

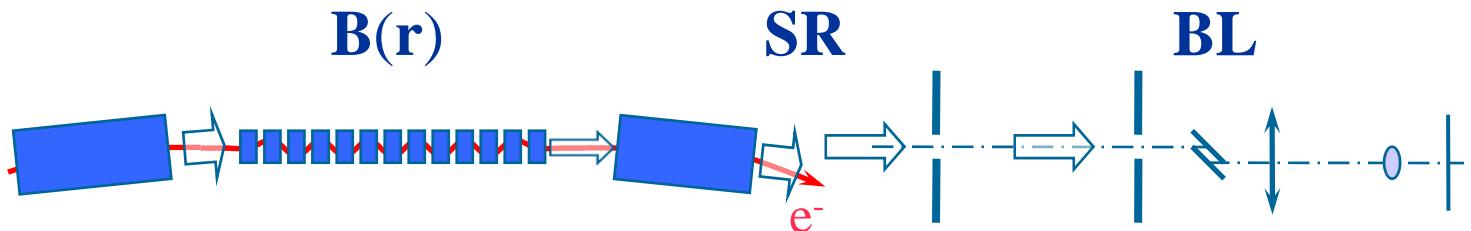
# Numerical Methods and Simulation Software for the Emission and Propagation of Fully- and Partially-Coherent Synchrotron Radiation Wavefronts

O. Chubar  
NSLS-II Project, BNL, USA

# Outline

- Introduction
  - Motivation
  - Existing Computer Codes
- Methods
  - Synchrotron Radiation:
    - Frequency Domain Electric Field from Liénard-Wiechert Potentials
  - Wavefront Propagation:
    - Kirchhoff Theorem for Single-Electron SR
    - Fourier Optics
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  - Radiation from Insertion Devices:
    - Spectral Flux and Brightness
    - Intensity Distributions
    - Peculiarities of the Phase
  - Wavefront Propagation in THz to Hard X-Ray Spectral Range
- Possible Evolution

# Motivation



- Computation of **Magnetic Fields** produced by Permanent Magnets, Coils and Iron Blocks and in 3D space, optimized for the design of **Accelerator Magnets, Undulators and Wigglers**
- Fast computation of **Synchrotron Radiation** emitted by relativistic electrons in Magnetic Field of arbitrary configuration
- SR Wavefront Propagation (Physical Optics)

RADIA

SRW

# Some Computer Codes

- For Synchrotron Radiation (Spontaneous Emission) and Wavefront Propagation Simulations
  - URGENT (R.Walker, ELETTRA)
  - XOP (S.Rio, ESRF, R.Dejus, APS)
  - WAVE + PHASE (J.Bahrdt, M.Scheer, BESSY)
  - SPECTRA (T.Tanaka, H.Kitamura, SPring-8)
  - SRW (O.Chubar, P.Elleaume, ESRF-SOLEIL, 1997-...)

# Growing Importance of Physical Optics Calculations

Example: NSLS-II (operation to start in ~2015)

Approved Beamlines (December 2008)	Requires Physical Optics Simulations?
Inelastic Scattering Beamline (0.1 – 1 meV spectral resolution)	yes
Nanoprobe Beamline	yes
Coherent Hard X-ray Beamline	yes
Coherent Soft X-ray Beamline	yes
X-ray Absorption Spectroscopy Beamline	?
Powder Diffraction Beamline	yes

# Spontaneous Emission by One Relativistic Electron Moving in Free Space

Lienard-Wiechert Potentials for One Electron:

(Gaussian CGS)

$$\vec{A} = e \int_{-\infty}^{+\infty} \vec{\beta}_e R^{-1} \delta(\tau - t + R/c) d\tau, \quad \varphi = e \int_{-\infty}^{+\infty} R^{-1} \delta(\tau - t + R/c) d\tau$$



Electric Field in Frequency Domain (exact expression!!!):

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

I.M.Ternov used this approach  
in Far Field approximation

$$\vec{E}_\omega = \frac{e}{c} \int_{-\infty}^{+\infty} \frac{\vec{n} \times \left[ (\vec{n} - \vec{\beta}_e) \times \dot{\vec{\beta}}_e \right] + cR^{-1}\gamma^{-2}(\vec{n} - \vec{\beta}_e)}{R \cdot (1 - \vec{n} \cdot \vec{\beta}_e)^2} \cdot \exp[i\omega(\tau + R/c)] d\tau \quad \text{J.D.Jackson}$$

Equivalence of the two expressions can be shown by integration by parts

# Spontaneous Emission by One Relativistic Electron

Electric Field in Frequency Domain:

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

$$\vec{n} = \vec{R}/R, \quad n_x \approx \frac{x - x_e}{z - c\tau}, \quad n_y \approx \frac{y - y_e}{z - c\tau}$$

Phase Expansion (valid in the Near- and in the Far Field):

$$\omega \cdot (\tau + R/c) \approx \Phi_0 + \frac{k}{2} \left[ c\tau\gamma^{-2} + c \int_0^\tau |\vec{\beta}_{e\perp}|^2 d\tilde{\tau} + \frac{|\vec{r}_\perp - \vec{r}_{e\perp}|^2}{z - c\tau} \right]$$

Asymptotic Expansion to accelerate computation and "improve" numerical convergence:

$$\int_{-\infty}^{+\infty} F \exp(i\Phi) ds = \int_{\tau_1}^{\tau_2} F \exp(i\Phi) ds + \int_{-\infty}^{\tau_1} F \exp(i\Phi) ds + \int_{\tau_2}^{+\infty} F \exp(i\Phi) ds$$

$$\int_{-\infty}^{\tau_1} F \exp(i\Phi) ds + \int_{\tau_2}^{+\infty} F \exp(i\Phi) ds \approx \left[ \left( \frac{F}{i\Phi'} + \frac{F'\Phi' - F\Phi''}{\Phi'^3} + \dots \right) \exp(i\Phi) \right]_{\tau_2}^{\tau_1}$$

# Incoherent and Coherent Emission by Many Electrons

Electron Dynamics:

$$\begin{pmatrix} x_e \\ y_e \\ z_e \\ \beta_{xe} \\ \beta_{ye} \\ \delta\gamma_e \end{pmatrix} = \mathbf{A}(\tau) \begin{pmatrix} x_{e0} \\ y_{e0} \\ z_{e0} \\ x'_{e0} \\ y'_{e0} \\ \delta\gamma_{e0} \end{pmatrix} + \mathbf{B}(\tau)$$

← Initial Conditions

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

$$\frac{dN_{ph}}{dt dS(d\omega/\omega)} = \frac{c^2 \alpha I}{4\pi^2 e^3} \left\langle \left| \vec{E}_\omega \right|^2 \right\rangle$$

“Incoherent” SR

$$\left\langle \left| \vec{E}_\omega \right|^2 \right\rangle = \int \left| \vec{E}_{\omega 0}(\vec{r}; x_{e0}, y_{e0}, z_{e0}, x'_{e0}, y'_{e0}, \delta\gamma_{e0}) \right|^2 f(x_{e0}, y_{e0}, z_{e0}, x'_{e0}, y'_{e0}, \delta\gamma_{e0}) dx_{e0} dy_{e0} dz_{e0} dx'_{e0} dy'_{e0} d\delta\gamma_{e0} +$$

$$+ (N_e - 1) \left| \int \vec{E}_{\omega 0}(\vec{r}; x_{e0}, y_{e0}, z_{e0}, x'_{e0}, y'_{e0}, \delta\gamma_{e0}) f(x_{e0}, y_{e0}, z_{e0}, x'_{e0}, y'_{e0}, \delta\gamma_{e0}) dx_{e0} dy_{e0} dz_{e0} dx'_{e0} dy'_{e0} d\delta\gamma_{e0} \right|^2$$

“Coherent” SR

Common Approximation for CSR: “Thin” Electron Beam:  $\left\langle \left| \vec{E}_\omega \right|^2 \right\rangle_{CSR} \approx N_e \left| \int_{-\infty}^{\infty} \tilde{f}(z_{e0}) \exp(ikz_{e0}) dz_{e0} \right|^2 \left| \vec{E}_{\omega 1} \right|^2$

For Gaussian Longitudinal Bunch Profile:  $\left\langle \left| \vec{E}_\omega \right|^2 \right\rangle_{CSR} \approx N_e \exp(-k^2 \sigma_b^2) \left| \vec{E}_{\omega 1} \right|^2$

However, if  $f(x_{e0}, y_{e0}, z_{e0}, x'_{e0}, y'_{e0}, \delta\gamma_{e0})$  is Gaussian, the 6-fold integration can be done analytically (!)

⇒ Efficient method for CSR computation taking into account 6D phase space distribution of electrons

# Self-Amplified Spontaneous Emission Described by Paraxial FEL Equations

## Approximation of Slowly Varying Amplitude of Radiation Field

Particles' dynamics  
in undulator and radiation fields  
(averaged over many periods):

$$\frac{d\theta}{dz} = k_u - k_r \frac{1 + p_\perp^2 + a_u^2 - 2a_r a_u \cos(\theta + \phi_r)}{2\gamma^2}$$

$$\frac{d\gamma}{dz} = -\frac{k_r f_c a_r a_u}{\gamma} \sin(\theta + \phi_r)$$

$$\frac{d\vec{p}_\perp}{dz} = -\frac{1}{2\gamma} \frac{\partial a_u^2}{\partial \vec{r}_\perp} + \mathbf{k}_{foc} \vec{r}_\perp$$

$$\frac{d\vec{r}_\perp}{dz} = \frac{\vec{p}_\perp}{\gamma}$$

$$\left[ 2ik_r \frac{\partial}{\partial z} + \nabla_\perp^2 \right] a_r \exp(i\phi_r) = -\frac{e\epsilon_0 I f_c a_u}{mc} \left\langle \frac{\exp(-i\theta)}{\gamma} \right\rangle$$

W.B. Colson  
J.B. Murphy  
C. Pellegrini  
E. Saldin  
E. Bessonov  
et. al.

