High-Accuracy Partially- and Fully-Coherent Wavefront Propagation Calculations for Storage Ring and FEL Sources





O. Chubar, NSLS-II, BNL "Software for Optical Simulations" Workshop Trieste, Italy, October 3 - 7, 2016



Outline

- Basics of Synchrotron Radiation (SR) calculation
- Basics of radiation Wavefront Propagation using Fourier Optics and compatible methods
- SR calculation examples; comparison with experiments
- Examples of Partially-Coherent SR propagation calculations for beamlines in Low-Emittance storage rings
- Example of Time-/Frequency-dependent Wavefront Propagation calculation for X-FEL applications
- Summary and comments

Emission by a Relativistic Charged Particle in Free Space: Retarded Potentials Approach

Exact expression, valid in the Near Field:

$$\vec{E}_{\omega} = iec^{-1}\omega \int_{-\infty} [\vec{\beta}_e - [1 + ic/(\omega R)] \cdot \vec{n}] R^{-1} \exp[i\omega(\tau + R/c)] d\tau \qquad (\checkmark)$$

The equivalence of ($\sqrt{}$) to the well-known expression of Jackson can be shown by integration by parts

$$\vec{E}_{\omega} = ec^{-1} \int_{-\infty}^{+\infty} \frac{\vec{n} \times [(\vec{n} - \vec{\beta}_e) \times \vec{\beta}_e] + cR^{-1}\gamma^{-2}(\vec{n} - \vec{\beta}_e)}{R \cdot (1 - \vec{n} \cdot \vec{\beta}_e)^2} \cdot \exp[i\omega(\tau + R/c)]d\tau$$

Emission by a Relativistic Charged Particle Efficient Computation

Exact expression obtained from Retarded Potentials:

$$\vec{E}_{\omega} = iec^{-1}\omega \int_{-\infty}^{+\infty} [\vec{\beta}_e - [1 + ic/(\omega R)] \cdot \vec{n}] R^{-1} \exp[i\omega(\tau + R/c)] d\tau$$

Phase expansion valid in the Near Field:

$$\omega \cdot (\tau + R/c) \approx \Phi_0 + \frac{\pi}{\lambda} \left[s\gamma^{-2} + \int_0^S |\vec{\beta}_{e\perp}|^2 d\vec{s} + \frac{(x - x_e)^2 + (y - y_e)^2}{z - s} \right]$$

Particle dynamics in external magnetic field:

$$\vec{r}_e = \vec{r}_e(s, \vec{r}_{e0}, \vec{\beta}_{e0}); \ \vec{\beta}_e \approx d\vec{r}_e/ds$$

Asymptotic expansion of the radiation integral (to accelerate computation):

$$\int_{-\infty}^{+\infty} F \exp(i\Phi) ds = \int_{s_1}^{s_2} F \exp(i\Phi) ds + \int_{-\infty}^{s_1} F \exp(i\Phi) ds + \int_{s_2}^{+\infty} F \exp(i\Phi) ds$$
$$\int_{-\infty}^{s_1} F \exp(i\Phi) ds + \int_{s_2}^{+\infty} F \exp(i\Phi) ds \approx \left[\left(\frac{F}{i\Phi'} + \frac{F'\Phi' - F\Phi''}{\Phi'^3} + \dots \right) \exp(i\Phi) \right]_{s_2}^{s_1}$$

Temporally-Incoherent and Coherent Spontaneous Emission by Many Electrons

Electron Dynamics:

$$\begin{array}{c} x_{e} \\ y_{e} \\ z_{e} \\ \beta_{xe} \\ \beta_{xe} \\ \beta_{ye} \\ \delta\gamma_{e} \end{array} \right| = \mathbf{A}(\tau) \begin{pmatrix} x_{e0} \\ y_{e0} \\ z_{e0} \\ x'_{e0} \\ y'_{e0} \\ \delta\gamma_{e0} \end{pmatrix} + \mathbf{B}(\tau) + \mathbf{B}(\tau)$$

Spectral Photon Flux per unit Surface emitted by the whole Electron Beam:

$$\frac{dN_{ph}}{dtdS(d\omega/\omega)} = \frac{c^{2}\alpha I}{4\pi^{2}e^{3}} \left\langle \left| \vec{E}_{\omega} \right|^{2} \right\rangle \qquad \text{``Incoherent'' SR} \\ \left\langle \left| \vec{E}_{\omega} \right|^{2} \right\rangle = \int \left| \vec{E}_{\omega0}(\vec{r}; x_{e0}, y_{e0}, z_{e0}, x'_{e0}, y'_{e0}, \delta\gamma_{e0}) \right|^{2} f(x_{e0}, y_{e0}, z_{e0}, x'_{e0}, y'_{e0}, \delta\gamma_{e0}) dx_{e0} dy_{e0} dz_{e0} dx'_{e0} dy'_{e0} d\delta\gamma_{e0} + (N_{e} - 1) \left| \int \vec{E}_{\omega0}(\vec{r}; x_{e0}, y_{e0}, z_{e0}, x'_{e0}, \delta\gamma_{e0}) f(x_{e0}, y_{e0}, z_{e0}, x'_{e0}, \delta\gamma_{e0}) dx_{e0} dy_{e0} dz_{e0} dx'_{e0} dy'_{e0} d\delta\gamma_{e0} \right|^{2} \\ \uparrow \\ \text{Coherent SR} \\ \text{Common Approximation for CSR: ``Thin'' Electron Beam: } \left\langle \left| \vec{E}_{\omega} \right|^{2} \right\rangle_{CSR} \approx N_{e} \left| \int_{-\infty}^{\infty} \widetilde{f}(z_{e0}) \exp(ikz_{e0}) dz_{e0} \right|^{2} \left| \vec{E}_{\omega1} \right|^{2} \\ \text{For Gaussian Longitudinal Bunch Profile: } \left\langle \left| \vec{E}_{\omega} \right|^{2} \right\rangle_{CSR} \approx N_{e} \exp(-k^{2}\sigma_{b}^{2}) \left| \vec{E}_{\omega1} \right|^{2} \\ \end{array}$$

If $f(x_{e0}, y_{e0}, z_{e0}, x'_{e0}, y'_{e0}, \delta \gamma_{e0})$ is Gaussian, 6-fold integration over electron phase space can be done analytically for the (Mutual) Intensity of Incoherent SR and for the Electric Field of CSR

Self-Amplified Spontaneous Emission Described by Paraxial FEL Equations

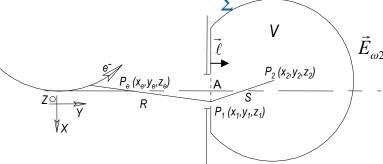
Approximation of Slowly Varying Amplitude of Radiation Field

 $\frac{d\theta}{dz} = k_u - k_r \frac{1 + p_\perp^2 + a_u^2 - 2a_r a_u \cos(\theta + \phi_r)}{2\nu^2}$ Particles' dynamics in undulator and radiation fields $\frac{d\gamma}{dz} = -\frac{k_r f_c a_r a_u}{v} \sin(\theta + \phi_r)$ W.B.Colson (averaged over many periods): J.B.Murphy C.Pellegrini $\frac{d\vec{p}_{\perp}}{dz} = -\frac{1}{2\nu} \frac{\partial a_u^2}{\partial \vec{r}_{\perp}} + \mathbf{k}_{foc} \vec{r}_{\perp}$ E.Saldin E.Bessonov et. al. $\frac{d\vec{r}_{\perp}}{dz} = \frac{\vec{p}_{\perp}}{v}$ Paraxial wave equation $\left[2ik_r\frac{\partial}{\partial z} + \nabla_{\perp}^2\right]a_r \exp(i\phi_r) = -\frac{e\varepsilon_0 If_c a_u}{mc} \left\langle \frac{\exp(-i\theta)}{v} \right\rangle$ with current: Solving this system gives Electric Field at the FEL exit for one "Slice": $E_{slice}\Big|_{z=z_{ovil}} \sim a_r \exp(i\phi_r)\Big|_{z=z_{ovil}}$ Loop on "Slices" (copying Electric Field to a next slice from previous slice, starting from back) Popular TD 3D FEL computer code: **GENESIS** (S.Reiche)

One run provides Time-Domain Electric Field in transverse plane at FEL exit: $E(x, y, z_{exit}, t)$ Electric Field in **Frequency** domain: $\vec{\tilde{E}}(\vec{r}, \omega) = \int_{0}^{\infty} \vec{E}(\vec{r}, t) \exp(i\omega t) dt$

Wavefront Propagation in the Case of Full Transverse Coherence

Kirchhoff Integral Theorem applied to Spontaneous Emission by One Electron



$$\vec{E}_{\omega^{2\perp}}(P_2) \approx \frac{k^2 e}{4\pi} \int_{-\infty}^{+\infty} d\tau \iint_{A} \frac{\vec{\beta}_{e\perp} - \vec{n}_{\perp}}{RS} \exp[ik(c\tau + R + S)] \cdot (\vec{\ell} \cdot \vec{n}_{p_e p_1} + \vec{\ell} \cdot \vec{n}_{p_1 p_2}) d\Sigma$$

Valid at large observation angles; Is applicable to complicated cases of diffraction inside vacuum chamber

Huygens-Fresnel Principle $\vec{E}_{\omega_{2\perp}}(P_2) \approx \frac{k}{4\pi i} \iint_A \vec{E}_{\omega_{1\perp}}(P_1) \frac{\exp(ikS)}{S} (\vec{\ell} \cdot \vec{\tilde{n}} + \vec{\ell} \cdot \vec{n}_{p_1p_2}) d\Sigma$

Fourier Optics

Free Space: (between parallel planes perpendicular to optical axis)

"Thin" Optical Element:

"Thick" Optical Element: (propagation from transverse plane before the element to a transverse plane just after it)

$$\vec{E}_{\omega^{2\perp}}(x_2, y_2) \approx \frac{k}{2\pi i L} \iint \vec{E}_{\omega^{1\perp}}(x_1, y_1) \exp[ik[L^2 + (x_2 - x_1)^2 + (y_2 - y_1)^2]^{1/2}] dx_1 dy_1$$
Assumption of small angles

$$\vec{E}_{\omega 2 \perp}(x, y) \approx \mathbf{T}(x, y, \omega) \, \vec{E}_{\omega 1 \perp}(x, y)$$

$$\vec{E}_{\omega 2 \perp}(x_2, y_2) \approx \mathbf{G}(x_2, y_2, \omega) \exp[ik\Lambda(x_2, y_2, k)] \vec{E}_{\omega 1 \perp}(x_1(x_2, y_2), y_1(x_2, y_2))$$

"Economic" and Numerically Stable Version of the Free-Space Fourier-Optics Propagator

Huygens-Fresnel Principle:

(paraxial approximation)

$$\vec{E}_{\omega_{2\perp}}(x_2, y_2) \approx \frac{k}{2\pi i L} \iint \vec{E}_{\omega_{1\perp}}(x_1, y_1) \exp[ik[L^2 + (x_2 - x_1)^2 + (y_2 - y_1)^2]^{1/2}] dx_1 dy_1$$

Analytical Treatment of **Quadratic Phase Term**:

Before Propagation:

$$\vec{E}_{\omega 1 \perp}(x_1, y_1) = \vec{F}_{\omega 1}(x_1, y_1) \exp\left[ik\frac{(x_1 - x_0)^2}{2R_x} + ik\frac{(y_1 - y_0)^2}{2R_y}\right]$$

After Propagation:

$$\begin{split} \vec{E}_{\omega 2 \perp}(x_2, y_2) &\approx \frac{k}{2\pi i L} \exp(ikL) \iint_{\Sigma} \vec{F}_{\omega 1}(x_1, y_1) \exp\left[ik \frac{(x_1 - x_0)^2}{2R_x} + ik \frac{(y_1 - y_0)^2}{2R_y} + ik \frac{(x_2 - x_1)^2 + (y_2 - y_1)^2}{2L}\right] dx_1 dy_1 \\ &= \frac{k}{2\pi i L} \exp\left[ikL + ik \frac{(x_2 - x_0)^2}{2(R_x + L)} + ik \frac{(y_2 - y_0)^2}{2(R_y + L)}\right] \times \\ &\times \iint_{\Sigma} \vec{F}_{\omega 1}(x_1, y_1) \exp\left[ik \frac{R_x + L}{2R_x L} \left(x_1 - \frac{R_x x_2 + L x_0}{R_x + L}\right)^2 + ik \frac{R_y + L}{2R_y L} \left(y_1 - \frac{R_y y_2 + L y_0}{R_y + L}\right)^2\right] dx_1 dy_1 \\ &= \vec{F}_{\omega 2}(x_2, y_2) \exp\left[ik \frac{(x_2 - x_0)^2}{2(R_x + L)} + ik \frac{(y_2 - y_0)^2}{2(R_y + L)}\right] \end{split}$$

