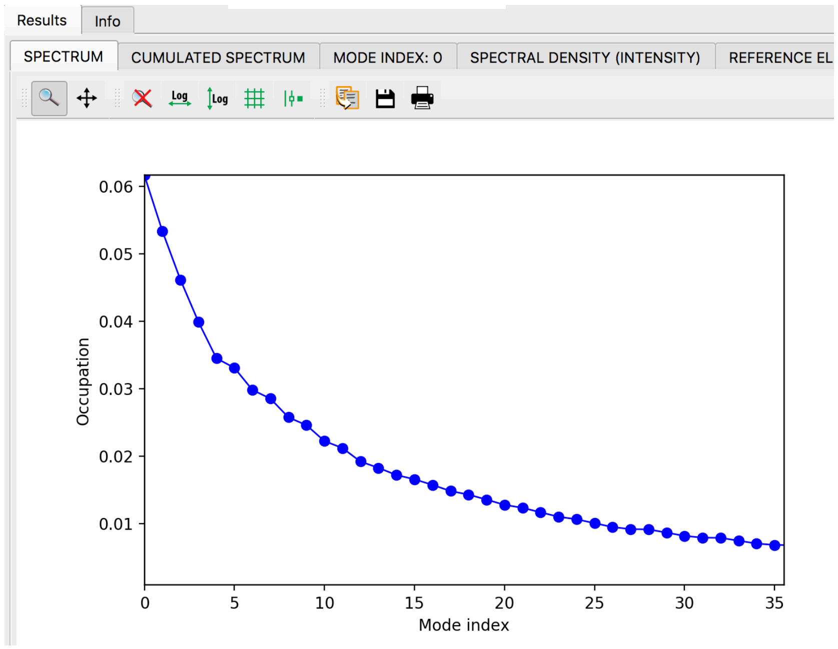
- Add-on
- Download 2 files (one BIG!!) from:
  https://anl.box.com/s/l9grzeul9d445eb1lijhxbkw46zdlkry
  or
  https://tinyurl.com/vcm6k2p