Paraxial wave equation  
with current:

Solving this system gives Electric Field at the FEL exit for one "Slice":  $E_{slice}|_{z=z_{exit}} \sim a_r \exp(i\phi_r)|_{z=z_{exit}}$

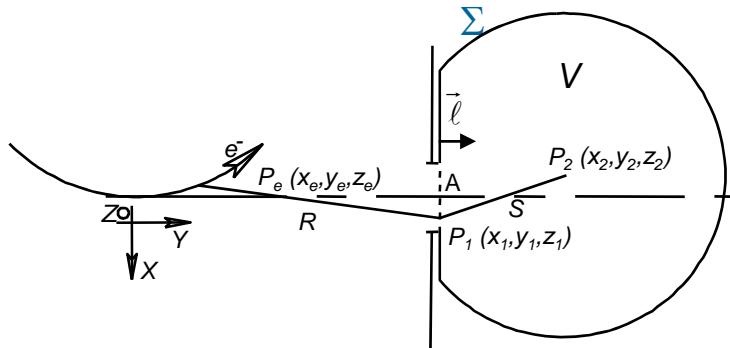
Loop on "Slices" (copying Electric Field to a next slice from previous slice, starting from back)

Time- (and Frequency-) Domain Electric Field in transverse plane at FEL exit:  $E(x, y, z_{exit}, t) \leftrightarrow E_\omega(x, y, z_{exit})$

- Popular TD 3D FEL computer code: **GENESIS** (S.Reiche)  
Integrated to SRW on C++ level

# Wavefront Propagation: Case of Full Transverse Coherence

Kirchhoff Integral Theorem applied to Spontaneous Emission by One Electron



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

$k = \omega/c$

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

Huygens-Fresnel Principle

$$\vec{E}_{\omega 2\perp}(P_2) \approx \frac{k}{4\pi i} \iint_A \vec{E}_{\omega 1\perp}(P_1) \frac{\exp(ikS)}{S} (\vec{l} \cdot \vec{n} + \vec{l} \cdot \vec{n}_{p_1 p_2}) d\Sigma$$

Fourier Optics

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

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

Assumption of small angles

"Thin" Optical Element:

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

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

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

E.g. from Stationary Phase method

# "Economic" Version of Free-Space Fourier-Optics Propagator

**Huygens-Fresnel Principle:**  
(paraxial approximation)

$$\vec{E}_{\omega 2\perp}(\vec{r}_2) \approx \frac{k}{2\pi i} \iint_{\Sigma_1} \vec{E}_{\omega 1\perp}(\vec{r}_1) \frac{\exp[ik|\vec{r}_2 - \vec{r}_1|]}{|\vec{r}_2 - \vec{r}_1|} d\Sigma_1$$

$$|\vec{r}_2 - \vec{r}_1| = [L^2 + (x_2 - x_1)^2 + (y_2 - y_1)^2]^{1/2}$$

**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:

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

# Wavefront Propagation: Taking Into Account Partial Coherence

## Averaging of Propagated One-Electron Intensity over Phase-Space Volume occupied by Electron Beam:

$$I_\omega(x, y) = \int I_{\omega 0}(x, y; x_{e0}, y_{e0}, x'_{e0}, y'_{e0}, \delta\gamma_{e0}) f(x_{e0}, y_{e0}, x'_{e0}, y'_{e0}, \delta\gamma_{e0}) dx_{e0} dy_{e0} dx'_{e0} dy'_{e0} d\delta\gamma_{e0}$$

**Convolution** is valid in many cases:

- projection geometry;
- focusing by a thin lens;
- diffraction on one slit (/pinhole);
- ...

$$I_\omega(x, y) \approx \iint_{-\infty-\infty}^{+\infty+\infty} \tilde{I}_{\omega 0}(x - \tilde{x}_e, y - \tilde{y}_e) \tilde{f}(\tilde{x}_e, \tilde{y}_e) d\tilde{x}_e d\tilde{y}_e$$

OR:

## Propagation of Mutual Intensity

Kwang-Je Kim

Mutual Intensity:

$$\begin{aligned} M_\omega(x, y; \tilde{x}, \tilde{y}) &= \int \vec{E}_{\omega 0\perp}(x, y; x_{e0}, y_{e0}, x'_{e0}, y'_{e0}, \delta\gamma_{e0}) \vec{E}_{\omega 0\perp}^*(\tilde{x}, \tilde{y}; x_{e0}, y_{e0}, x'_{e0}, y'_{e0}, \delta\gamma_{e0}) \\ &\quad \times f(x_{e0}, y_{e0}, x'_{e0}, y'_{e0}, \delta\gamma_{e0}) dx_{e0} dy_{e0} dx'_{e0} dy'_{e0} d\delta\gamma_{e0} \end{aligned}$$

Wigner Distribution (or mathematical Brightness):

$$B_\omega(x, y; \theta_x, \theta_y) = \frac{1}{2\pi} \iint_{-\infty-\infty}^{+\infty+\infty} M_\omega(x, y; \tilde{x}, \tilde{y}) \exp[ik(\theta_x \tilde{x} + \theta_y \tilde{y})] d\tilde{x} d\tilde{y}$$

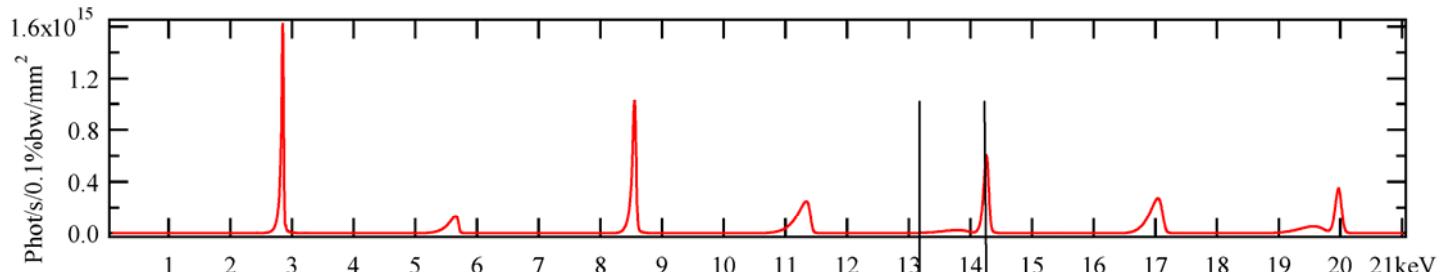
# Examples: Undulator Radiation

## On-Axis Spectrum (taking into account e-beam Emittance)

Undulator:

$$\lambda_u = 35 \text{ mm}$$

$$K = 2.2$$



e-Beam:

$$E = 6 \text{ GeV}$$

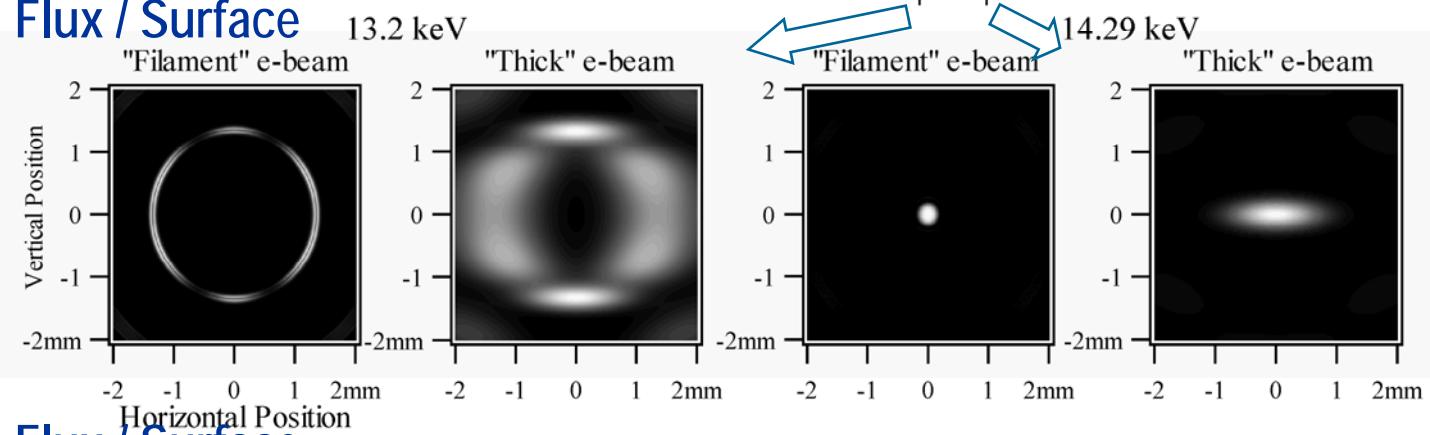
$$\sigma_{x \text{ eff}} / R = 16.2 \mu\text{m}$$