An Approach to High-Accuracy Partially-Coherent Emission and Wavefront Propagation Simulations

Averaging (over phase-space volume occupied by e-beam) of the intensity (or mutual intensity, or mathematical brightness) obtained from electric field emitted by an electron and propagated through an optical system:

$$\begin{split} I_{\omega}(x,y) &= \int I_{\omega 1}(x,y;x_{e},y_{e},z_{e},x'_{e},y'_{e},\delta\gamma_{e}) f(x_{e},y_{e},z_{e},x'_{e},y'_{e},\delta\gamma_{e}) dx_{e} dy_{e} dz_{e} dx'_{e} dy'_{e} d\delta\gamma_{e} \\ I_{\omega 1}(x,y;x_{e},y_{e},z_{e},x'_{e},y'_{e},\delta\gamma_{e}) &= \left| \mathbf{E}_{\omega 1 \perp}(x,y;x_{e},y_{e},z_{e},x'_{e},y'_{e},\delta\gamma_{e}) \right|^{2} \\ M_{\omega 1}(x,y,\tilde{x},\tilde{y};x_{e},y_{e},z_{e},x'_{e},y'_{e},\delta\gamma_{e}) &= \mathbf{E}_{\omega 1 \perp}(x,y;x_{e},y_{e},z_{e},x'_{e},y'_{e},\delta\gamma_{e}) \mathbf{E}_{\omega 1 \perp}^{*}(\tilde{x},\tilde{y};x_{e},y_{e},z_{e},x'_{e},y'_{e},\delta\gamma_{e}) \\ B_{\omega 1}(x,y,\theta_{x},\theta_{y};x_{e},y_{e},z_{e},x'_{e},y'_{e},\delta\gamma_{e}) \sim \mathbf{E}_{\omega 1 \perp}(x,y;x_{e},y_{e},z_{e},x'_{e},\gamma'_{e},\delta\gamma_{e}) \int \mathbf{E}_{\omega 1 \perp}^{*}(\tilde{x},\tilde{y};x_{e},y_{e},z_{e},x'_{e},y'_{e},\delta\gamma_{e}) \exp\left[i\frac{\omega}{c}(\theta_{x}\tilde{x}+\theta_{y}\tilde{y})\right] d\tilde{x}d\tilde{y} \end{split}$$

This method is **general** and **accurate**. For the most part, it is already implemented in SRW code. However, it can be **CPU-intensive**, requiring **parallel calculations** on a multi-core server or a small cluster. Several approaches are considered for increasing the efficiency, including use of low-discrepancy sequences (collaboration with R. Lindberg, K.-J. Kim, X. Shi, ANL), "improved Monte-Carlo" type techniques, as well as "coherent mode decomposition".

NOTE: the **smaller** the **e-beam emittance** (the higher the radiation coherence) – the **faster** is the **convergence** of simulations with this general method.

NOTE: **convolution** can be valid in some cases, such as pure projection geometry, focusing by a thin lens, diffraction at one slit, etc.

$$I_{\omega}(x,y) \approx \int \widetilde{I}_{\omega 1}(x-\widetilde{x}_{e},y-\widetilde{y}_{e})\widetilde{f}(\widetilde{x}_{e},\widetilde{y}_{e}) d\widetilde{x}_{e}d\widetilde{y}_{e}$$

If convolution is valid, the **calculations can be accelerated** dramatically. The validity of the convolution relation can be easily verified numerically.

All calculations presented below were done with "Synchrotron Radiation Workshop" code

First work on Wavefront Propagation applied to SR beamlines (PHASE code): J. Bahrdt, Appl. Opt. 36 (19) 4367 (1997)

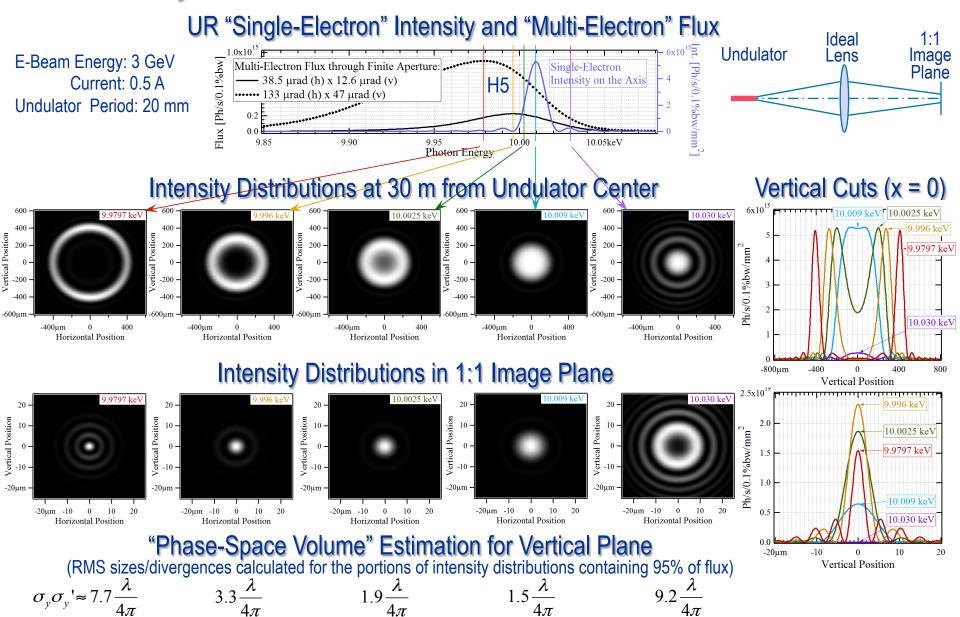
- First official version of SRW was developed at ESRF in 1997-98 (written in C++, interfaced to IGOR Pro); compiled versions are distributed from: http://www.esrf.eu/Accelerators/Groups/InsertionDevices/Software/SRW
- SRW was released to Open Source in 2012 under BSD type license. To make the release possible, permissions were obtained from all previously contributed Institutes: ESRF, European XFEL, SOLEIL, DIAMOND, BNL, and from US DOE



The main Open Source repository, containing all C/C++ sources, C API, all interfaces and project development files, is on GitHub: https://github.com/ochubar/SRW

- SRW for Python (2.7.x and 3.x, 32- and 64-bit) cross-platform versions were released in 2012
- SRW development is partially supported by US DOE SBIR Program (BNL acts as subcontractor of RadiaSoft LLC, headed by D. Bruhwiler) Aradiasoft

Single-Electron (Fully Transversely-Coherent) UR Intensity Distributions, "in Far Field" and "at Source"

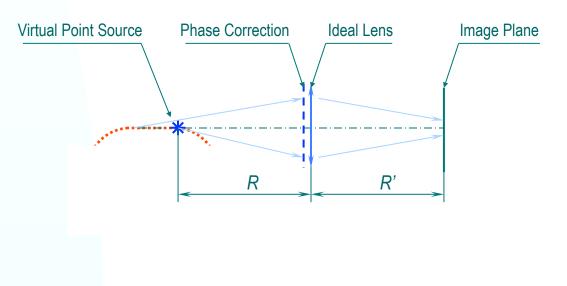


"Phase Correction" for Coherent Radiation

"Real Wave Front" + "Phase Correction" = "Spherical Wave Front" $E_{out}(x, y) = T(x, y)E_{in}(x, y) = A(x, y) \exp[i\pi(x^{2} + y^{2})/(\lambda R)]$ $T(x, y) = \exp[i\Phi_{cor}(x, y)]$

 $\Phi_{cor}(x,y) = \arg[\exp[i\pi(x^2+y^2)/(\lambda R)+i\Phi_0]/E_{in}(x,y)]$

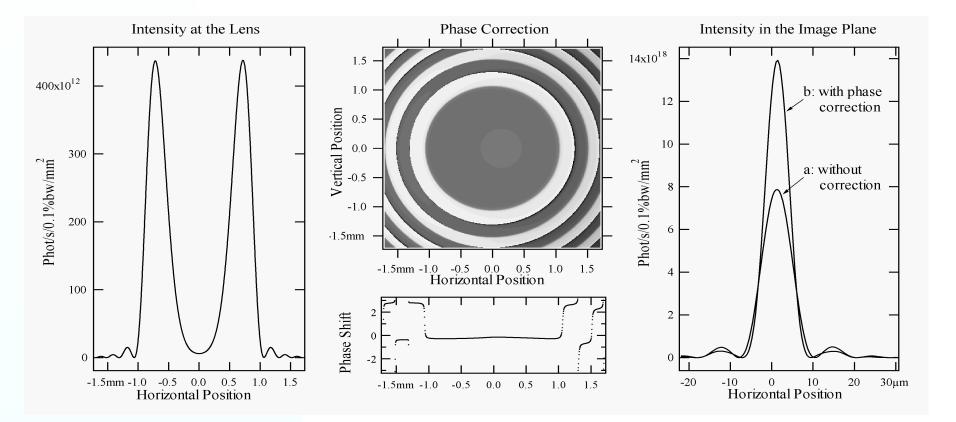
Testing Efficiency of Phase Corrections



Phase Corrections for Single-Electron UR (I)

Planar undulator, odd harmonics

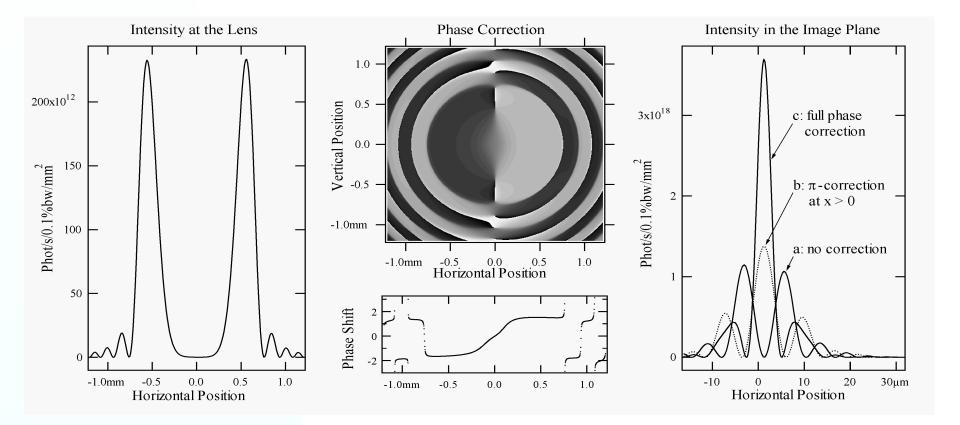
E = 6 GeV; K = 2.2; 38 x 42 mm; $\varepsilon = 2.36 \text{ keV}$ (~ fundamental) 1 : 1 imaging; 30 m from middle of Undulator to Thin Lens & Phase Correction



Phase Corrections for Single-Electron UR (II)

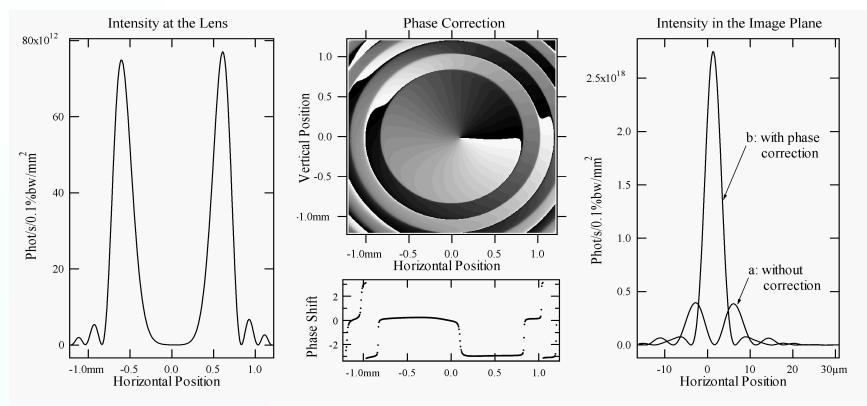
Planar undulator, even harmonics

E = 6 GeV; K = 2.2; 38 x 42 mm; $\varepsilon = 4.775$ keV (2^{-nd} harmonic) 1 : 1 imaging; 30 m from middle of Undulator to Thin Lens & Phase Correction



Phase Corrections for Single-Electron UR (III)

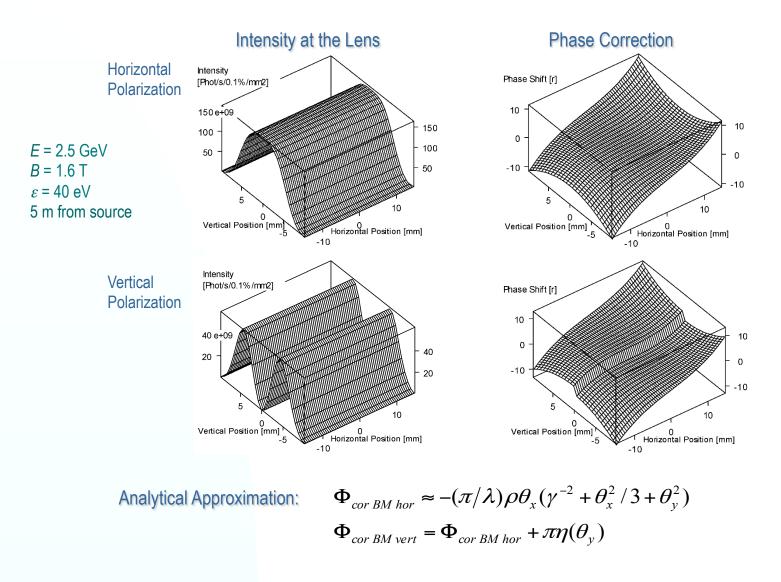
Helical undulator, harmonics n > 1 E = 6 GeV; $B_{x max} = B_{z max} = 0.3$ T; 28 x 52 mm; $\varepsilon = 4.20$ keV (2^{-nd} harmonic) 1 : 1 imaging; 30 m from middle of Undulator to Thin Lens & Phase Correction



O. Chubar, P. Elleaume, A. Snigirev, NIMA 435 (1999) 495 - 508

S. Sasaki, I. McNulty, PRL 100, 124801 (2008) interpreted of this effect – azimuthal phase dependence – as "Orbital Angular Momentum"; several other publications followed.