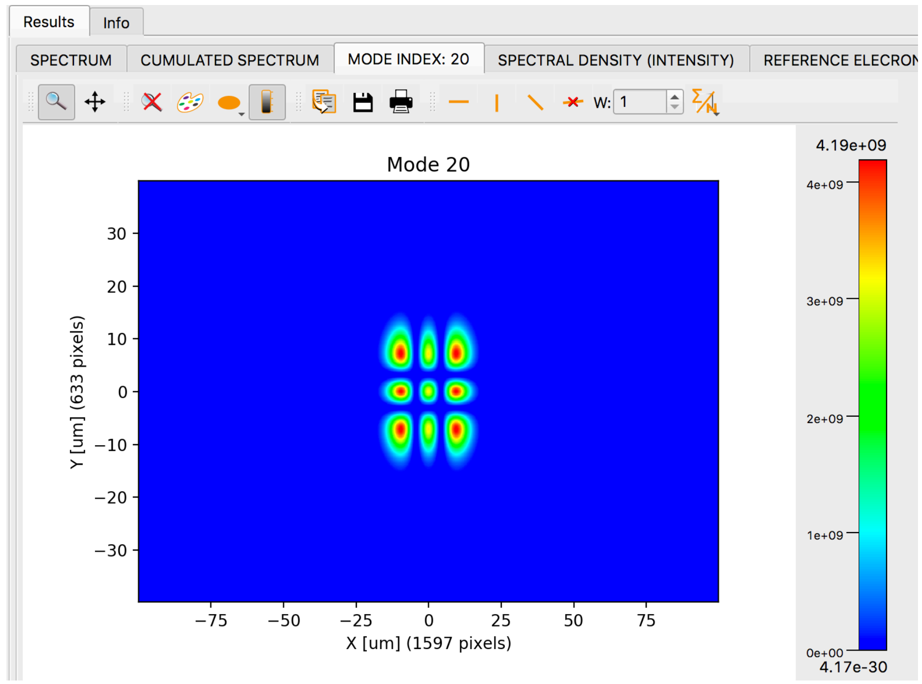
OASYS-COMSYL

Modes loader

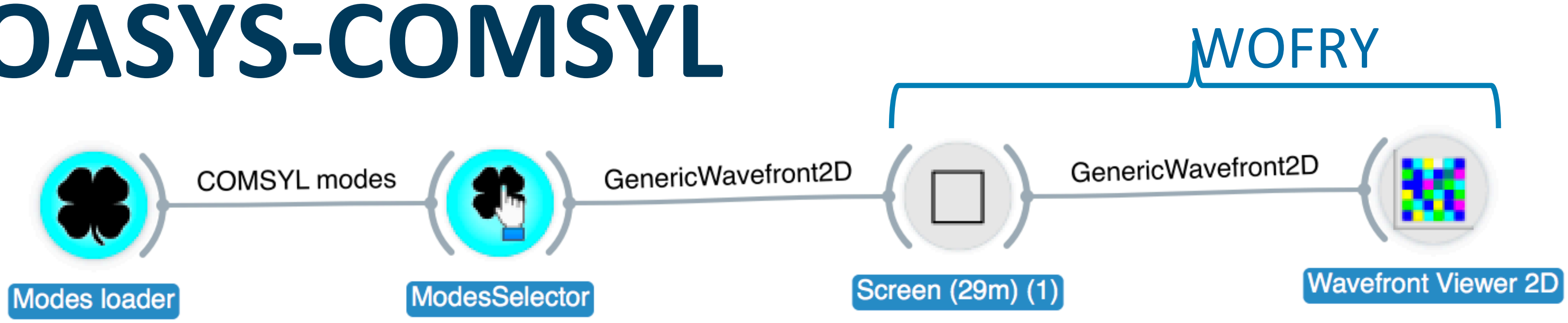
Read and visualize COMSYL calculations

Undulator ISN 25KeV: u_25keV_s10.0.npy



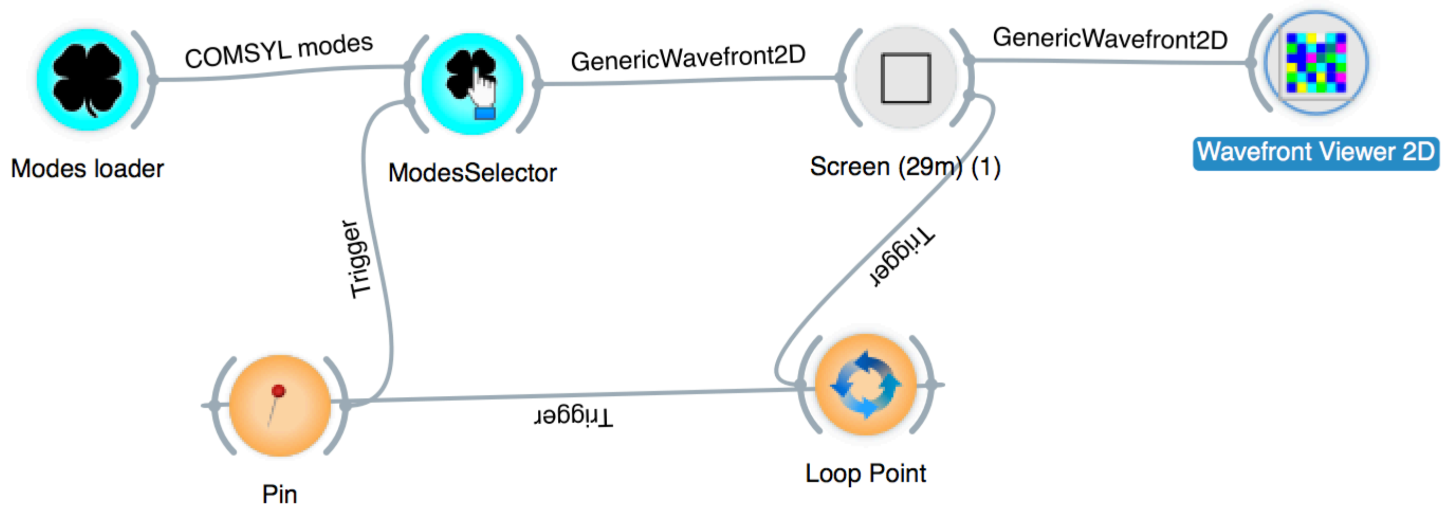


OASYS-COMSYL



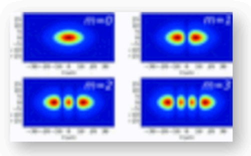
Extract wavefronts to propagate with WOFRY or SRW

Loop over number of modes:



COMSYL: ESRF ID16A

J. Synchrotron Rad. (2019). **26**, 1887-1901
https://doi.org/10.1107/S160057751901213X



A hierarchical approach for modeling X-ray beamlines: application to a coherent beamline

M. Sanchez del Rio, R. Celestre, M. Glass, G. Pirro, J. R. Herrera, R. Barrett, J. C. da Silva, P. Cloetens, X. Shi and **L. Rebuffi**

A hierarchical scheme of the calculations of an X-ray beamline for coherent applications is presented. Starting from simple calculations to partial coherence calculations, ray-tracing and wave optics software are applied to simulate the beamline performances

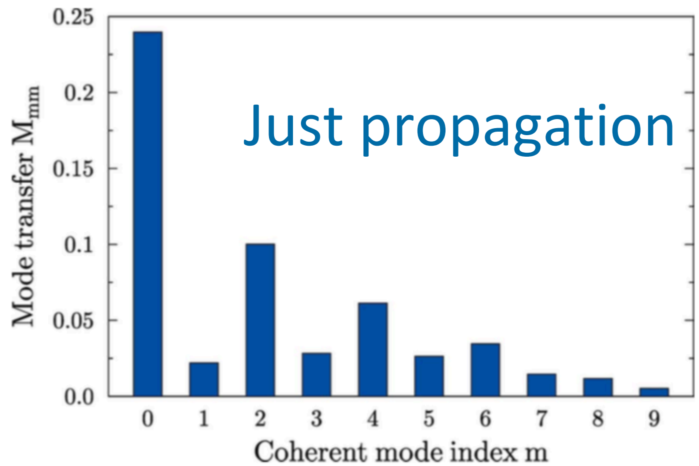


Figure 10
Transmission M_{mm} [see equation (11)] of the different modes of the EBS source due to the effect of propagation and cropping by the beamline optics.