$$\sigma_{z \text{ eff}} / R = 3.96 \mu\text{m}$$

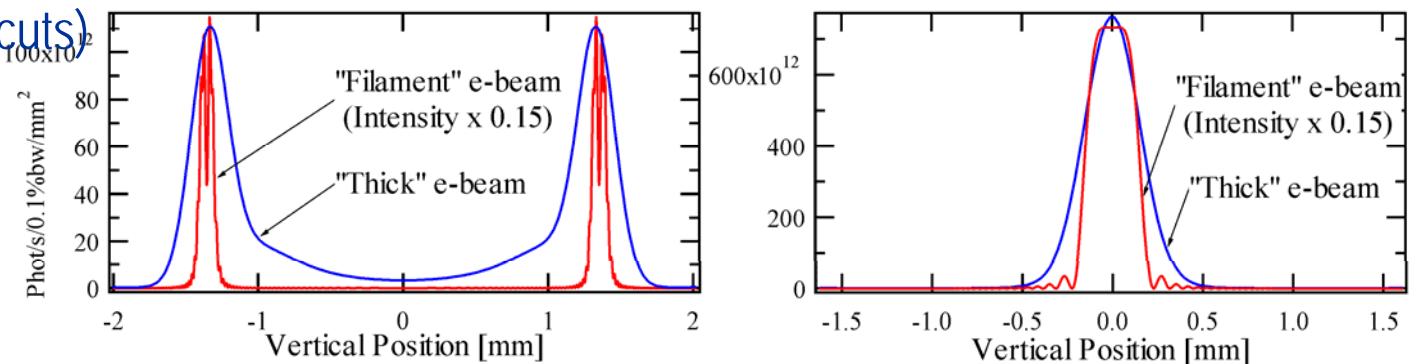
$$\sigma_E / E = 10^{-3}$$

$$R = 30 \text{ m}$$

## Spectral Flux / Surface

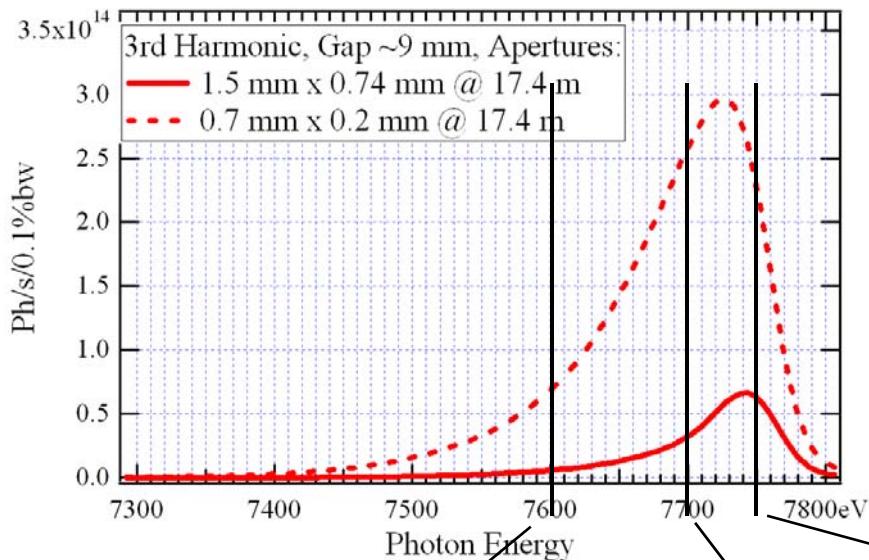


## Spectral Flux / Surface (vertical cuts)

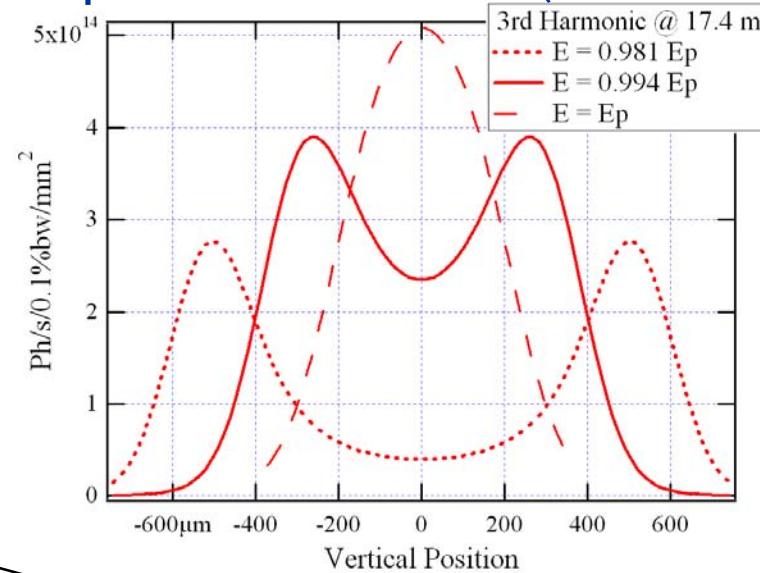


# Examples: Undulator Radiation U20 (SOLEIL) Spectra and Intensity Distributions @ H3

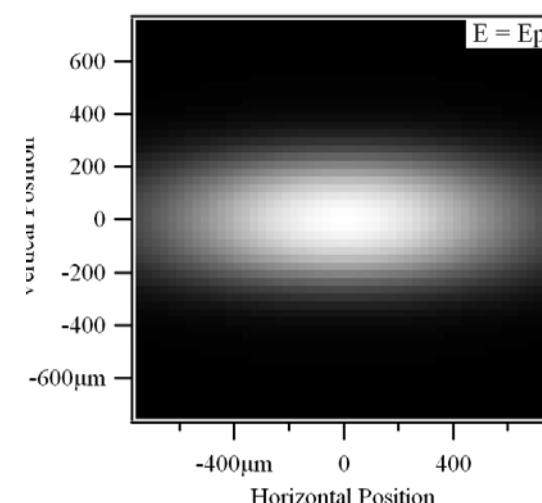
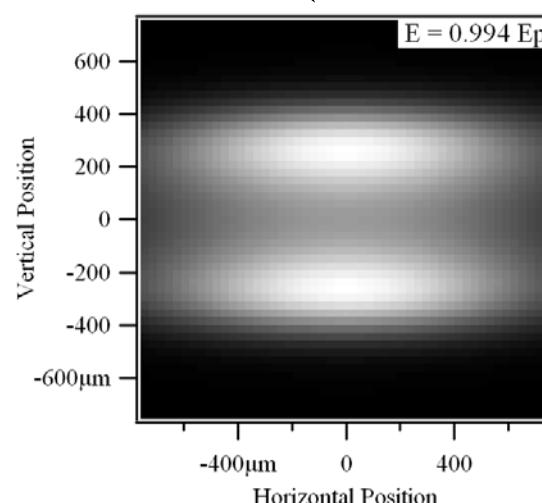
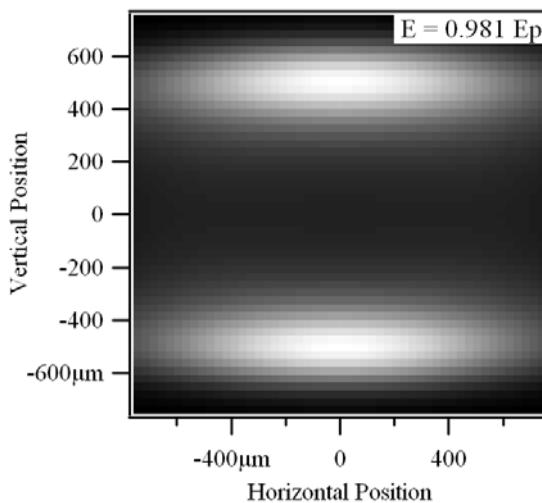
Spectral Flux



Spectral Flux / Surface (vertical cuts)