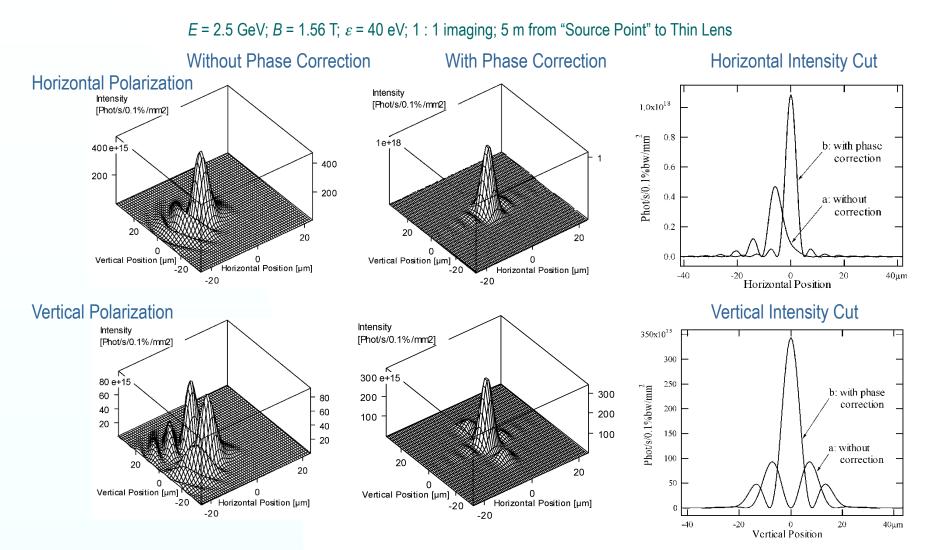
Phase Corrections for Bending Magnet SR



O. Chubar, P. Elleaume, A. Snigirev, NIMA 435 (1999) 495 - 508

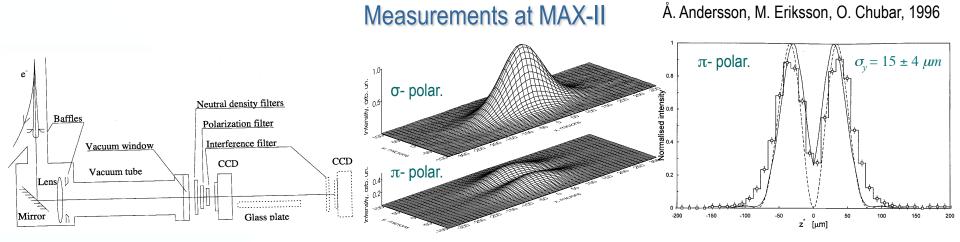
Phase Corrections for Bending Magnet SR

Intensity in the Image Plane



O. Chubar, P. Elleaume, A. Snigirev, NIMA 435 (1999) 495 - 508

Determining Electron Beam Size from Focused Visible Bending Magnet SR



Measurements at MAX-IV

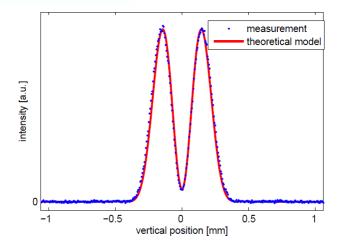
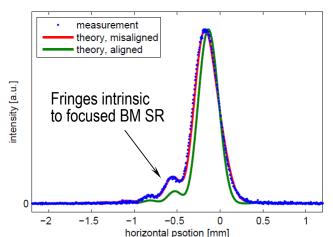


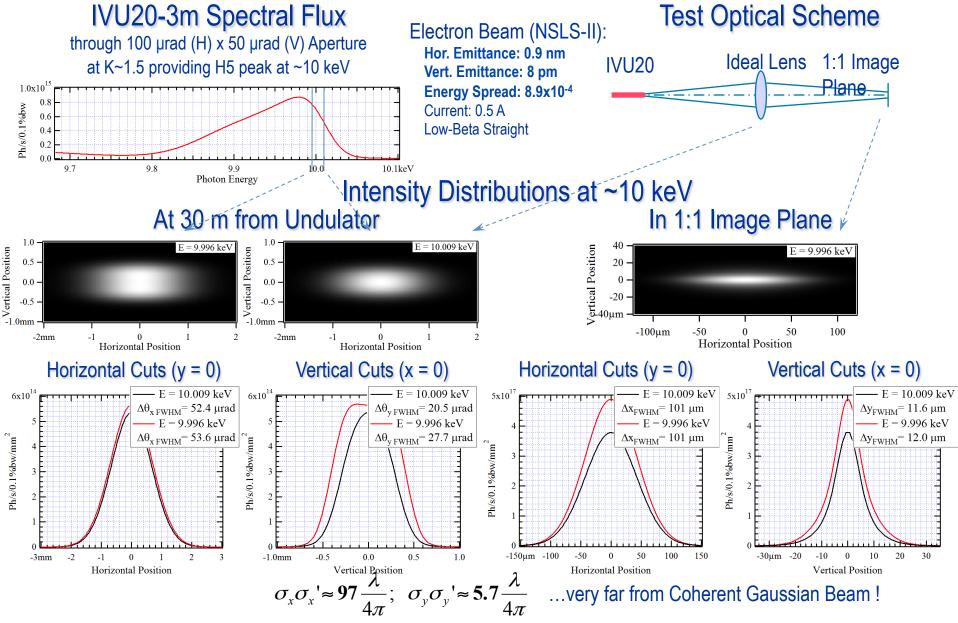
Figure 3: Vertical profile of imaged π -polarized SR at 488 nm wavelength. Measurement (blue dots) and SRW calculation (red lines). The vertical beam size is 11.5 µm.



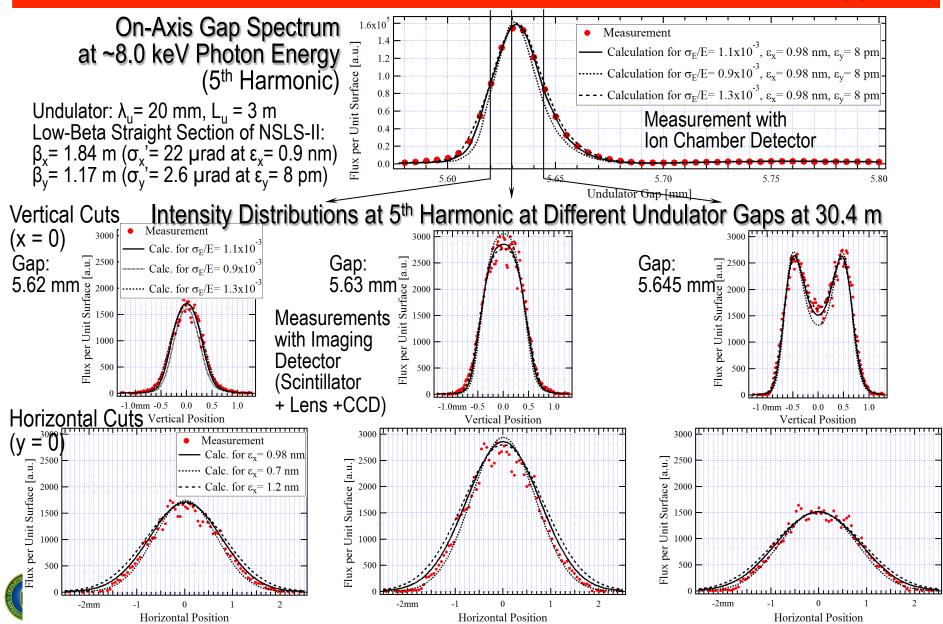
J. Breunlin, Å.Andersson, 2015

Figure 7: Horizontal profiles of σ -polarized SR at 930 nm for 8.2 mrad horizontal opening angle. The horizontal beam size is 24.5 µm.

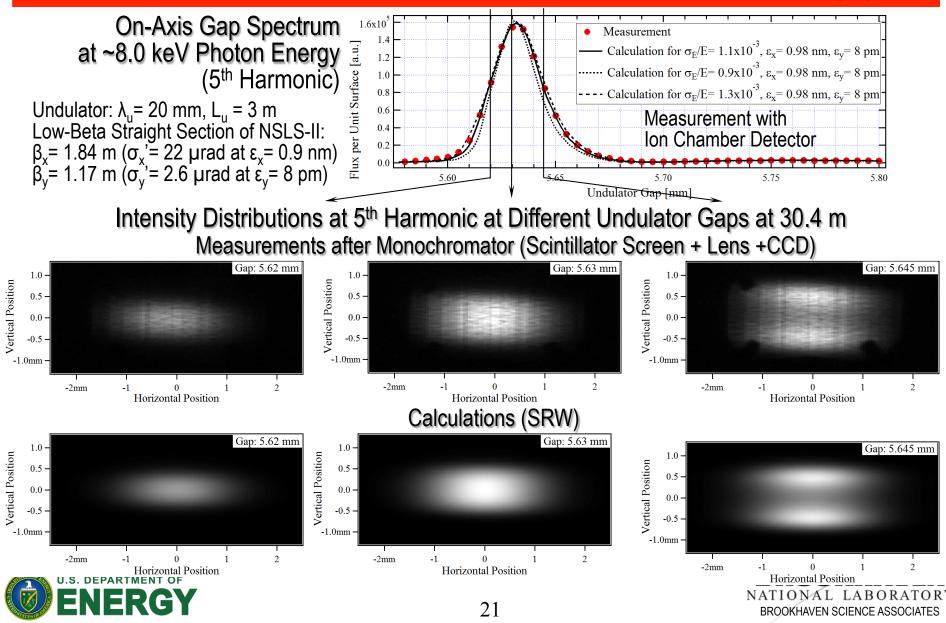
Calculated UR Intensity Distributions from Finite-Emittance Electron Beam, "in Far Field" and "at Source"



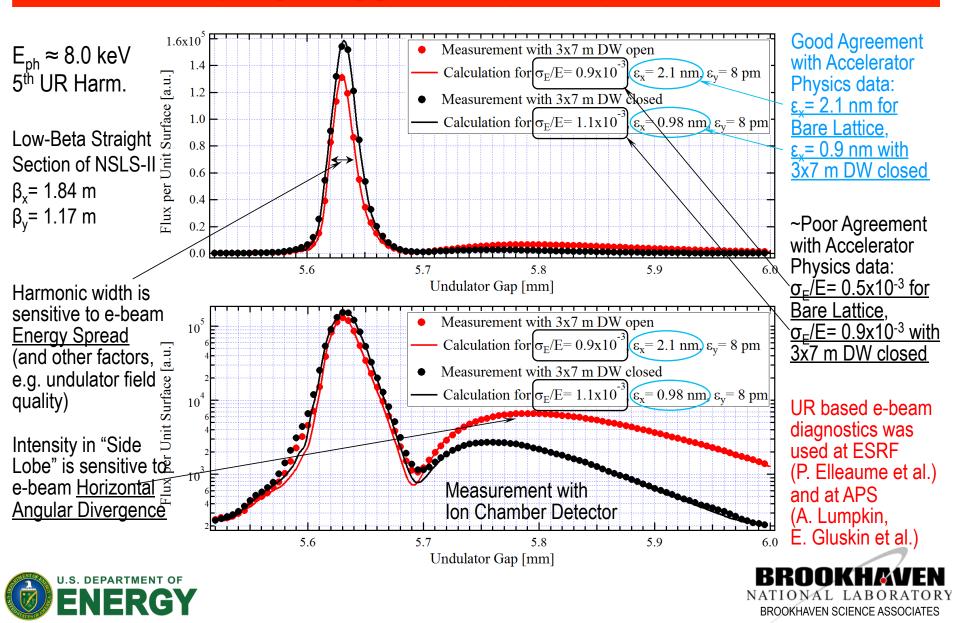
On-Axis "Gap Spectrum" and Intensity Distributions of Radiation from IVU20 at HXN Beamline (I)