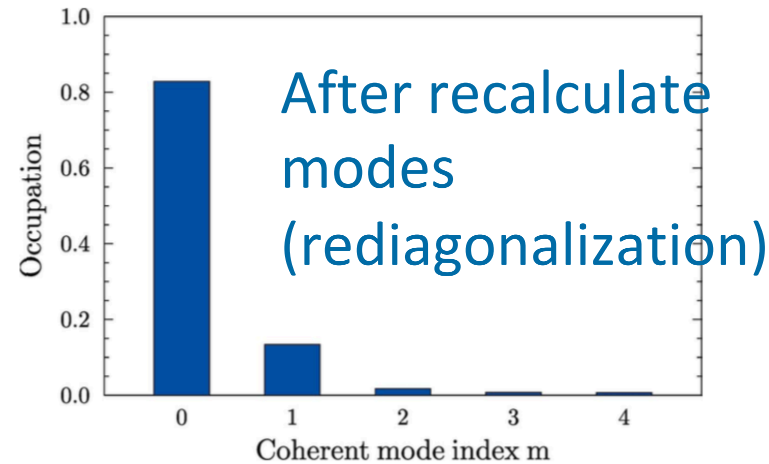
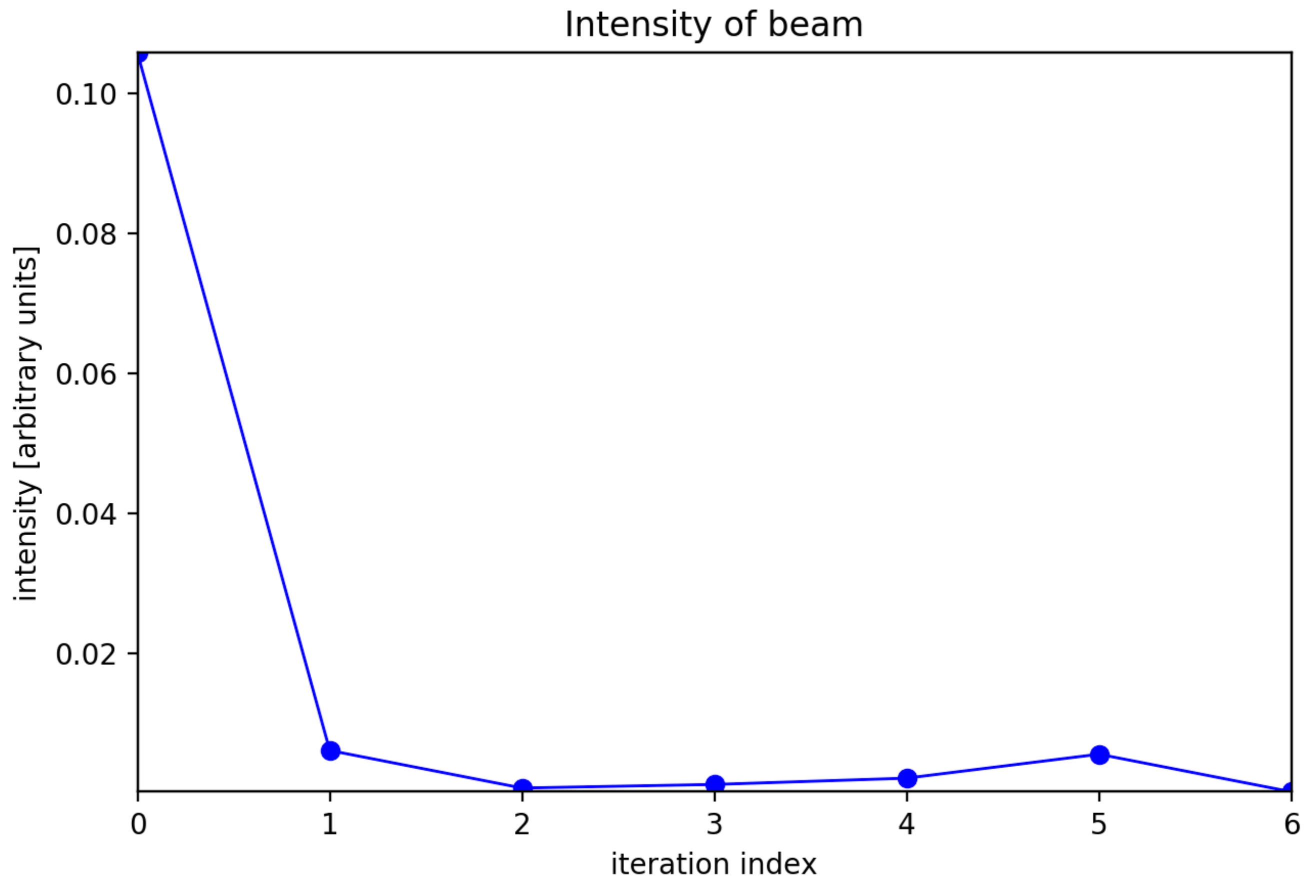


Figure 11
Occupation of the coherent modes of the final focused beam.