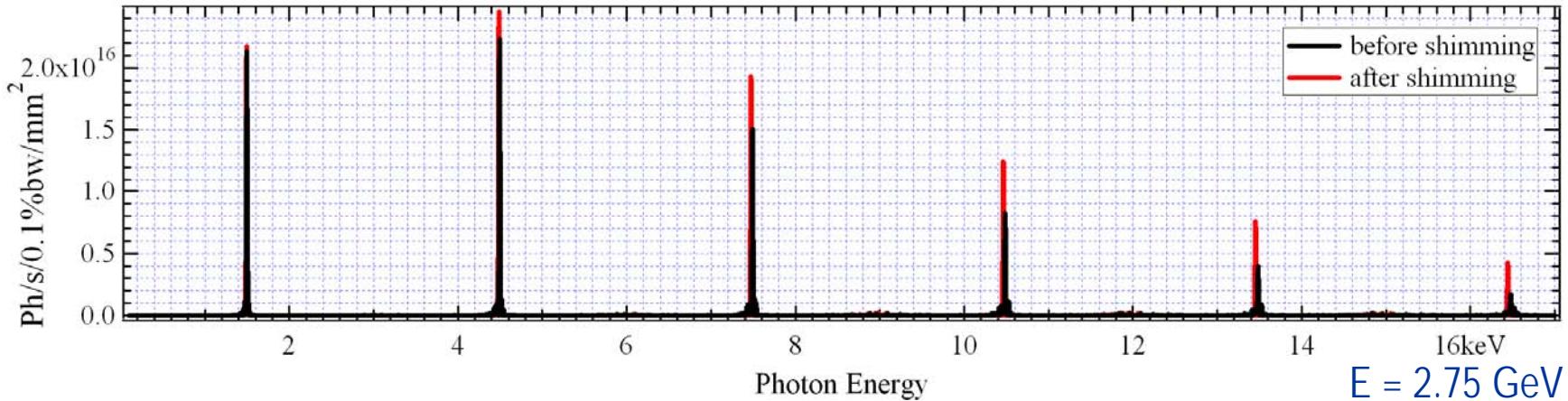


Spectral Flux / Surface @ 17.4 m

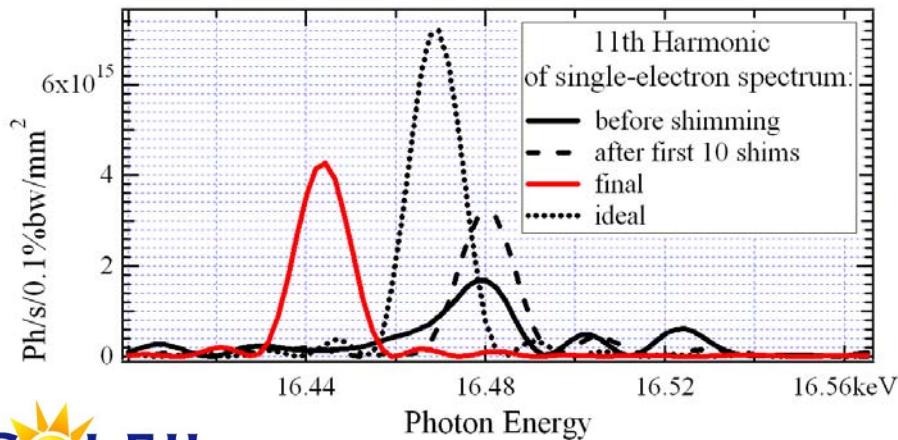


# In-Vacuum Hybrid Undulator U20 (SWING) Spectral Shimming Results

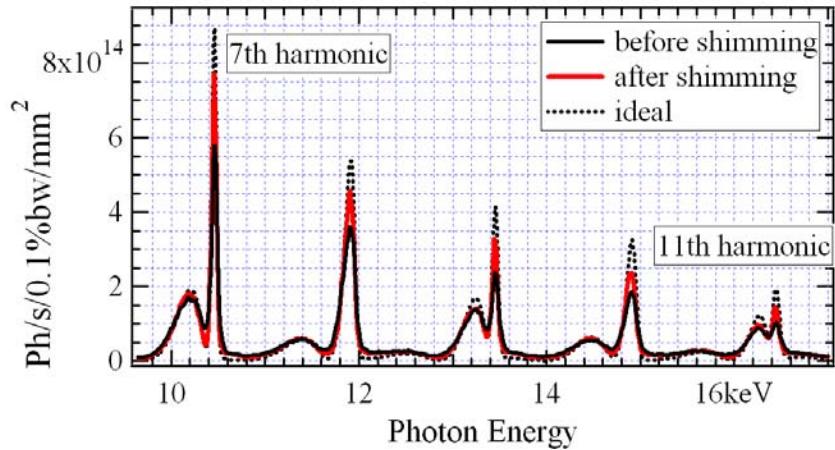
On-Axis Single-Electron Spectra Before and After Shimming (10 m from source)



Evolution of 11<sup>th</sup> Harmonic  
of Single-Electron Spectrum

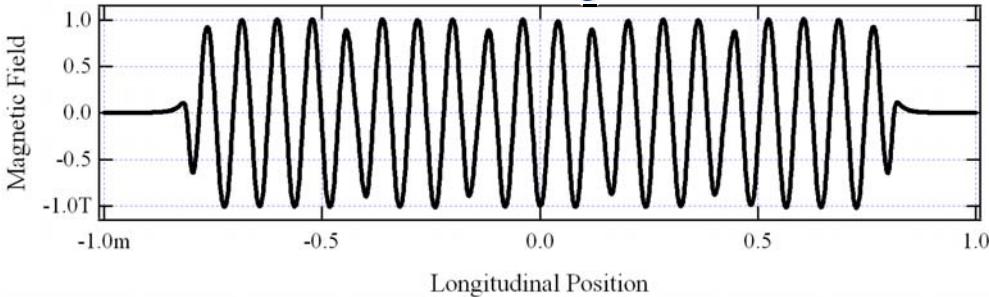


On-Axis Intensity Taking into account  
E-Beam Emittance and Energy Spread

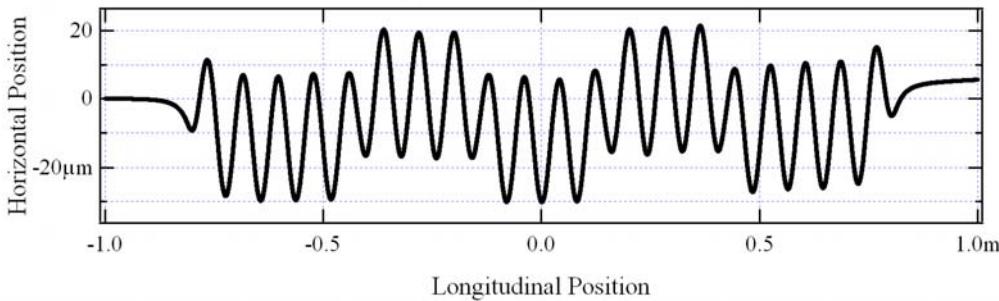


# APPLE-II Undulator HU80-PLEIADES: Quasi-Periodic Field, Trajectory, Spectra

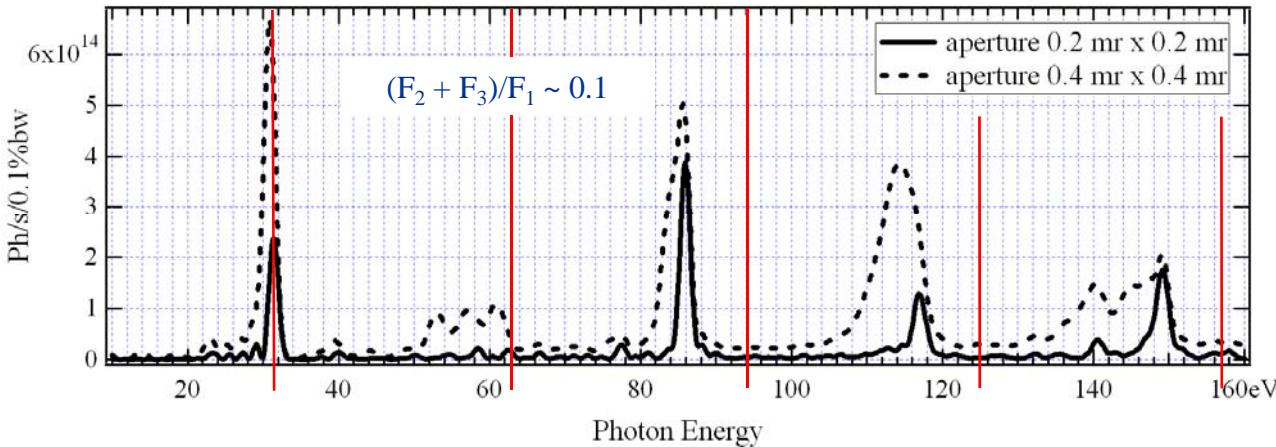
## Measured Vertical Magnetic Field



## Horizontal Trajectory



## Spectra Through Finite Apertures

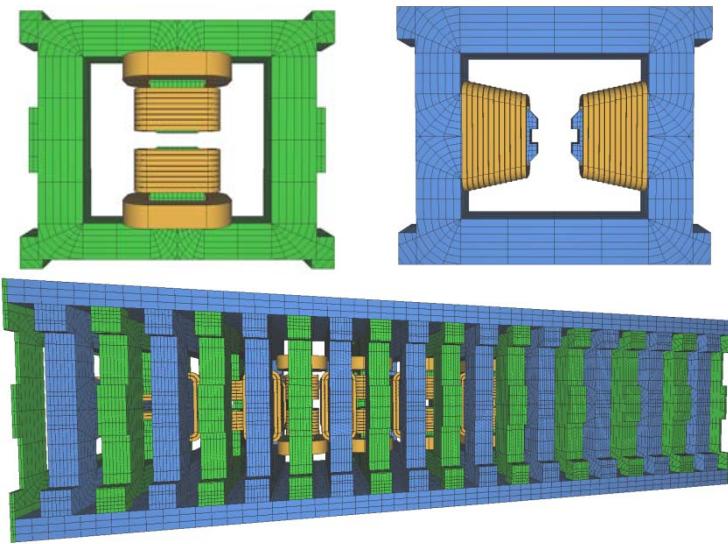


Quasi-Periodic Mode  
was realized by 11 mm  
displacement of some  
longitudinally-polarized  
magnet blocks

# RADIA-SRW Examples: Electromagnetic Elliptical Undulator HU256

The Structure (A.Dael, SOLEIL; P.Vobly, BINP)

RADIA Model



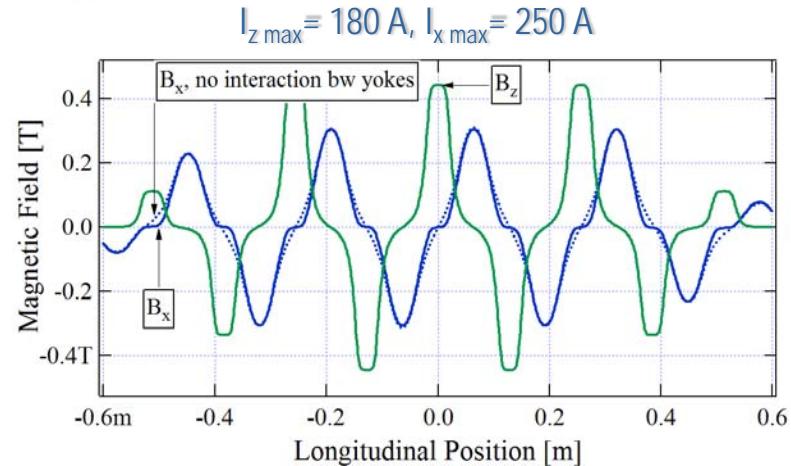
## Specifications:

Circular Polarization:  $\varepsilon_1 \text{ min} < 10 \text{ eV}$

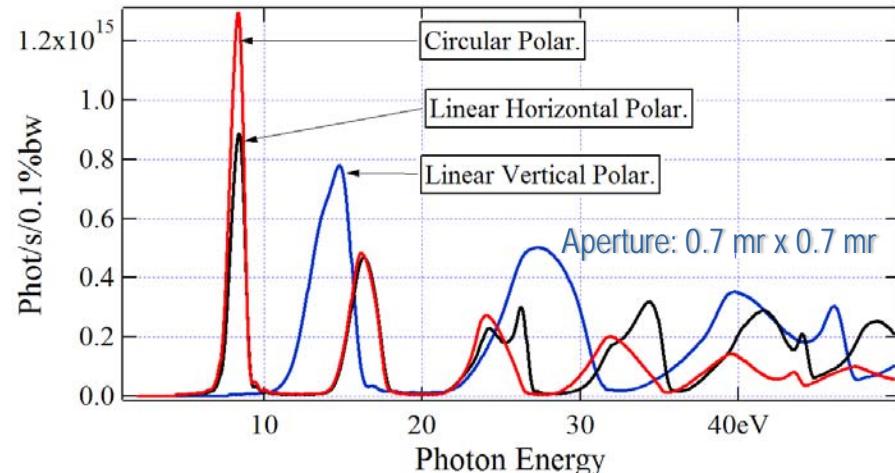
Linear Horiz. Polarization:  $\varepsilon_1 \text{ min} < 10 \text{ eV}$

Linear Vertical Polarization:  $\varepsilon_1 \text{ min} < 20 \text{ eV}$

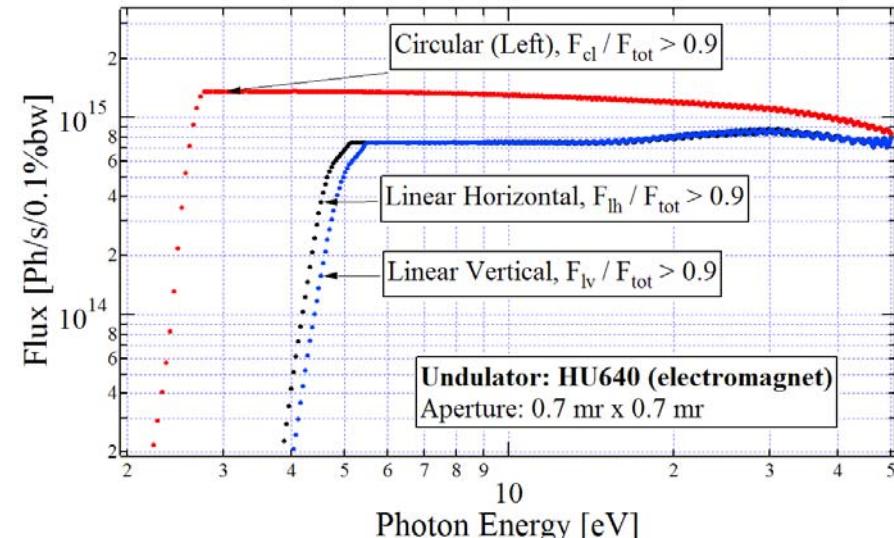
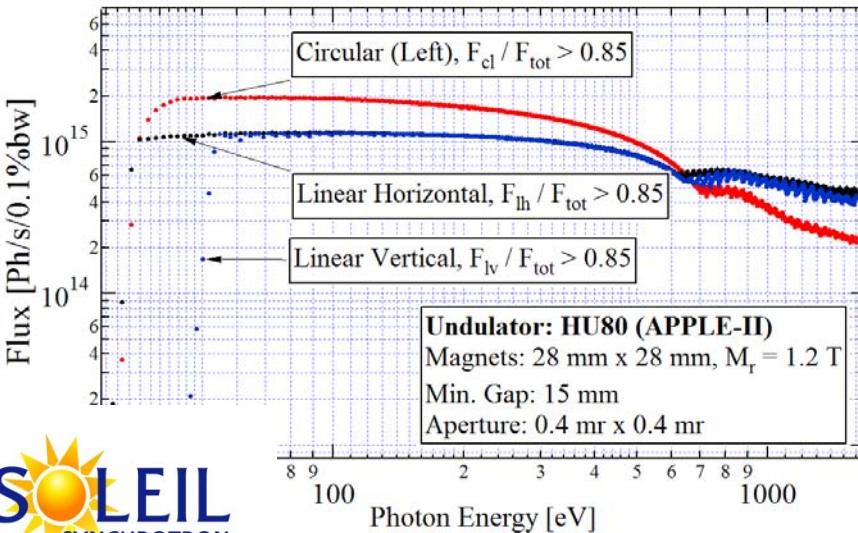
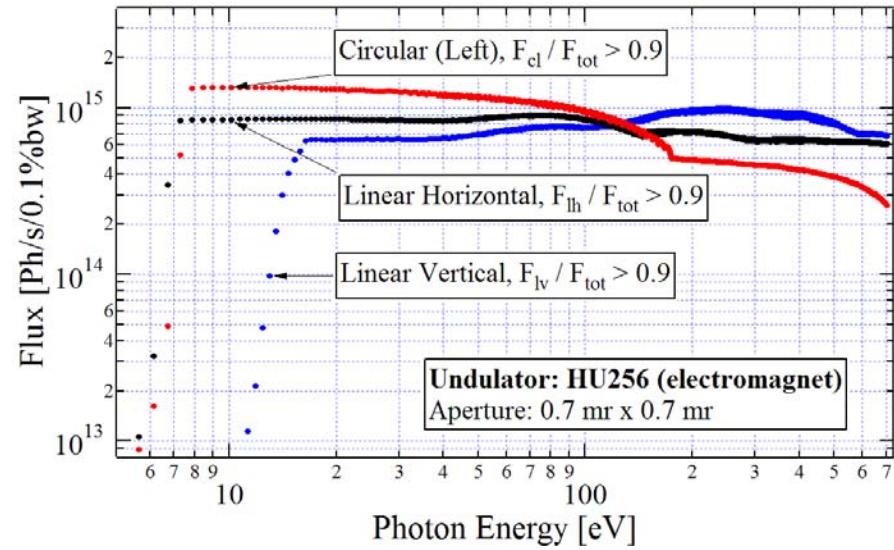
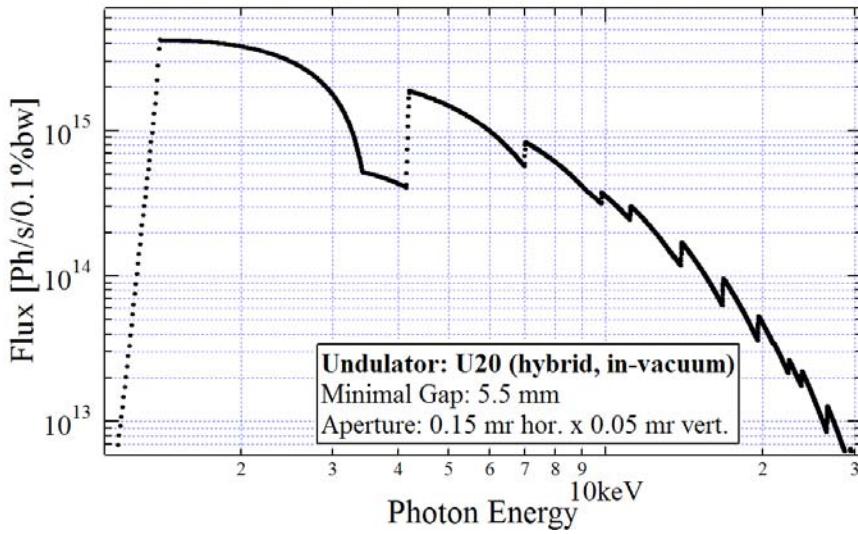
Magnetic Fields at Max. Currents (RADIA)



Calculated Spectra at Maximal Currents (SRW)

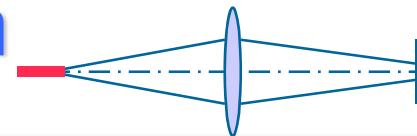


# Examples: Undulator Radiation Maximal Spectral Flux at Various Polarizations

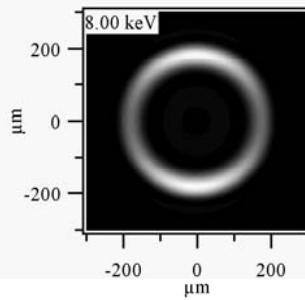
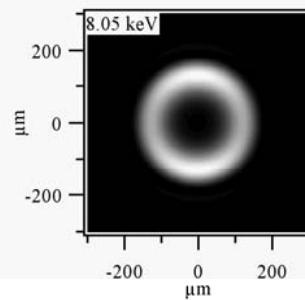
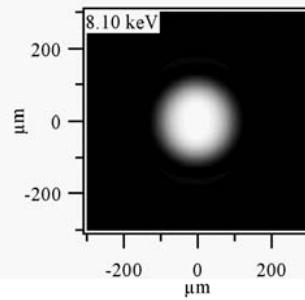
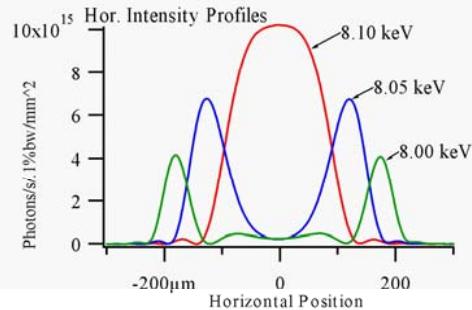