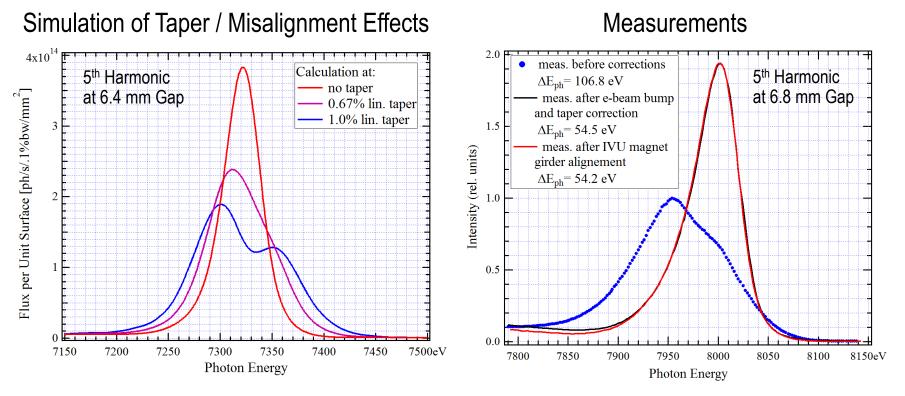
On-Axis "Gap Spectrum" and Intensity Distributions of Radiation from IVU20 at HXN Beamline (II)



IVU20 (HXN) On-Axis "Gap Spectra" with Damping Wiggler Gaps "Open" and "Closed"



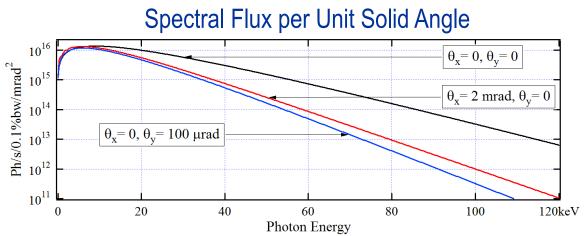
Example of Using High-Accuracy UR Calculation for Advanced Commissioning of SRX Beamline at NSLS-II



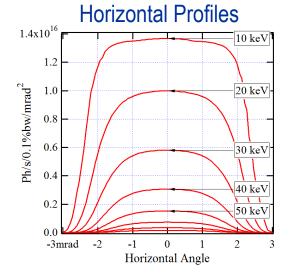
Undulator Radiation Simulations with SRW allowed to:

- Identify case of an under-performing In-Vacuum Undulator;
- Find reason for the reduction of spectral performance (small misalignment of magnet arrays);
- Implement most efficient correction and restore nearly ideal IVU spectrum.

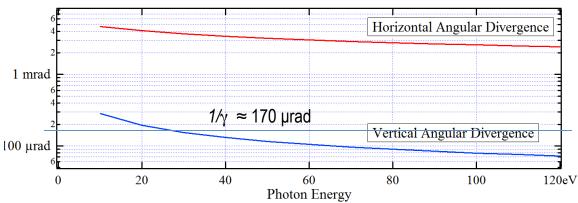
Spectral-Angular Distributions of Emission from NSLS-II 2 x 3.5 m Long Damping Wiggler in "Inline" Configuration

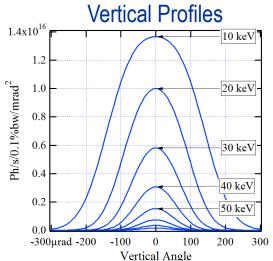


Angular Profiles of DW Emission at Different Photon Energies

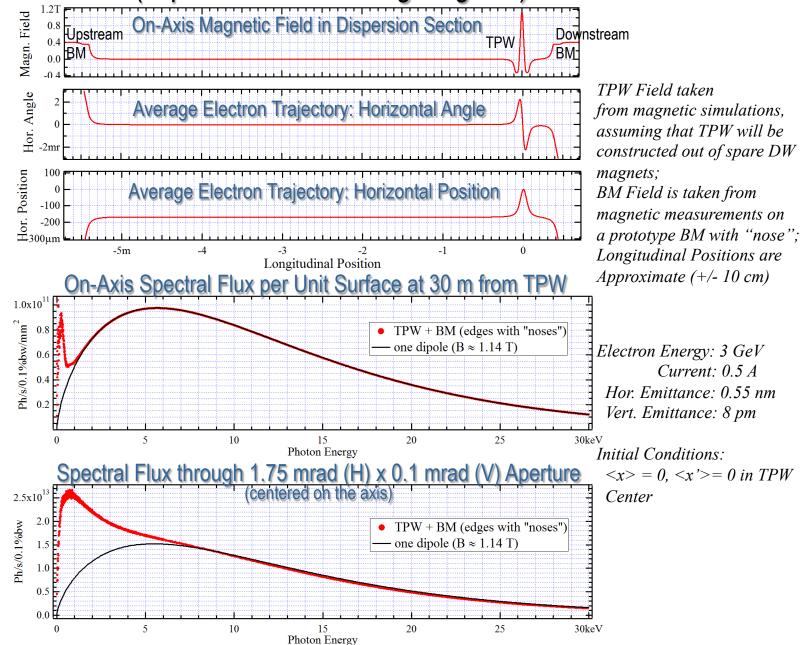


FWHM Angular Divergence of DW Emission



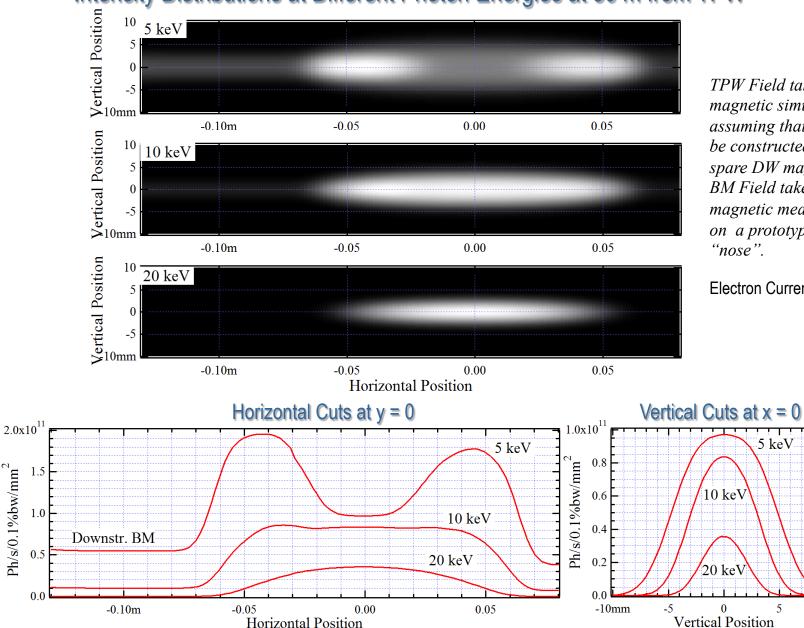


NSLS-II 3PW: Magn. Field, Electron Trajectory, Spectra (in presence of Bending Magnets)



NSLS-II 3PW+BM Radiation Intensity (Hard X-Rays)

Intensity Distributions at Different Photon Energies at 30 m from TPW



 $Ph/s/0.1\% bw/mm^2$

TPW Field taken from magnetic simulations, assuming that TPW will be constructed out of spare DW magnets; BM Field taken from magnetic measurements on a prototype BM with "nose".

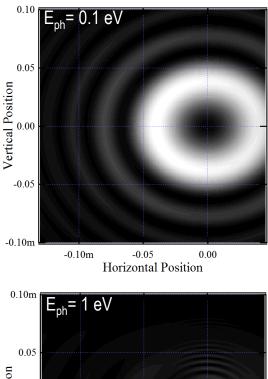
Electron Current: 0.5 A

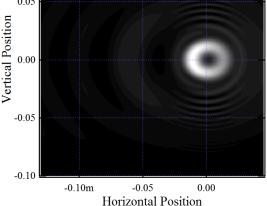
5

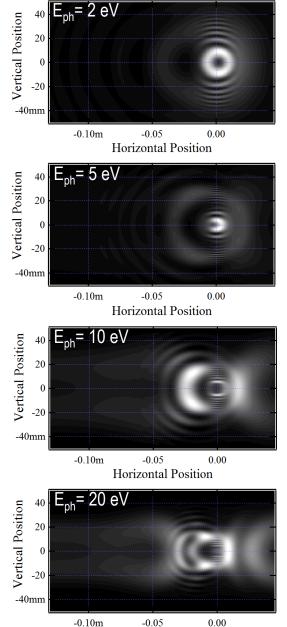
10

NSLS-II 3PW+BM Radiation Intensity (IR to Soft X-Rays)

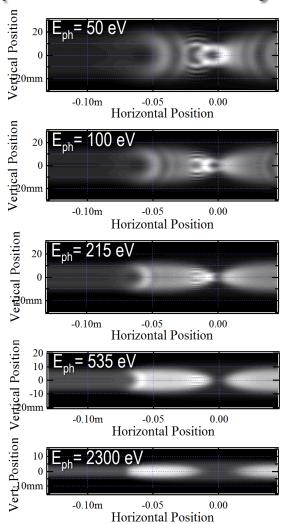
Observation Distance: 30 m (from TPW center)







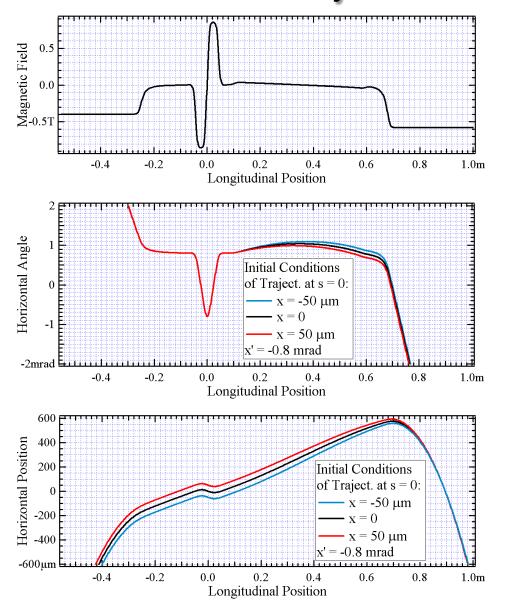
Horizontal Position



TPW Field taken from magnetic simulations, assuming that TPW will be constructed out of spare DW magnets;

BM Field taken from magnetic measurements on a prototype BM with "nose".