Mode transmission for ISN (draft!)



Exercise

- Couple COMSYL models with ISN beamline:
  - WOFRY
  - SRW (real optics, surface errors)
- Rediagonalize beam at focal position to compute coherent fraction

Advanced use of COMSYL
Study of singularities in W

PHYSICAL REVIEW A **100**, 043813 (2019)

Speckled cross-spectral densities and their associated correlation singularities for a modern source of partially coherent x rays

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Role of the phase of CSD

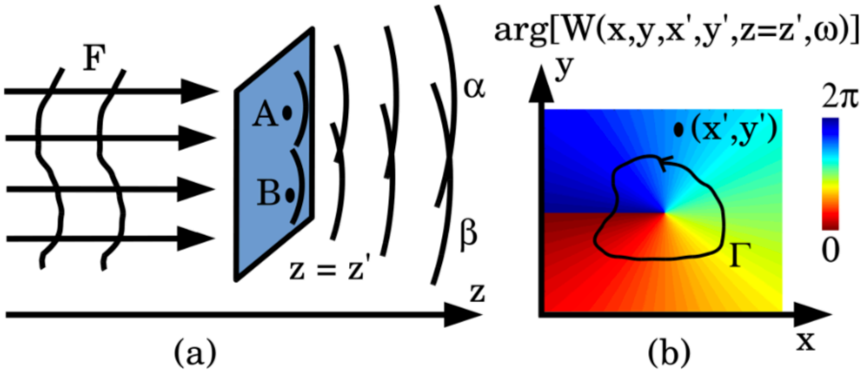


FIG. 1. (a) The cross-spectral density $W(x, y, x', y', z = z', \omega)$ associated with a statistically stationary field F quantifies the degree of correlation of the disturbance at points $(x, y, z) \equiv A$ and $(x', y', z' = z) \equiv B$. (b) For fixed (x', y'), ω and $z = z'$, the phase (arg) of $W(x, y, x', y', z = z', \omega)$ has a coherence vortex as a function of x and y, at a point enclosed within the contour Γ, about which the phase winds by an integer multiple m of 2π rad. Here $m = 1$. See Eq. (6).

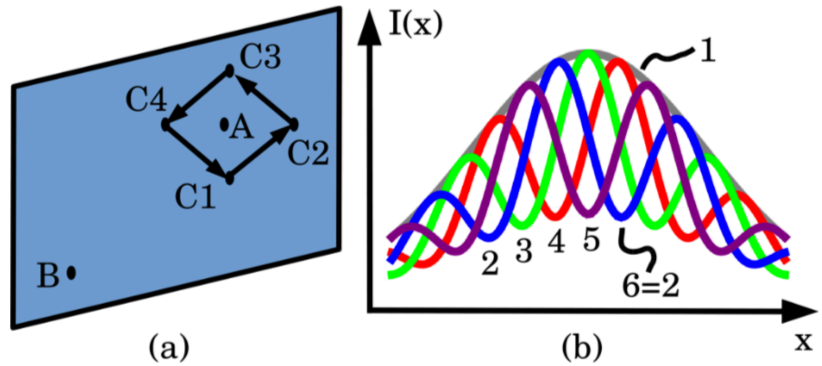
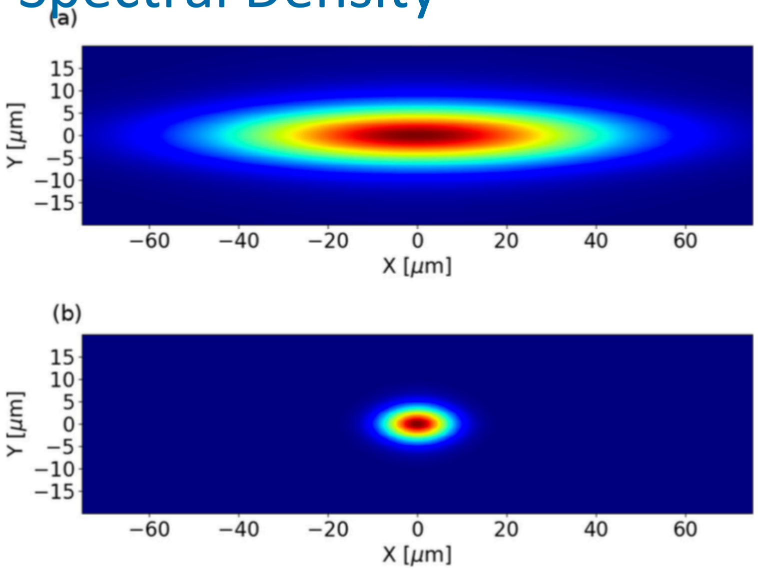


FIG. 2. Ratcheting of Young interferograms associated with $m = 1$ coherence vortex corresponding to the pair of points A, B. (a) A series of Young interferometers is constructed. In all setups, radiation illuminates a screen in which the first of two pinholes is always at B.