# Examples: Wavefront Propagation

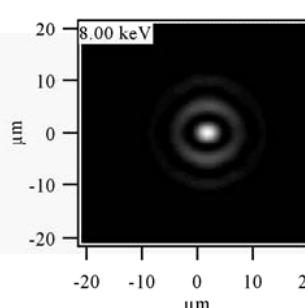
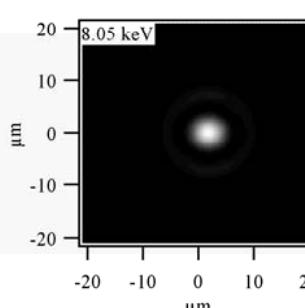
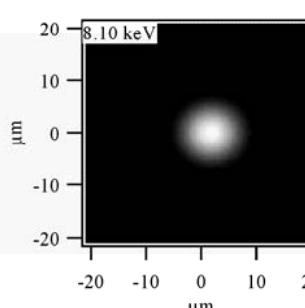
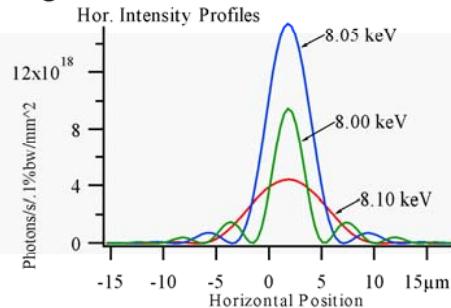
## Focusing of Undulator Radiation



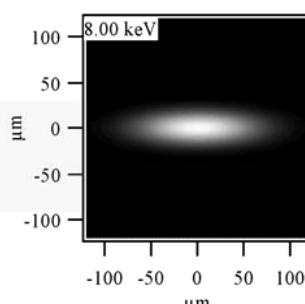
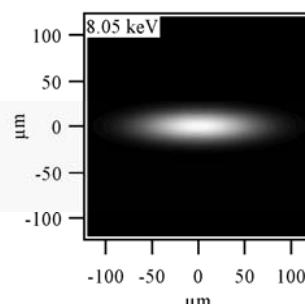
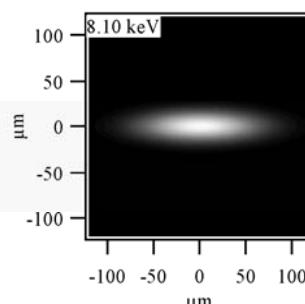
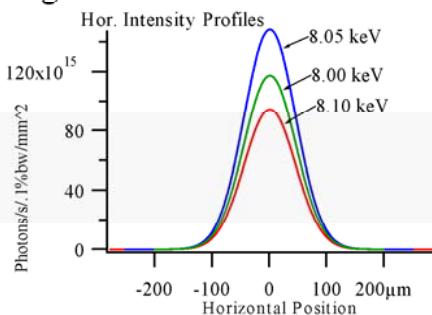
A: Lens Plane. "Filament" e-beam.



B: Image Plane. "Filament" e-beam.

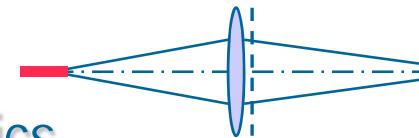


C: Image Plane. "Thick" e-beam.



# Examples: Wavefront Propagation

## Peculiarities of UR Wavefronts

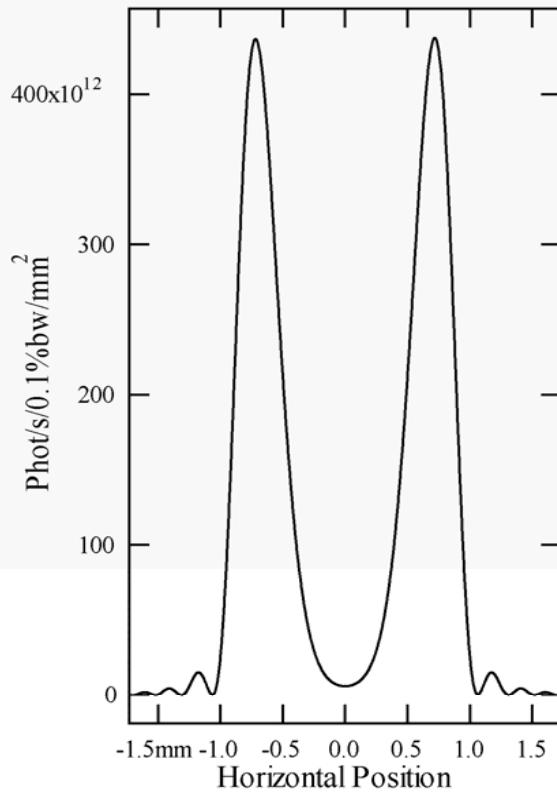


### Planar Undulator, Odd Harmonics

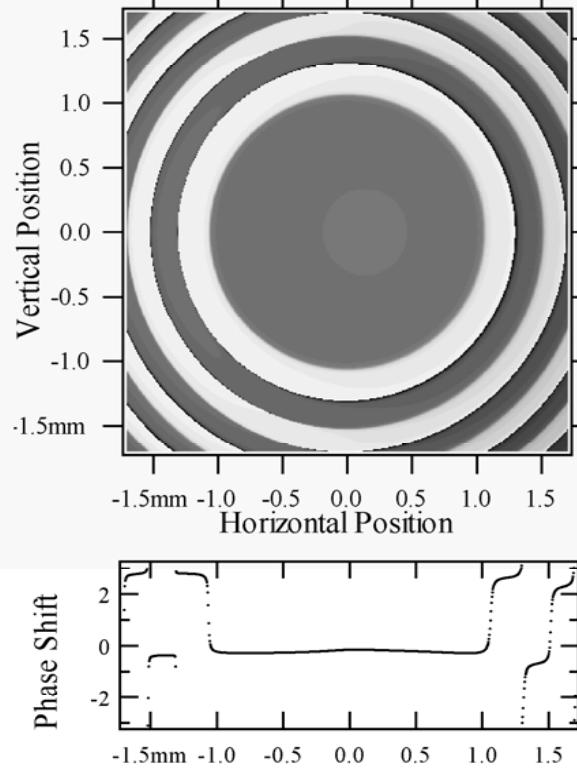
$E = 6 \text{ GeV}$ ;  $K = 2.2$ ;  $38 \times 42 \text{ mm}$ ;  $\varepsilon = 2.36 \text{ keV}$  (~ fundamental)