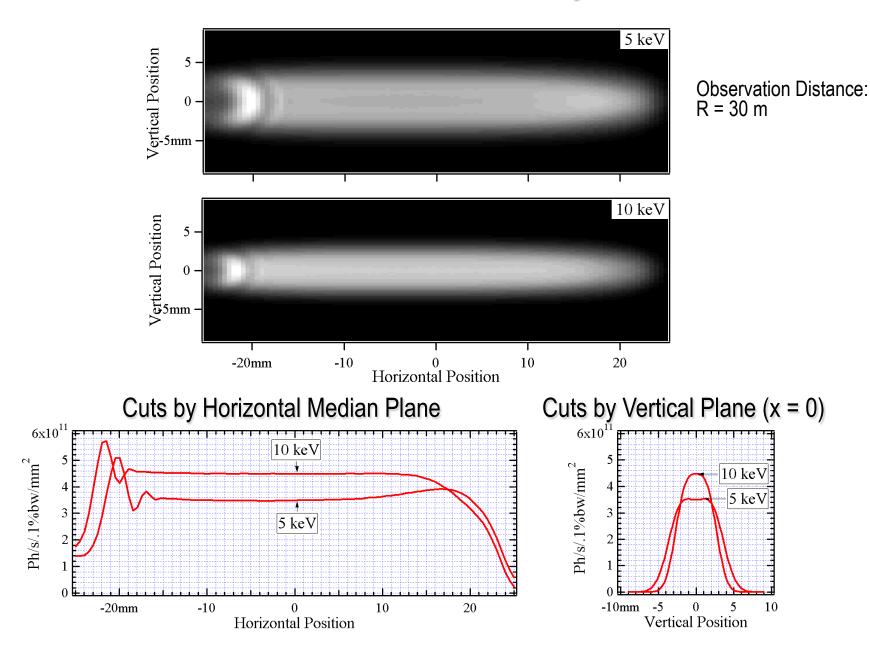
ESRF-U 2PW (option): Magnetic Field and Electron Trajectories

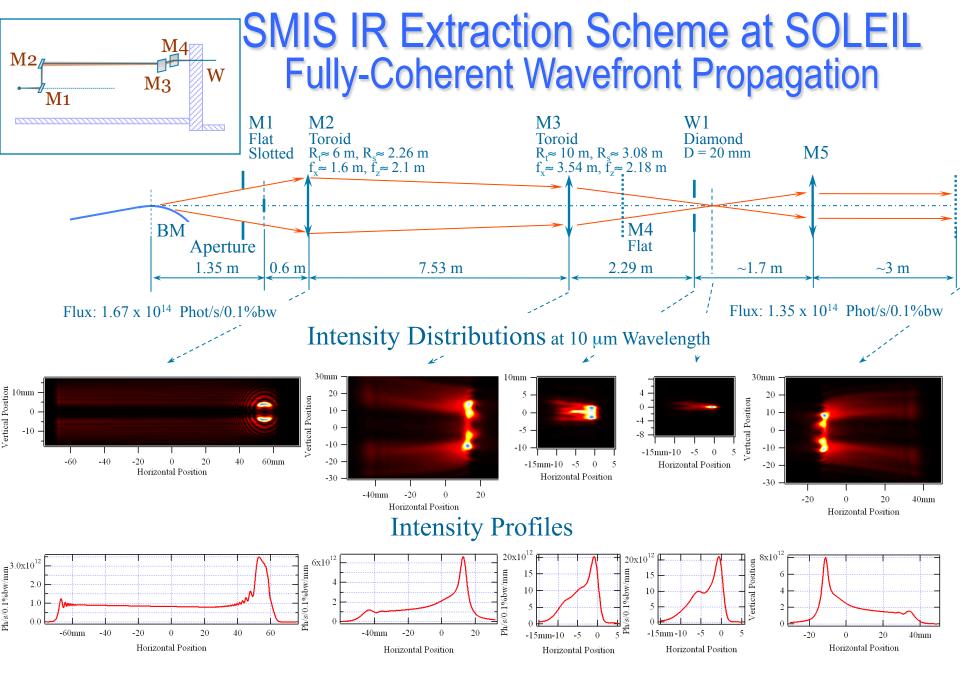


Magnetic design by J. Chavanne

Quadrupole Lens is included into analysis (under testing)

ESRF-U 2PW Radiation Intensity Distributions





Optical scheme: F. Polack, P. Dumas

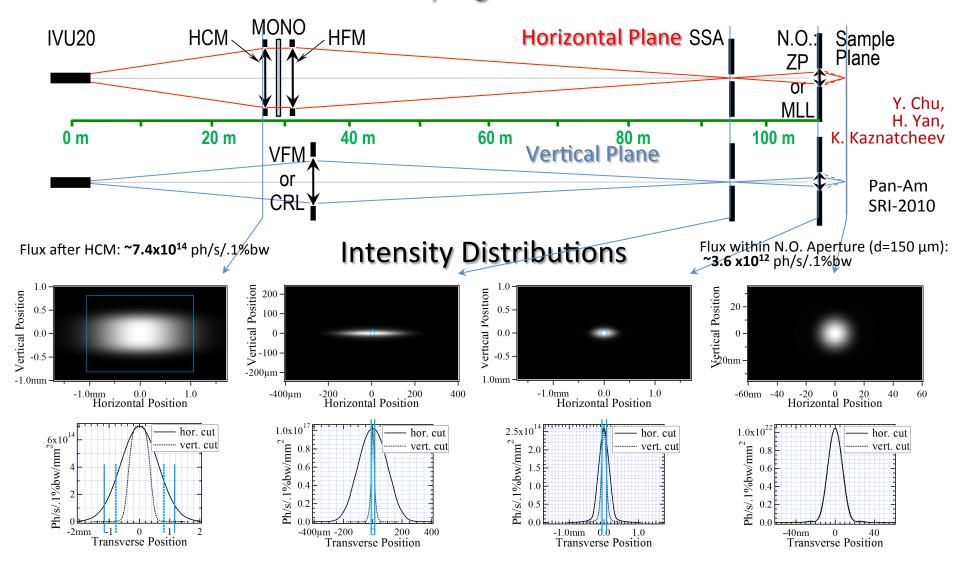
Updates of Core Functions in "Synchrotron Radiation Workshop" Code Enabling Physical-Optics Calculations for Beamlines in Low-Emittance Rings and X-FEL

- Accurate partially-coherent emission and wavefront propagation simulations for SR sources are possible with SRW since ~2009: O.Chubar, Y.S.Chu, K.Kaznatcheev, H.Yan, AIP Conf. Proc. Vol. 1234, pp.75-78 (2009) O.Chubar, Y.S.Chu, K.Kaznatcheev, H.Yan, Nucl. Instr. and Meth., vol. A649, Issue 1, pp.118-122 (2011)
- Parallel calculations of Partially-Coherent Emission and Wavefront Propagation are implemented in SRW for Python (based on MPI / mpi4py). Besides "normal" Intensity, calculation of Mutual Intensity / Degree of Coherence is possible:

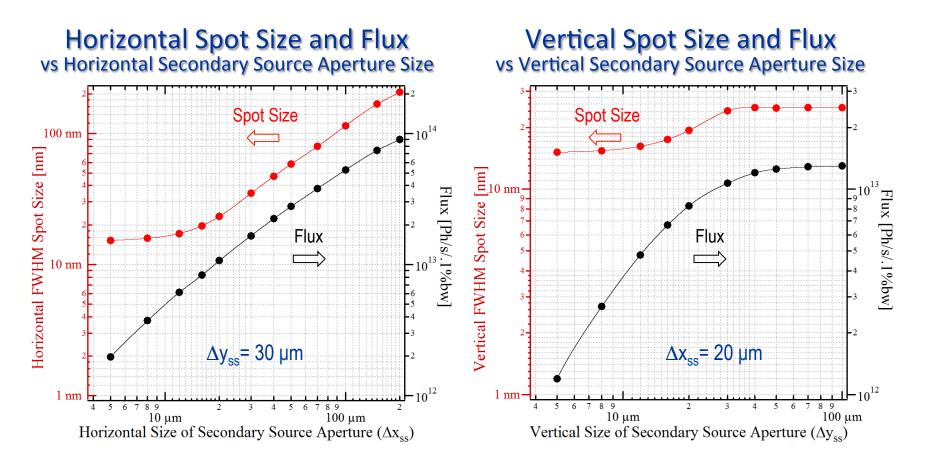
O.Chubar, A.Fluerasu, L.Berman, K.Kaznatcheev, L.Wiegart, J. Phys.: Conf. Ser. 425, 162001 (2013) D.Laundy, J.P.Sutter, U.H.Wagner, C.Rau, C.A.Thomas, K.J.S.Sawhney, and O.Chubar, J. Phys.: Conf. Ser. 425, 162002 (2013)

- Increased reliability of Time- / Frequency-Dependent FEL Pulse Propagation simulations: S.Roling, H.Zacharias, L.Samoylova, H.Sinn, Th.Tschentscher, O.Chubar, A.Buzmakov, E.Schneidmiller, M.V.Yurkov, F.Siewert, S.Braun, and P.Gawlitza, Phys. Rev. ST Accel. Beams 17, 110705 (2014)
- Physical-optics "propagators" are implemented for:
- Grazing-Incidence Focusing Mirrors, using the stationary phase method / "local ray-tracing": N.Canestrari, O.Chubar, R.Reininger, J. Synchrotron Rad. 21, 1110-1121 (2014)
- Perfect Crystals, using the X-ray Dynamical Diffraction methods: J.P.Sutter, O.Chubar, A.Suvorov, Proc. SPIE Vol. 9209, 92090L (2014) A.Suvorov, Y.Q.Cai, J.P.Sutter, O.Chubar, Proc. SPIE Vol. 9209, 92090H (2014) O.Chubar, G.Geloni, V.Kocharyan, A.Madsen, E.Saldin, S.Serkez, Y.Shvyd'ko, J.Sutter, JSR 23, 410-424 (2016)
- Variable Line Spacing Gratings, using the Stationary Phase method: N.Canestrari, V.Bisogni, A.Walter, Y.Zhu, J.Dvorak, E.Vescovo, O.Chubar, Proc. SPIE Vol. 9209, 92090I (2014)

NSLS-II Hard X-Ray Nanoprobe (HXN) Beamline Optical Scheme and Partially-Coherent Wavefront Propagation Simulation



Final Focal Spot Size and Flux at Sample vs Secondary Source Aperture Size (HXN, NSLS-II)

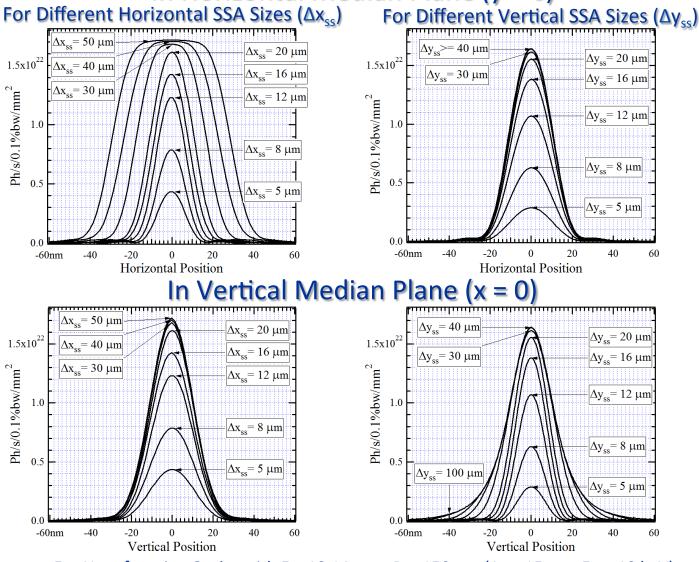


Pan-Am SRI-2010

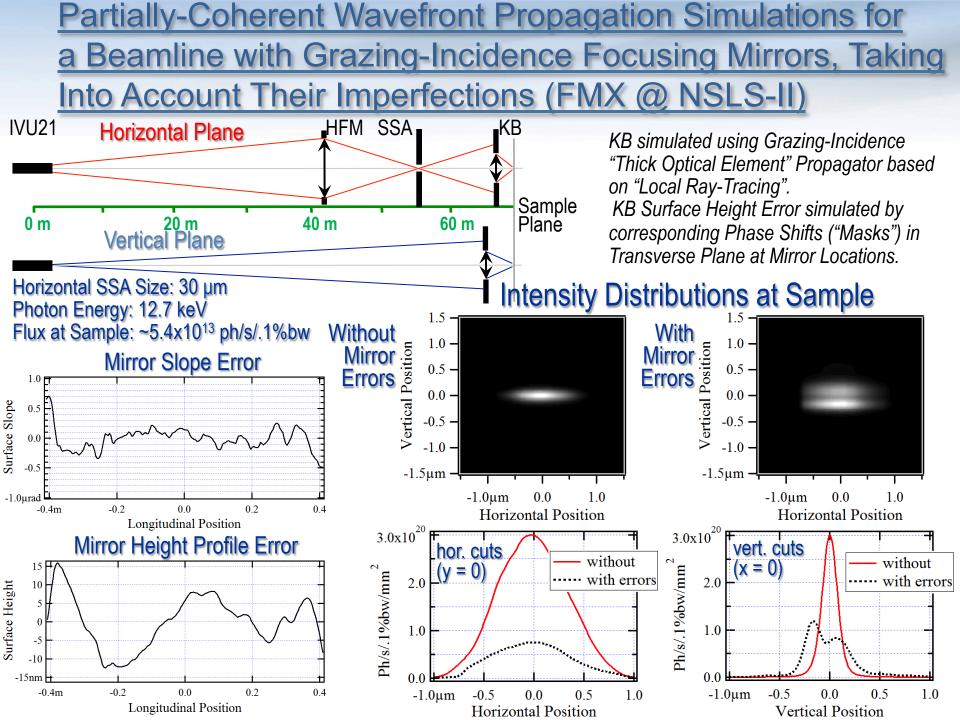
Secondary Source Aperture located at 94 m from Undulator Spot Size and Flux calculated for Nanofocusing Optics simulated by Ideal Lens with F = 18.14 mm, D = 150 μ m located at 15 m from Secondary Source (109 m from Undulator)

Intensity Distributions at Sample for Different Secondary Source Aperture Sizes at HXN (NSLS-II)

In Horizontal Median Plane (y = 0)