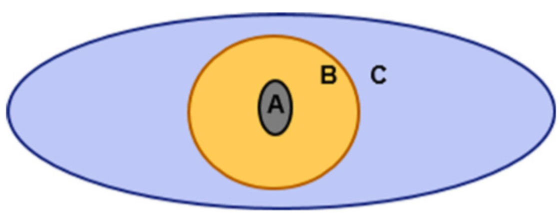
Arg[W] at Source position

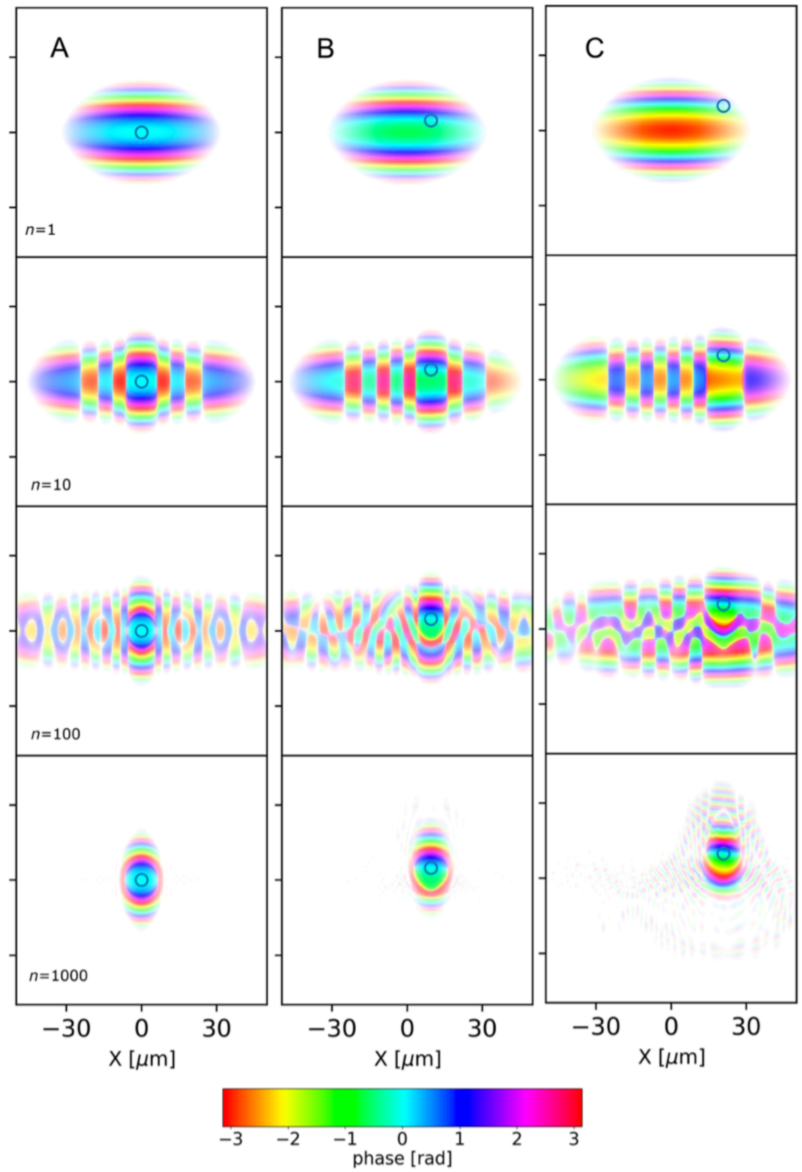
Spectral Density



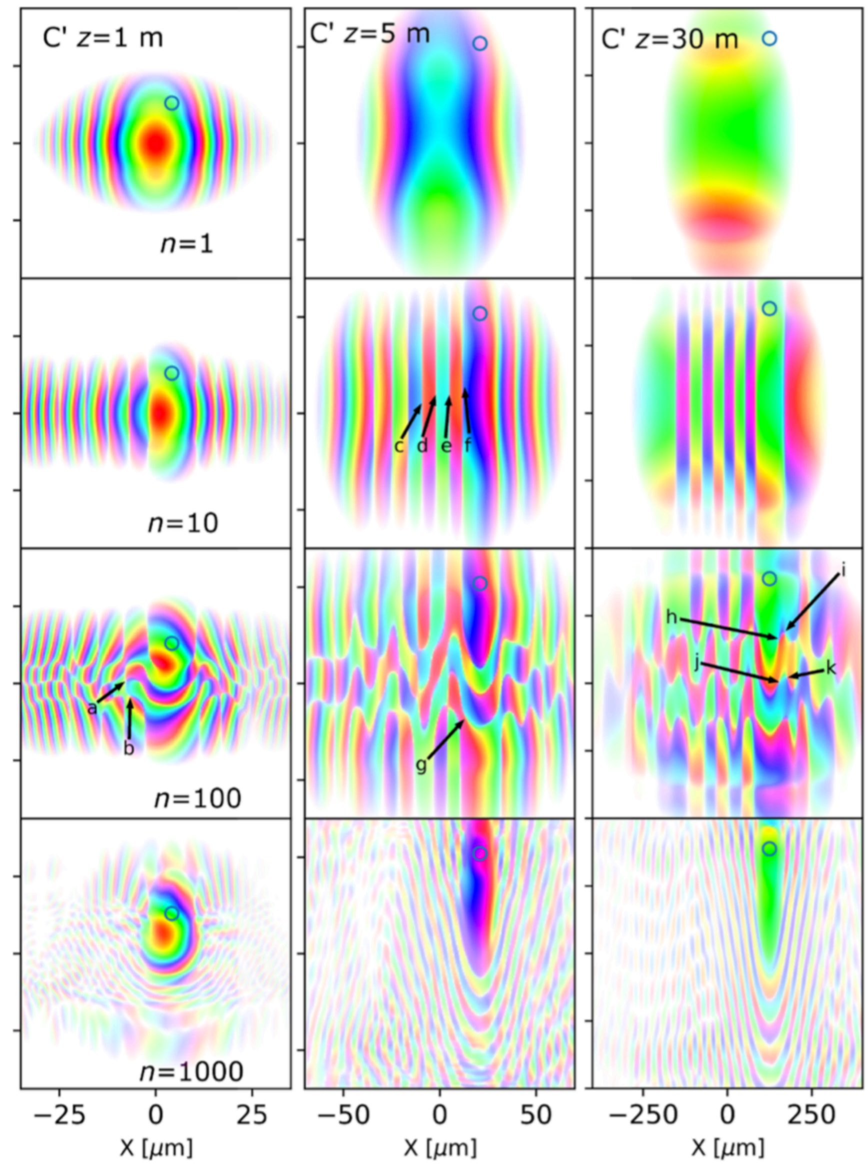
First coherent mode

Position of the fixed point



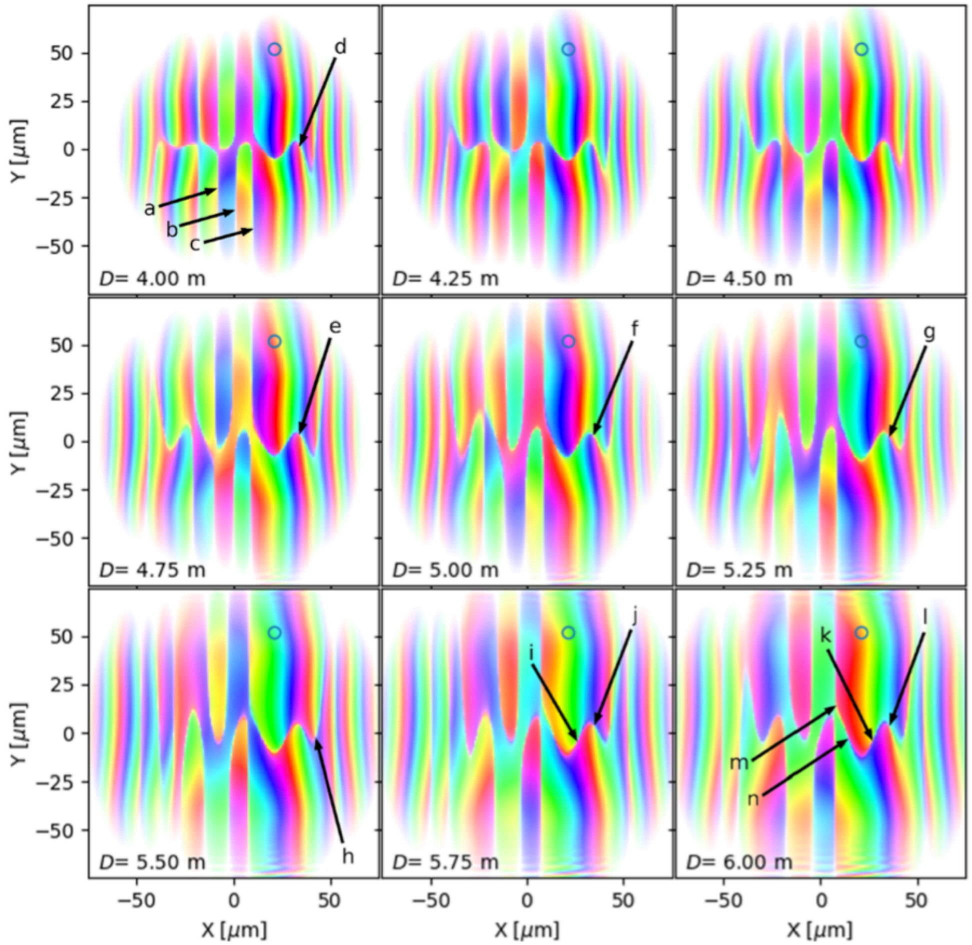


Propagated



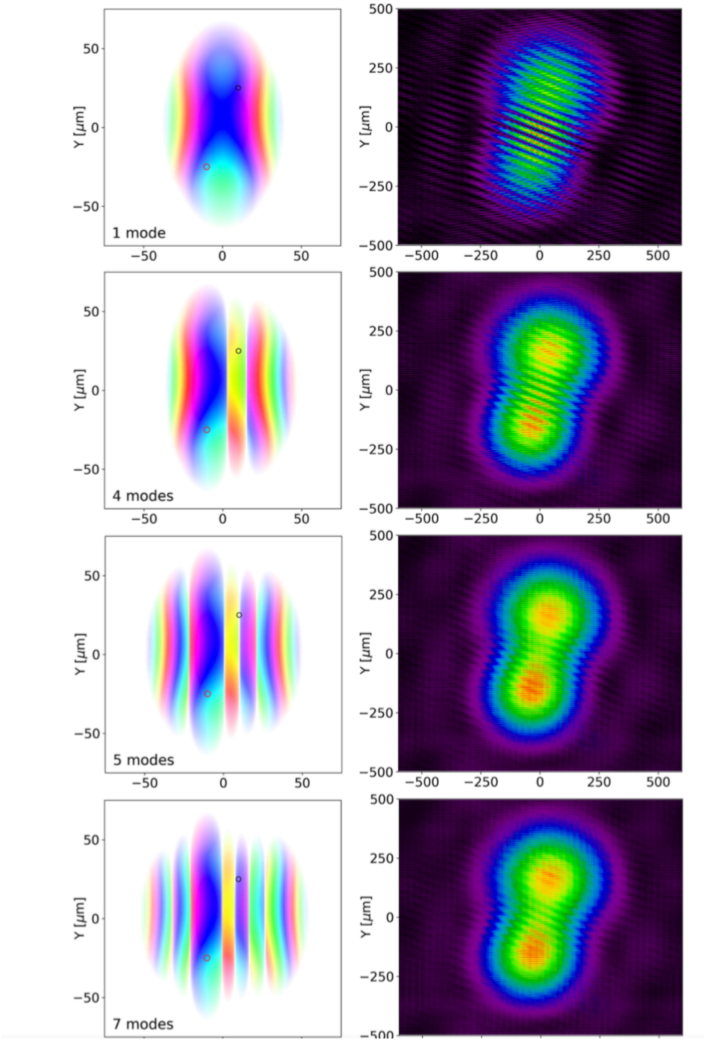
C' z=1 m
C' z=5 m
C' z=30 m
n=1
n=10
n=100
n=1000
a
b
c d e f
g
h
i
j
k
−25 0 25
X [μm]
−50 0 50
X [μm]
−250 0 250
X [μm]

Dynamics of singularities



- Coherence domain walls *a*, *b*, *c*
- Coherence vortices: *d* , *e*, *f* , *g*, *h*