1 : 1 imaging; 30 m from middle of Undulator to Thin Lens & Phase Correction

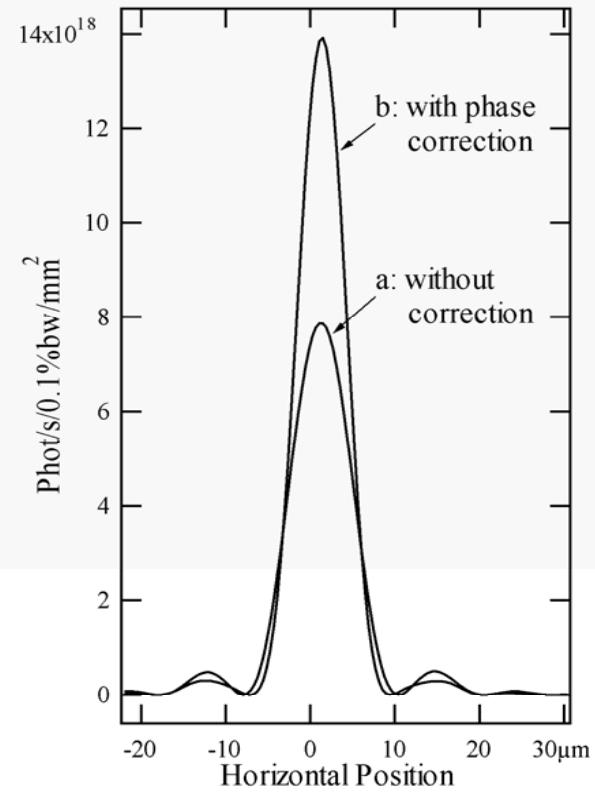
Intensity at the Lens



Phase Correction

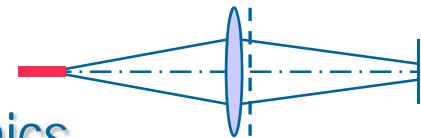


Intensity in the Image Plane



# Examples: Wavefront Propagation

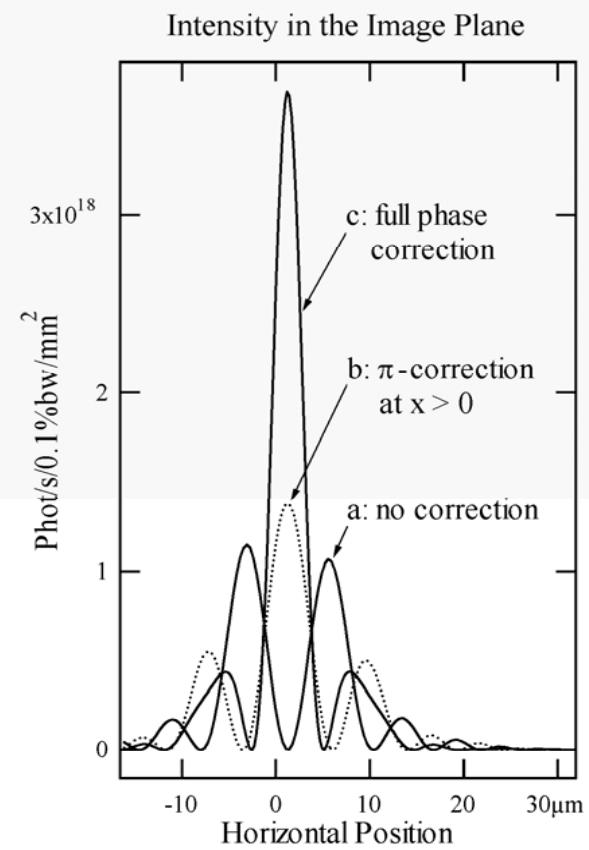
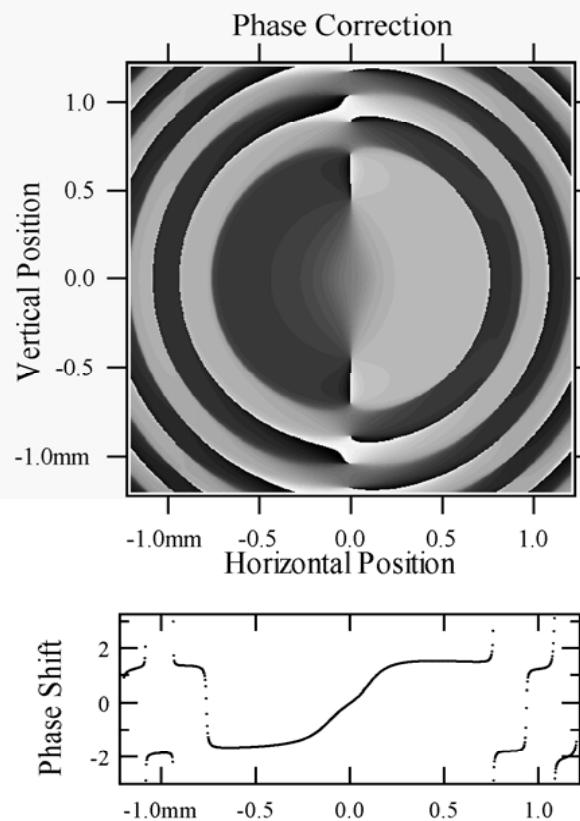
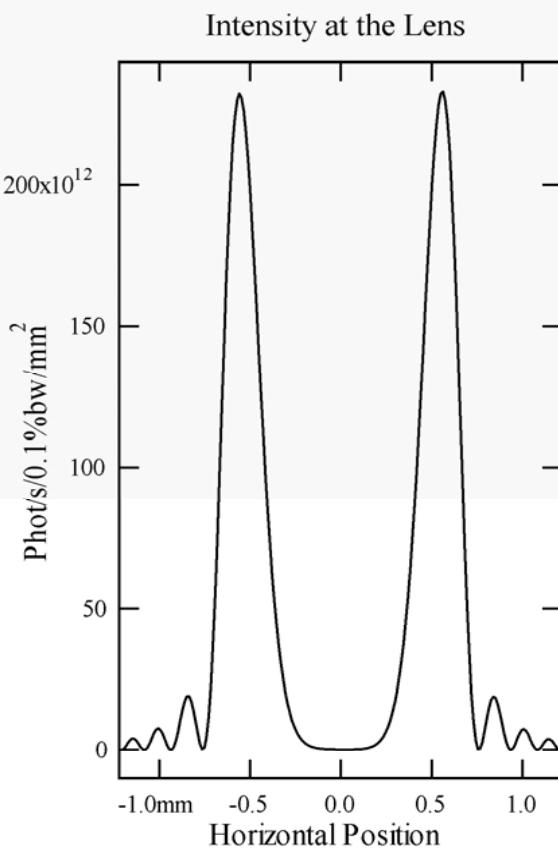
## Peculiarities of UR Wavefronts



### Planar Undulator, Even Harmonics

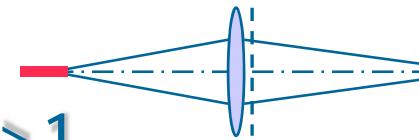
$E = 6 \text{ GeV}$ ;  $K = 2.2$ ;  $38 \times 42 \text{ mm}$ ;  $\varepsilon = 4.775 \text{ keV}$  (2<sup>-nd</sup> harmonic)

1 : 1 imaging; 30 m from middle of Undulator to Thin Lens & Phase Correction



# Examples: Wavefront Propagation

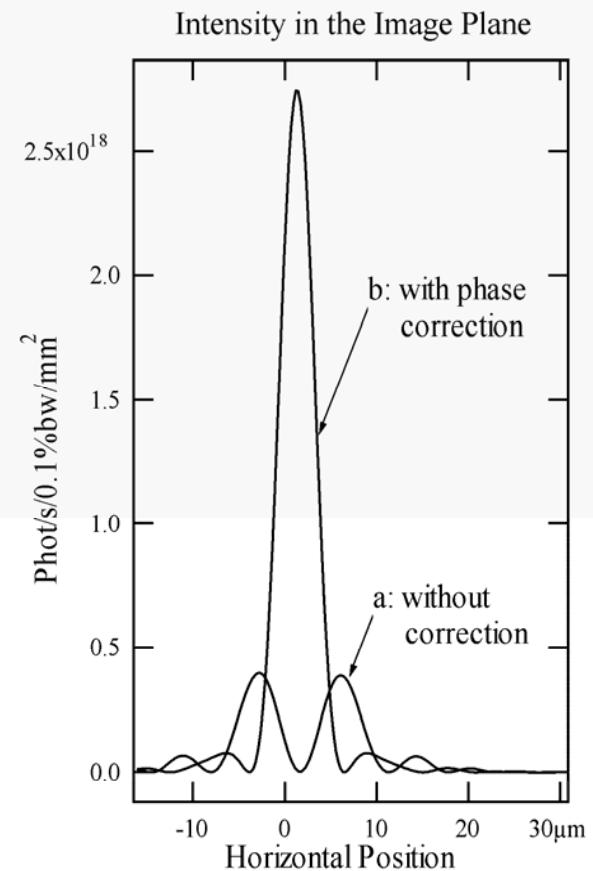
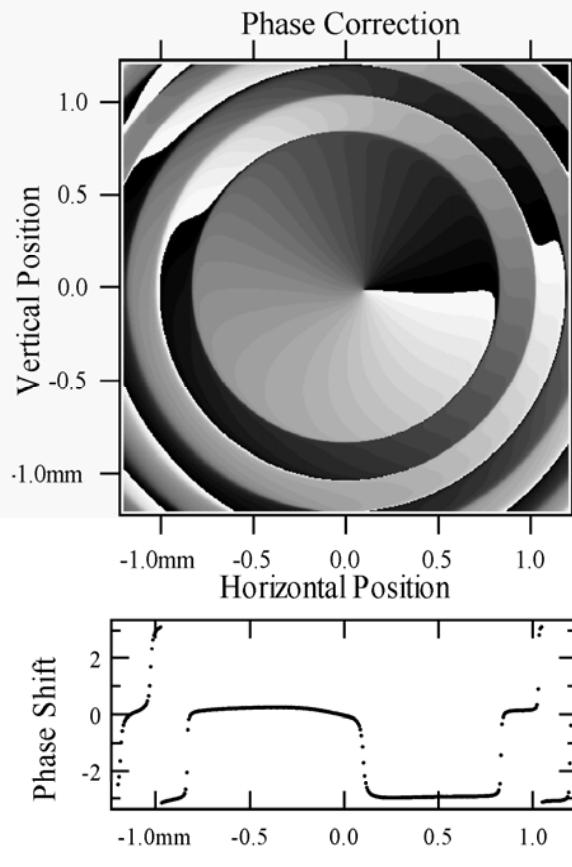
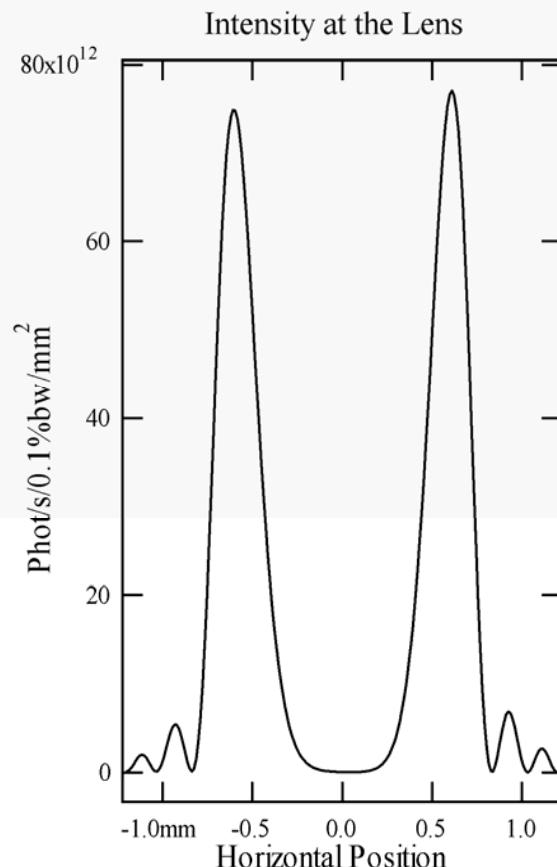
## Peculiarities of UR Wavefronts