For Nanofocusing Optics with F = 18.14 mm, D = 150 μ m ($\Delta r \approx 15$ nm; E_{ph} ≈ 10 keV) SSA located at 94 m, Nanofocusing Optics at 109 m from Undulator



Using CRL for Producing "Large Spot" at Sample of FMX Beamline @ NSLS-II **IVU21** HFM SSA CRL **■**KB Source: Horizontal Plane Electron Current: 0.5 A Sample Plane Horizontal Emittance: 0.55 nm ("ultimate") Vertical Emittance: 8 pm 20 m 40 m 0 m 60 m Undulator: IVU21-1.5 m centered at +1.25 m Vertical Plane from Low-Beta Straight Section Center Intensity Distributions at Sample Horizontal SSA Size: 30 µm With under the second s Without With Vertical Position 40 -Photon Energy: 12.7 keV 20 -0 -CRL "Transfocator": -20 Ž_{40μm} -8 Horizontally + 3 Vertically-Focusing Be Lenses R_{min} = 200 μm -40um-20 0 20 -40um-20 20 40 0 40 $F_h \approx 5.9 \text{ m}, F_v \approx 15.8 \text{ m}$ Horizontal Position Horizontal Position Geom. Ap.: 1 mm x 1 mm

1.2x10¹⁶ hor. cuts

0.8

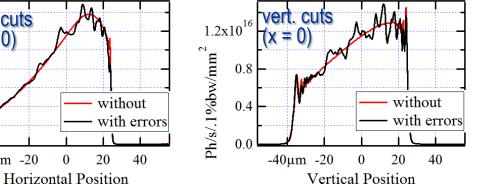
0.4

0.0

Ph/s/.1%bw/mm²

(y = 0)

-40µm -20

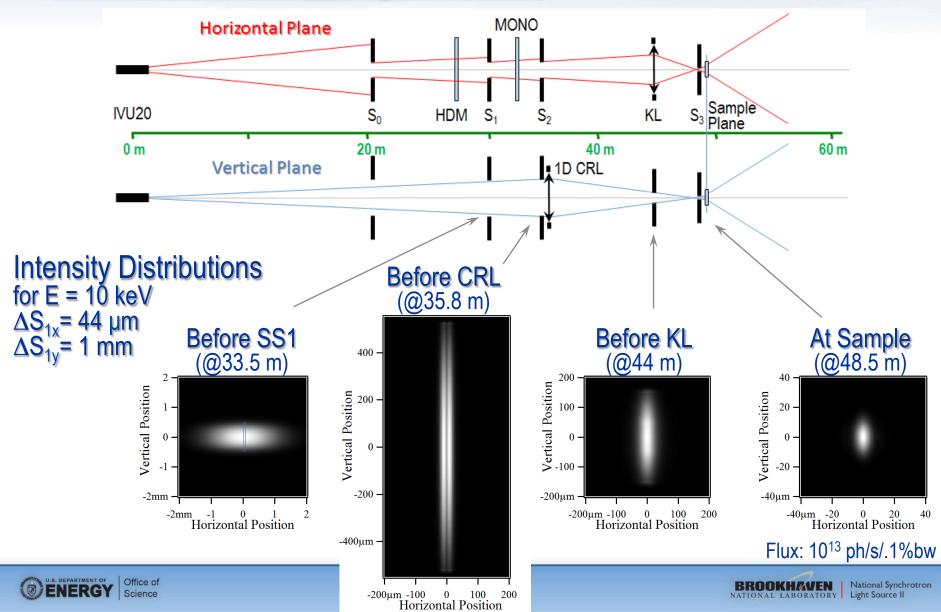


Located at 0.75 m before VKB edge (10 m after SSA)

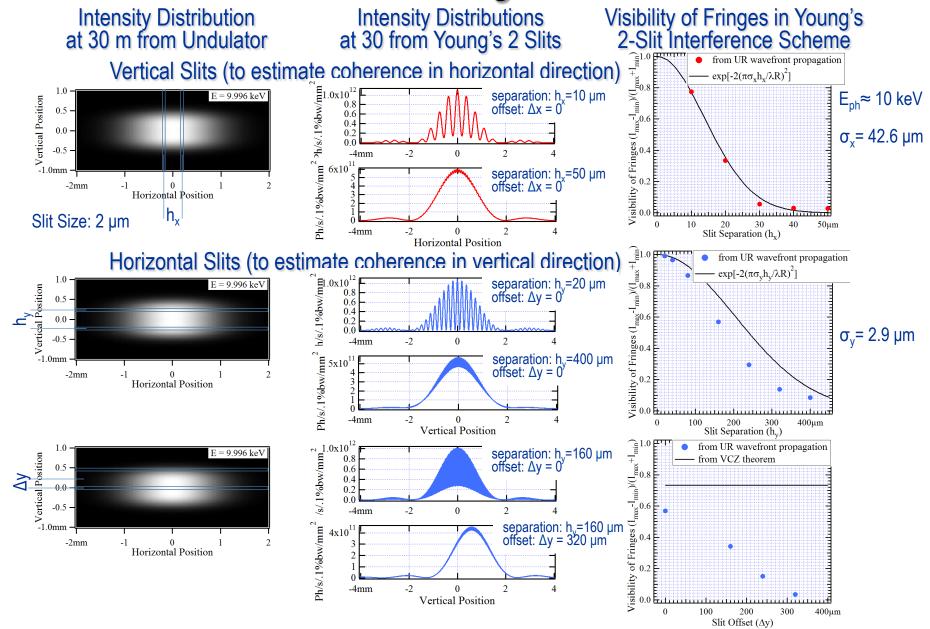
Flux Losses at CRL: ~1.6 times

J.S. DEPARTMENT OF Office of ENERGY Science

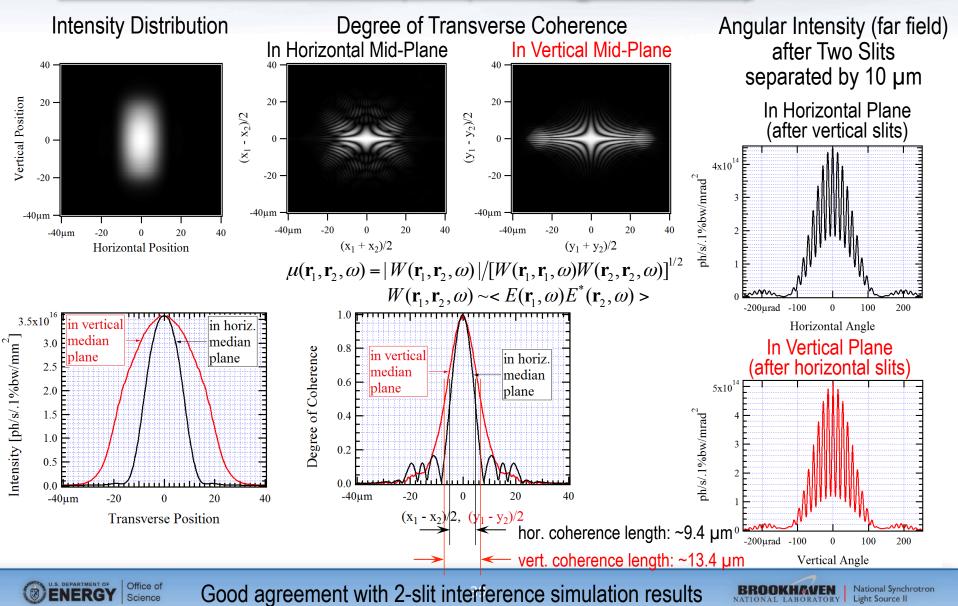
Partially-Coherent Wavefront Propagation Simulations for CHX Beamline @ NSLS-II

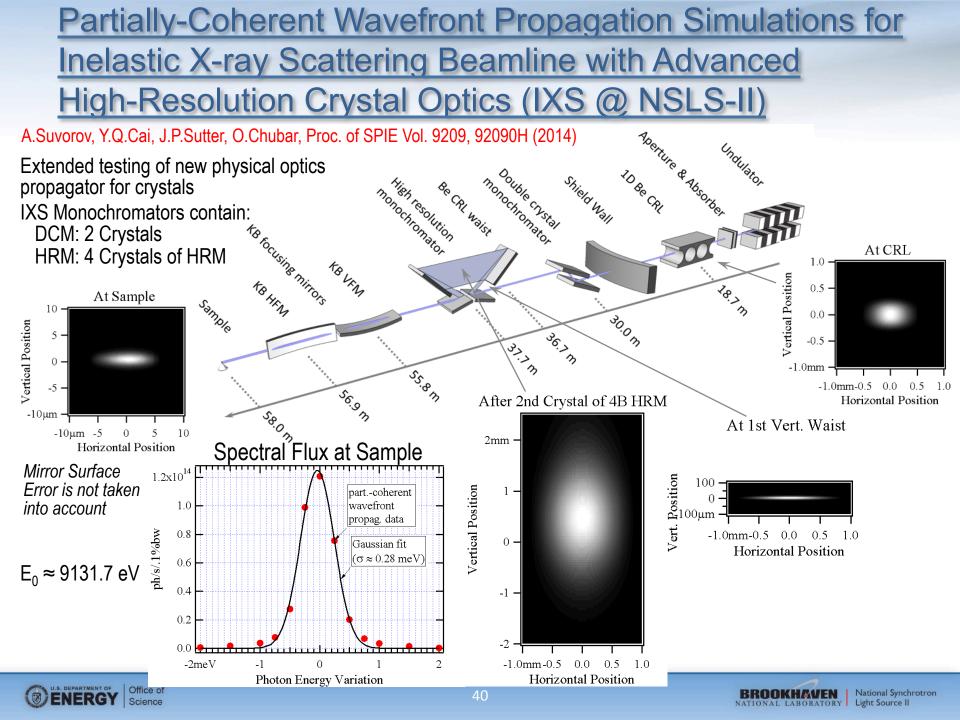


Estimating Degree of Coherence of Radiation from U20 Installed in Low-Beta Straight Section of NSLS-II



Tracking Intensity and Degree of Transverse Coherence at a Sample (CHX @ NSLS-II)





NSLS-II Soft Matter Interfaces beamline modelling 29.50 m White Beam Slits 34.88 m IVU23 Courtesy of M. Zhernenkov and M. Rakitin HFM 39.00 m VM 47.00 m DCM SRW modelling with: SSA 31.94 m Microfocusing VFM "True" partially-(57.5 m): ✓ actual measured SMI mirrors' profiles 59.00 m 38.30 m CRLS coherent calc. is ✓ FEA heat load on 1st DCM crystal Liquids Experiment (ES1) compared to a 50.90 m convolved zero-GI-SAXS/WAXS Experiment (ES2) 2.1 keV 20.4 **¢re**i₩ance calc. (obtained in 30 s) ES1 focus ES2 focus with CRLs Intensity (ph/s/0.1% by 7x10 - ME w/o energy spread 7x101 7x10¹ 6x10¹⁸ 6x10¹ 6x10¹¹ (ph/s/0.1% bw/mm2) 10 3x1017 4x10¹ 5x101 3.1x10¹ coordinate (µm) 5x10¹¹ horizontal 5 - 3x10¹⁵ 4x10¹⁸ 4x10¹ 3 2x10¹⁷ 2.5x10¹ 2x10¹⁵ 3x10¹⁵ 3x101 0 coordinate (µm) 2 1x10¹⁹ 1.8x10¹ 1x10¹⁷ 2x10¹⁵ 2x1018 -5 -1x10[°] 1.2x10¹ 1x10 × 10 0 -10 10 20 -30 -20 0 30 6.1x10¹⁶ 3x10¹¹ -15 -10 -5 50 100 150 -150 -100 -50 0 -15 -1 Y coordinate (µm) X coordinate (um) -150 -100 -50 0 50 100 150 2.0x10¹⁰ 2x10¹⁷ vertical X coordinate (um) -2 ES2 focus with CRLs -3 1x10¹¹ Intensity (ph/s/0.1% bw/mr -4 ME w/o energy spread 9x101 9x10 -30 -20 -10 ò 10 20 9x10 -2 -1 0 2 8x10¹⁶ -3 8x10¹⁶ X coordinate (µm) 7x10¹ beam coordinate (um) 7x10¹⁶ 7x1016 6x10¹⁶ coordinate (µm) 2 -6x10¹⁶ 6x10¹⁶ - 4x10¹⁶ 5x10¹⁶ 5x1016 ES2 focus no CRLs · 3x10¹⁶ 4x10¹⁶ 4x1016 1x10¹⁶ 3x10¹⁶ 3x1016 2x10¹⁶ 2x1016 Intensity 1x10¹⁶ (ph/s/0.1% bw/mm²) 6x10¹⁶ 6x10¹⁶ 20 -3 -40 -30 -20 -10 ò 10 20 30 40 horizontal -3 -2 -1 0 1 2 3 4 -4 5x10¹⁶ X coordinate (µm) 15 Y coordinate (µm) 4x10¹⁶ -30 -20 -10 0 10 20 30 4x10¹⁶ X coordinate (um) coordinate (μm) 10 ES2 focus no CRLs 2x10¹⁶ 3x10¹⁶ 5 -2x10¹⁶ Intensity (ph/s/0.1% bw/mm²) 0 ME w/o energy spread 2.0×10^{1} 10x10¹⁶ -200 -100 100 200 6x10¹⁶ 2x10¹⁵ 2x10¹⁵ 1.7x10¹⁵ -5 2x10¹ 20 coordinate (µm) 1.3x10¹⁵ 4x10¹⁶ vertical 2x10¹⁵ 1.5x10¹⁵ ×⁻¹⁰ 1.0x10¹⁵ 6.7x10¹ -15 2x10¹⁶ 1x10¹⁵ 1x10¹⁵ 3.3x10¹⁴