- Vortex-antivortex pair *i j* is nucleated in passing from *D* = 5.50 m to *D* = 5.75 m

Visibility vs coherence

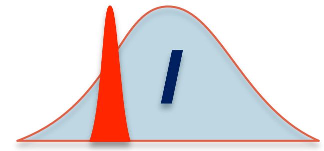


Coherence vortices and domain walls will exist in many nontrivial x-ray fields. Such correlation singularities influence the images that one takes, in ways that may lead to misleading results if one simply ignores their existence. Correlation singularities were seen to be present in the field generated by a modern x-ray undulator. Such singularities, which are not present in many simple models for partially coherent sources, were seen to imply a speckled structure in the associated cross-spectral density.

Gaussian Shell-Model

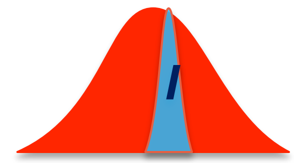
$$W(x_1, x_2, \omega) = A^2 e^{-(x_1^2+x_2^2)/(4\sigma_I^2)} e^{-(x_2-x_1)^2/(2\sigma_\mu^2)}$$

Both intensity (Spectral Density) and correlation (Spectral Degree of Coherence) are Gaussians



$S_I >> S_m$ the source is mostly incoherent (quasi homogeneous)

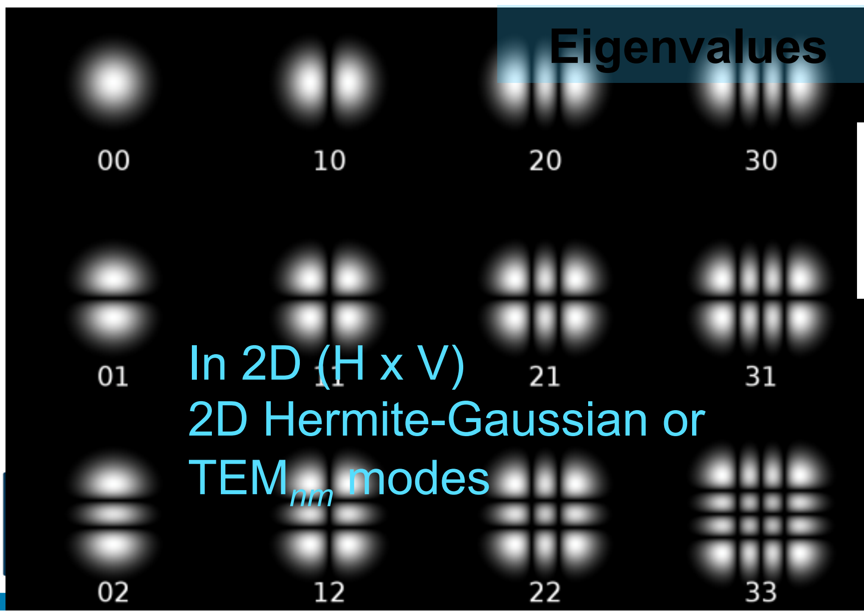
$S_I << S_m$ is mostly coherent



$$\beta = \frac{\sigma_\mu}{\sigma_I}$$

$$W(x_1, x_2, \omega) = \sum_n \boxed{\lambda_n(\omega)} \boxed{\phi_n^*(x_1, \omega)} \boxed{\phi_n(x_2, \omega)},$$