0.0

5x10¹⁴

-200 -100 5x10¹⁴

100 200

0

X coordinate (um)

-30 -20 -10 10 20

0

Y coordinate (µm)

-20

-200 -100 0 100 200

X coordinate (µm)

0

-20 -15 -10 -5 0 5

10 15

beam coordinate (um)

≻

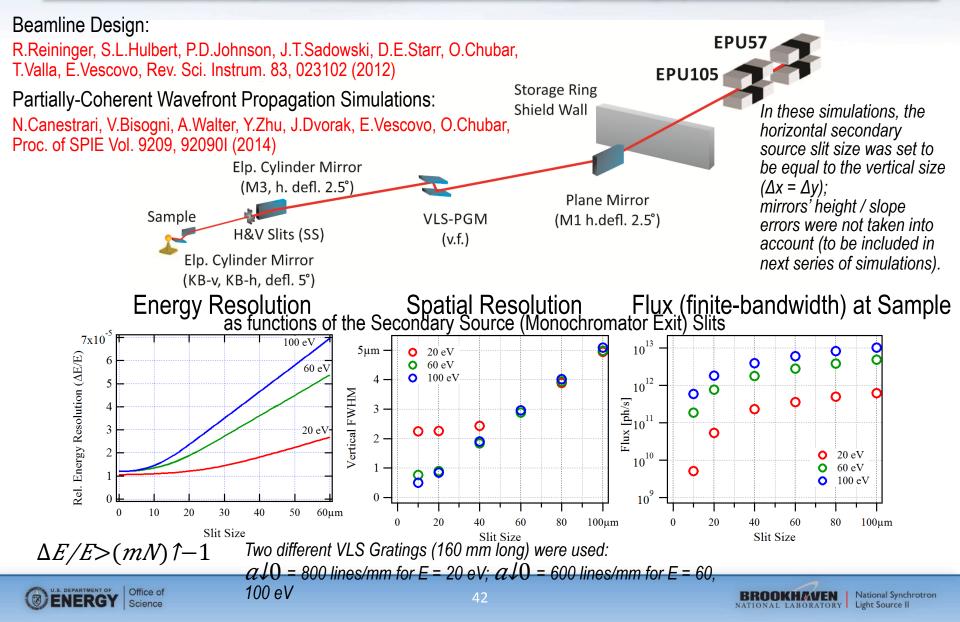
-20

-30

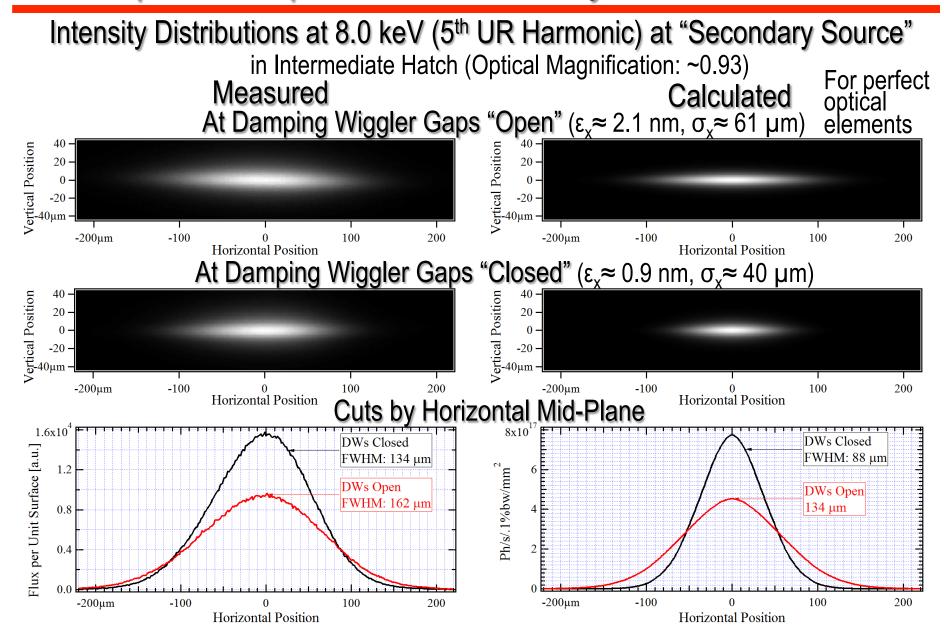
-200 -100 ò 100 200

X coordinate (µm)

Partially-Coherent Wavefront Propagation Simulations for a Soft X-ray Beamline with VLS grating (ESM @ NSLS-II)

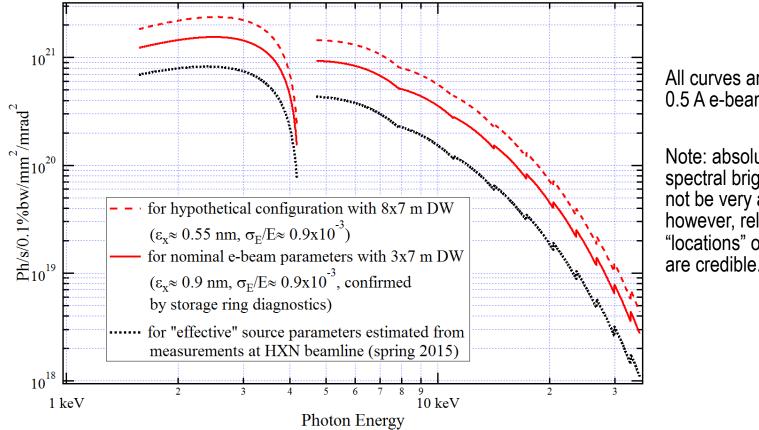


NSLS-II Emittance Reduction by DWs Observed after Imperfect Optics at "Secondary Source" of HXN



NSLS-II Brightness: Nominal and Estimated from Measurements at HXN Beamline

Approximate Spectral Brightness of IVU20 in Low-Beta Straight Section of NSLS-II



All curves are scaled for 0.5 A e-beam current.

> Note: absolute values of spectral brightness may not be very accurate, however, relative "locations" of the curves are credible.

The reduction of brightness "observed" at the beamline is attributed to imperfections of X-ray optics (horizontallyfocusing bendable mirrors, monochromator, vertically-focusing CRL) and undulator magnetic field.



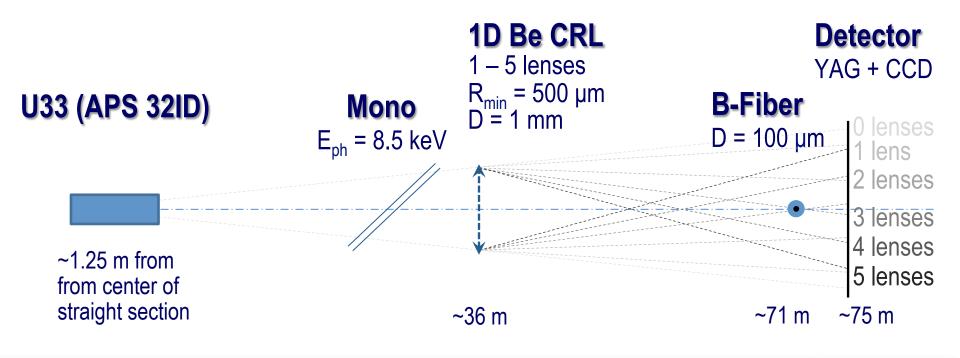
It will be possible to "restore" this "effective" brightness in the future (by further fine-tuning / processing / replacing of individual beamline components, identified from simulations and dedicated measurements).



Approach to Coherence Preservation Diagnostics Assisted by Simulations (Illustration)

V.Kohn, I.Snigireva and A.Snigirev, Phys. Rev. Lett., vol.85(13), p.2745 (2000) A.Snigirev, V.Kohn, I.Snigireva, B.Lengeler, Nature, vol.384, p.49 (1996) O.Chubar, A.Fluerasu, Y.S.Chu, L.Berman, L.Wiegart, W.-K.Lee, J.Baltser, J. Phys.: Conf. Ser. 425, 052028 (2013)

Optical scheme of test experiments with CRL and a Boron fiber probe

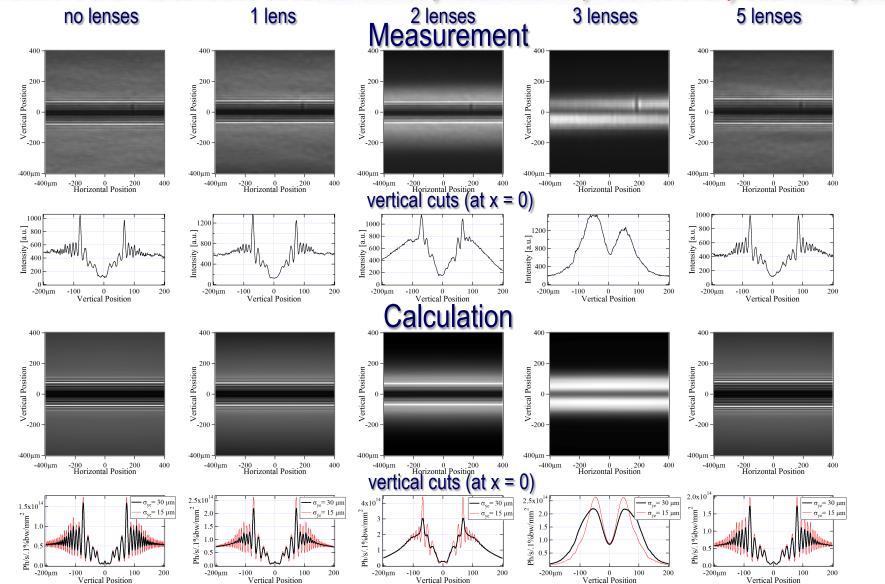


National Synchrotron

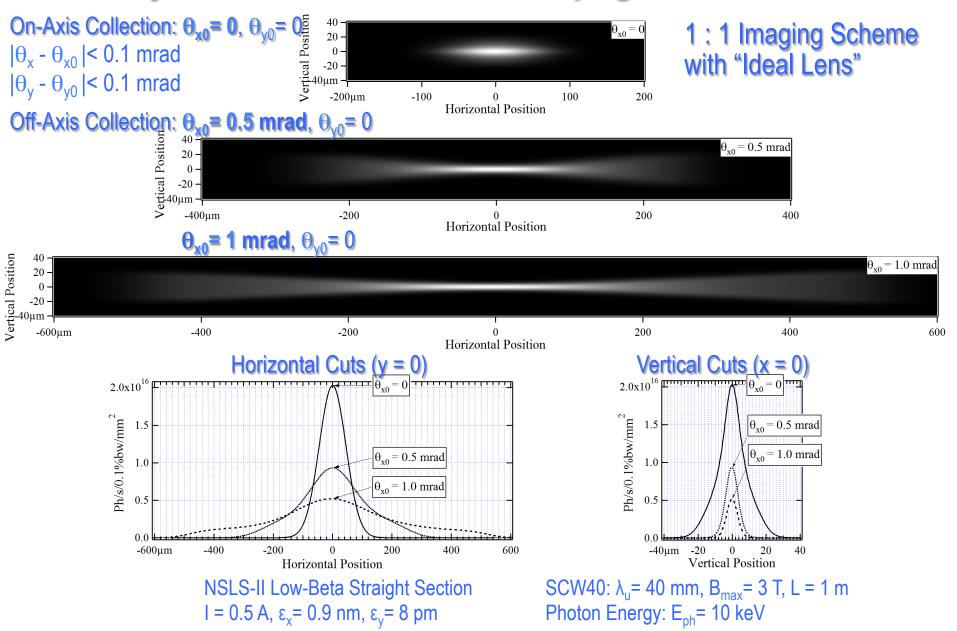
Light Source II

Intensity Distributions in the B-fiber Based Interference Scheme for Different Numbers of CRL in Optical Path