Eigenvalues



In 2D (H x V)
2D Hermite-Gaussian or TEM_{nm} modes

Eigenfunctions (Hermite-Gaussian modes)

$$\phi_n(x) = \left(\frac{2c}{\pi}\right)^{1/4} \frac{1}{\sqrt{2^n n!}} H_n(x\sqrt{2c}) e^{-cx^2}$$

Magic property: Propagation invariance

In the first mode (Gaussian) : $\boxed{\sigma_x \sigma_\theta = \frac{\lambda}{4\pi}}$

The spectrum of coherent modes

Eigenvalues

$$\lambda_n = A\left(\frac{\pi}{a+b+c}\right)^{1/2}\left(\frac{b}{a+b+c}\right)^n$$

$$a(\omega) = \frac{1}{4\sigma_I{}^2(\omega)}, \qquad b(\omega) = \frac{1}{2\sigma_\mu{}^2(\omega)} \qquad c = (a^2 + 2ab)^{1/2}$$

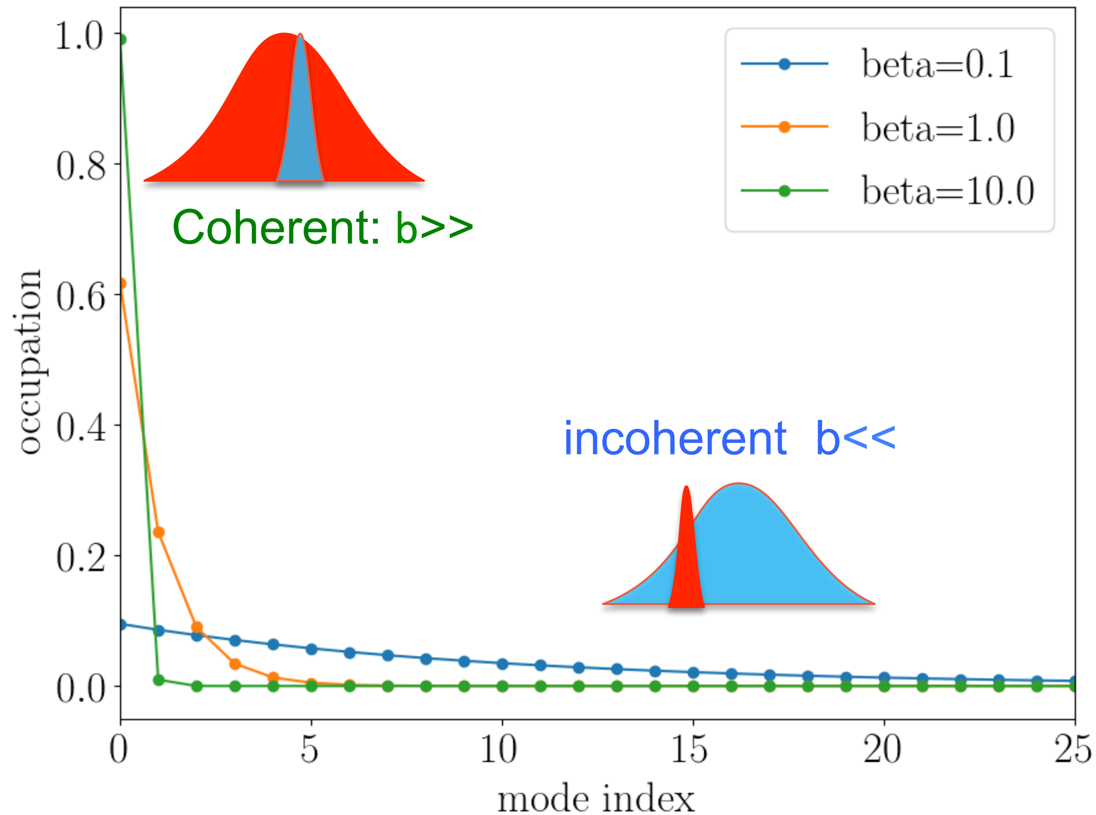
$$\beta = \frac{\sigma_\mu}{\sigma_I}$$

Mode occupation:

$$\eta_i(\omega) = \frac{\lambda_i(\omega)}{\sum_{n=0}^{\infty} \lambda_n(\omega)}$$

Coherent fraction:

$$CF = \frac{\lambda_0}{\sum \lambda_n}$$



In general we cannot apply Gaussian Shell-model to synchrotron