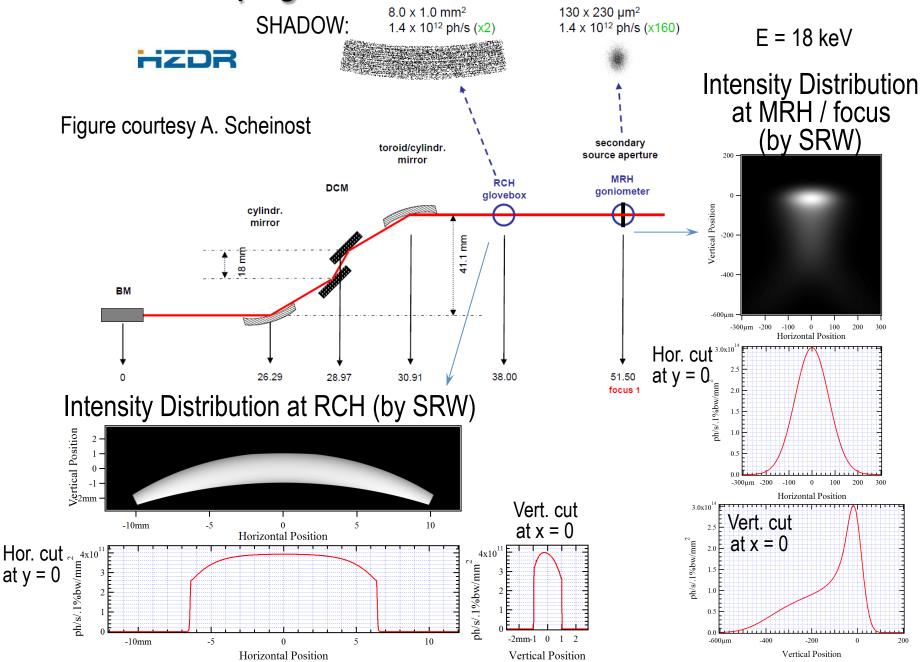
Simulations allow to conclude about coherence preservation in presence of any beamline optics!



Intensity Distributions of Focused Wiggler Radiation from Partially-Coherent Wavefront Propagation Calculations

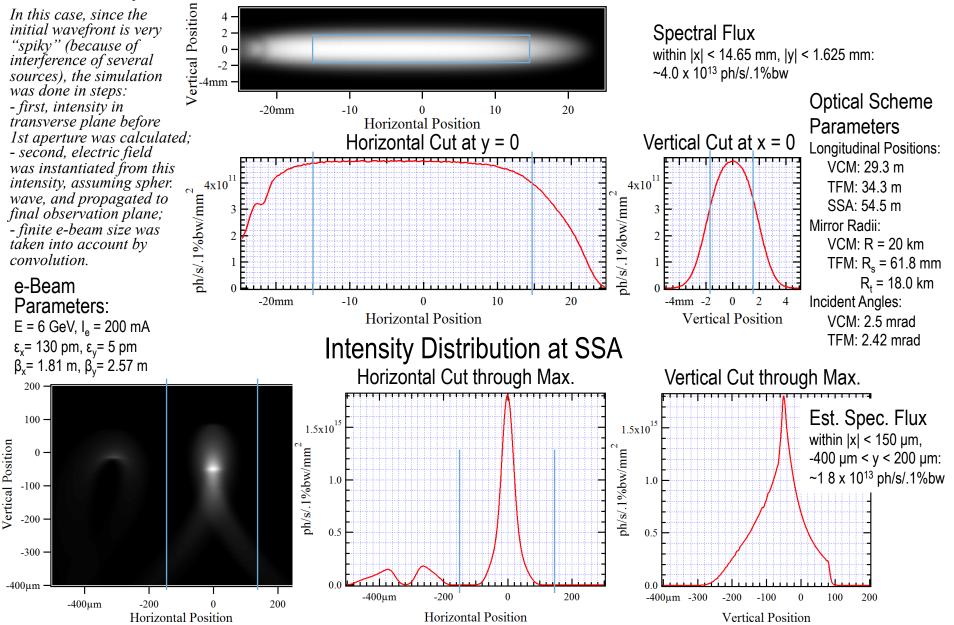


Wavefront Propagation Calculations for ROBL at ESRF

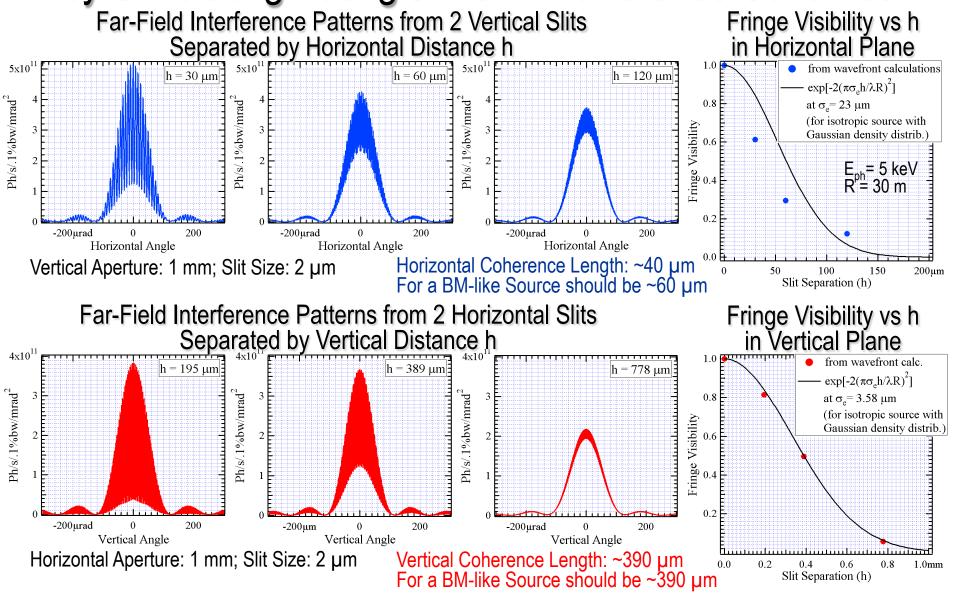


2PW-B Option for ROBL after ESRF Upgrade

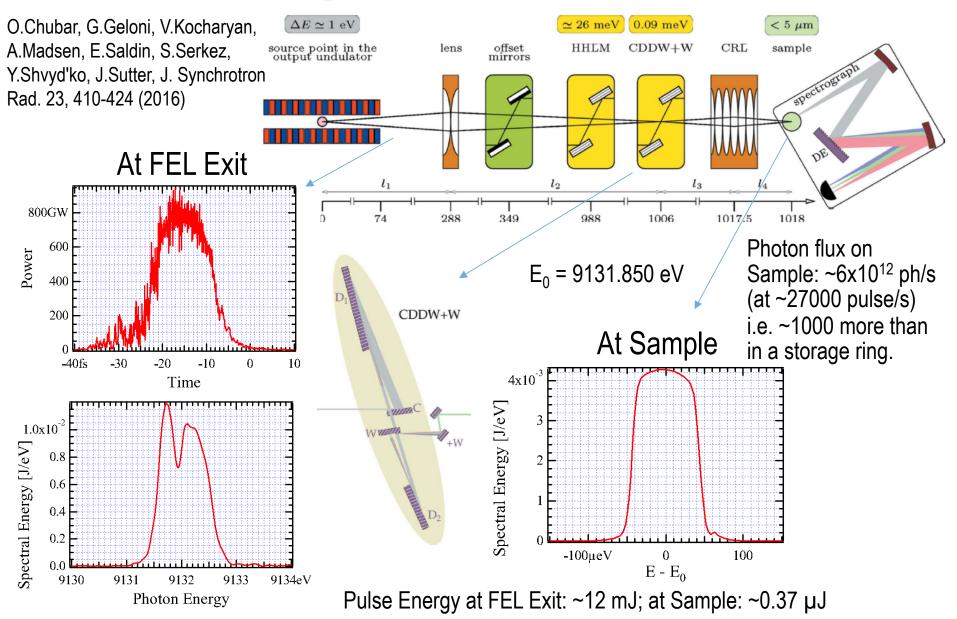
Intensity Distribution at 18 keV at ~29.3 m from Source (assuming no apertures upstream)



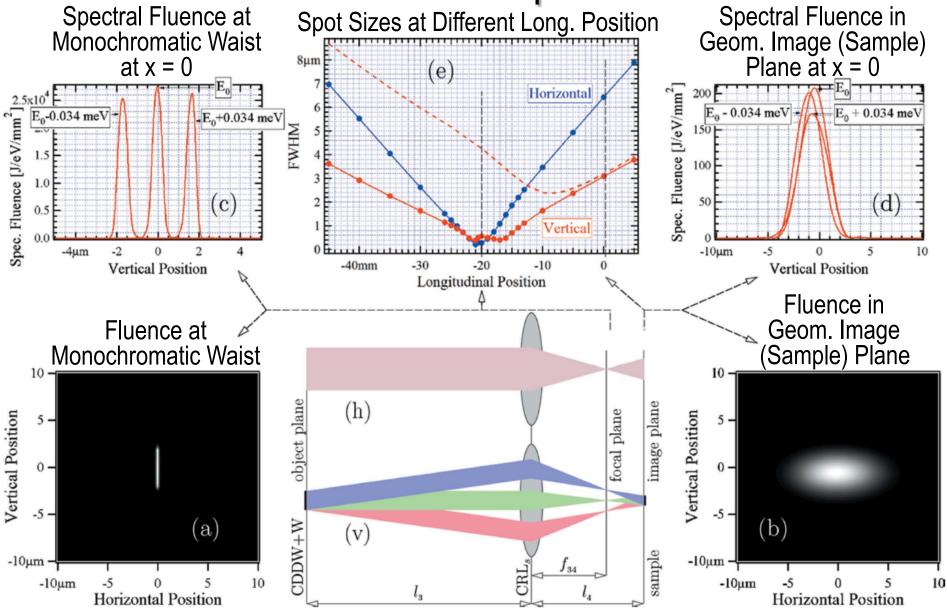
Estimating Degree of Coherence (/ Transverse Coherence Lengths) of Radiation from ESRF-U 2PW by Simulating Young's 2-Slit Interference Schemes



Testing Untra-High Resolution Inelastic X-ray Scattering Scheme at High-Rep-Rate Self-Seeded X-FEL



IXS at X-FEL: Radiation Pulse Characteristics Near Sample



Summary and Comments

- High-accuracy fully- and partially-coherent synchrotron emission and wavefront propagation calculations for sources and beamline optics are currently done routinely for beamlines at new storage rings and FEL (though performance can still be an issue in cases of low coherence).
- An advantage of high-accuracy wavefront calculations is very broad range of applications (because of their general electrodynamics basement): design of new sources and optics (maximizing performance of both), commissioning, diagnostics, simulation of user experiments, addressing misc. inverse problems of data processing, etc. Some interesting potential applications are not fully explored yet.
- Main disadvantage of these calculations is currently a ~low CPU performance in low-coherence cases compared to geometrical ray-tracing; however, it can be mitigated by parallelization, coherent mode decomposition and other methods.
 Note: the higher is the degree of coherence in a beamline, the easier is the treatment of partial coherence, which is very good for applications in FEL and MBA storage rings.
 Another "disadvantage" is higher complexity of these calculations compared to ray-tracing. It can be mitigated by programming more robust "propagators", propagation "drivers", as well as developing better user interfaces and writing better help.

Acknowledgments

- Pascal Elleaume, Jean-Louis Laclare
- Colleagues contributed to development of SRW: J. Sutter (DLS), D. Laundy (DLS), A. Suvorov (BNL), N. Canestrari (ESRF-BNL), R. Reininger (ANL), X. Shi (ANL), R. Lindberg (ANL), L. Samoylova (E-XFEL), A. Buzmakov (E-XFEL), D. Bruhwiler (RadiaSoft LLC), R. Nagler (RadiaSoft LLC), M. Rakitin (BNL)
- Management and colleagues who helped in transition to Open Source: G. Materlik (DLS, London Centre for Nanotechnology), K. Sawhney (DLS), J. Susini (ESRF), M. S. del Rio (ESRF), S. Dierker (BNL), Q. Shen (BNL), P. Zschack (BNL), S. Hulbert (BNL), H. Sinn (E-XFEL)
- NSLS-II scientists: A. Fluerasu, L. Wiegart, K. Kaznatcheev, E. Vescovo, V. Bisogni, M. Zhernenkov, E. DiMasi, Y. Cai, Y. Chu, I. Jarrige, D. Schneider, M. Fuchs, J. Thieme, L. Yang, T. Shaftan
- Many thanks to Luca and Manuel the S.O.S. Workshop Organizers!