### Helical Undulator, Harmonics $n > 1$

$E = 6 \text{ GeV}; B_{x \text{ max}} = B_{z \text{ max}} = 0.3 \text{ T}; 28 \times 52 \text{ mm}; \varepsilon = 4.20 \text{ keV}$  (2<sup>-nd</sup> harmonic)

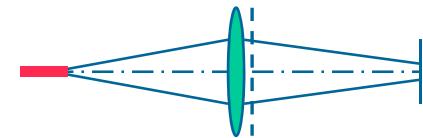
1 : 1 imaging; 30 m from middle of Undulator to Thin Lens & Phase Correction



Directly relevant to "OAM"! – S. Sasaki and I. McNulty, PRL, 2008

# Examples: Wavefront Propagation

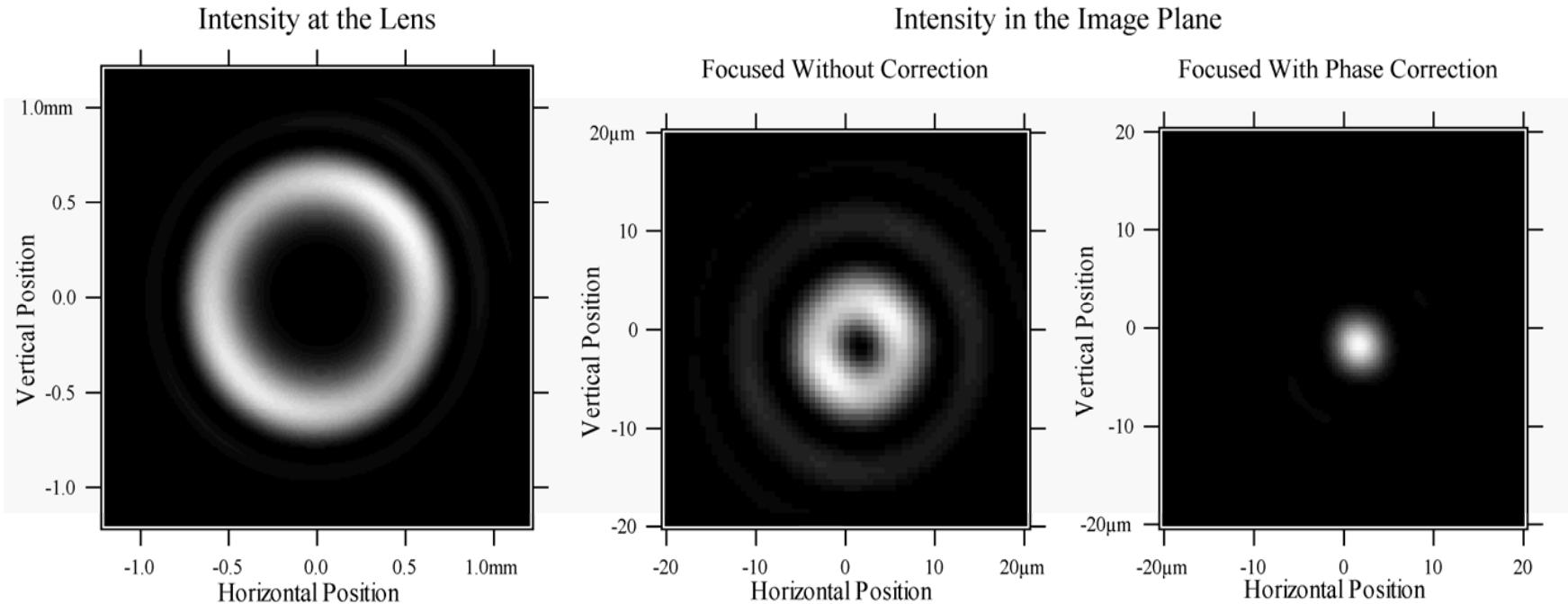
## Peculiarities of UR Wavefronts



### Focusing of Radiation from Helical Undulator, Harmonics $n > 1$

$E = 6 \text{ GeV}$ ;  $B_{x \text{ max}} = B_{z \text{ max}} = 0.3 \text{ T}$ ;  $28 \times 52 \text{ mm}$ ;  $\epsilon = 4.20 \text{ keV}$  (2<sup>nd</sup> harmonic)

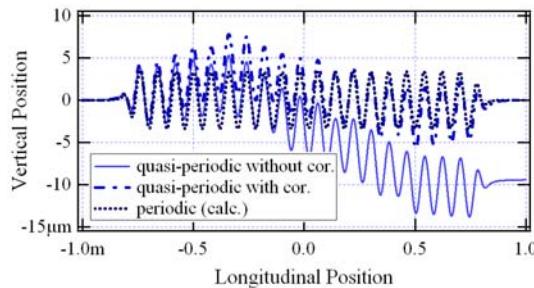
1 : 1 imaging; 30 m from middle of Undulator to Thin Lens & Phase Correction



# Wavefront Propagation Simulations for HU80- $\mu$ Foc

## Back-Propagation from M1 to Undulator Center ( $\approx 1:1$ Imaging)

In Vertical Plane

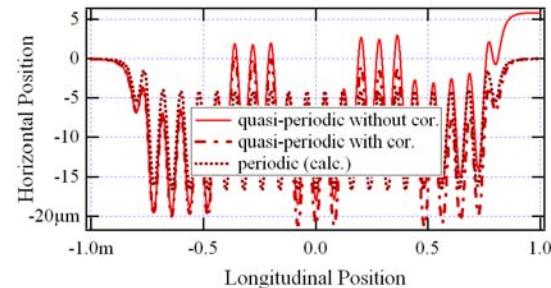


Electron Trajectories

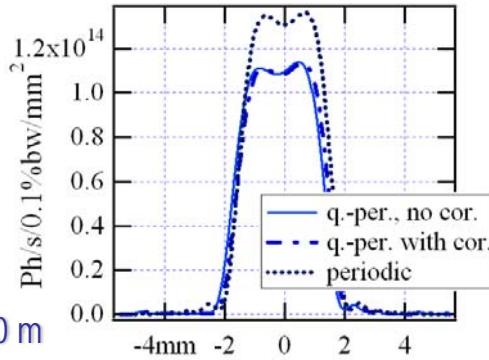
from Measured  
Magnetic Field

Gap: 30 mm  
Phase: -20 mm

In Horizontal Plane

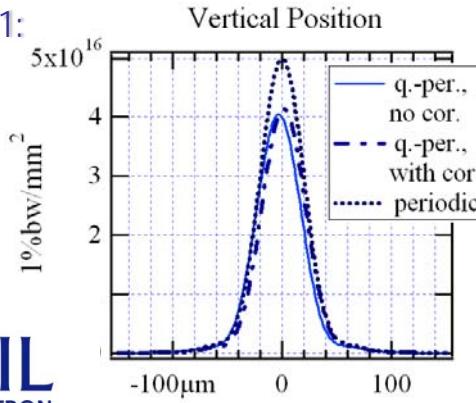


Vertical Cuts

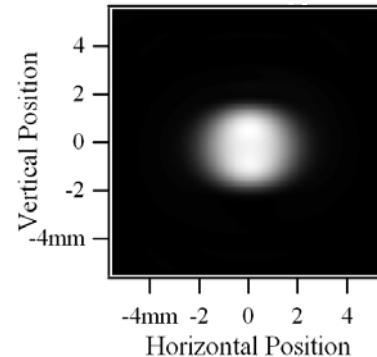


Distance from  
Und. to M1: 20 m

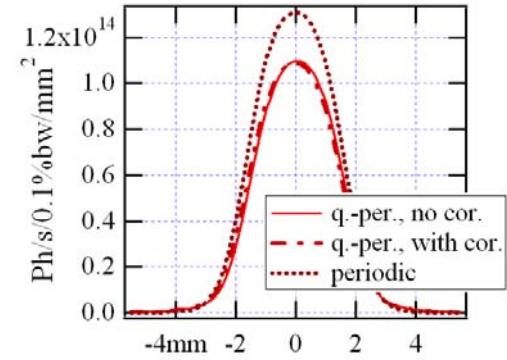
Aperture @ M1:  
5 mm (H) x  
4 mm (V)



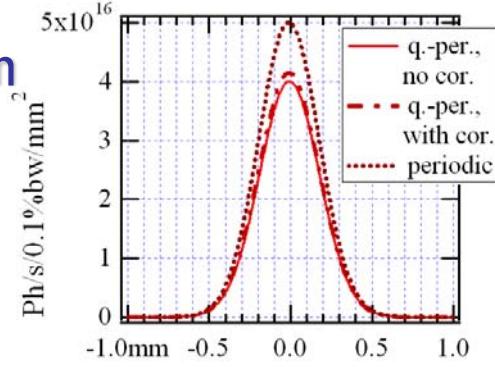
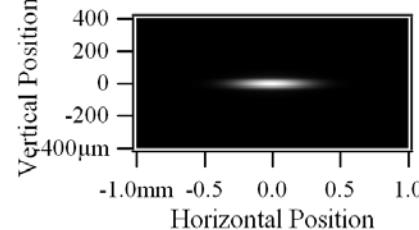
Intensity Distribution at M1  
Photon Energy: 163 eV



Horizontal Cuts

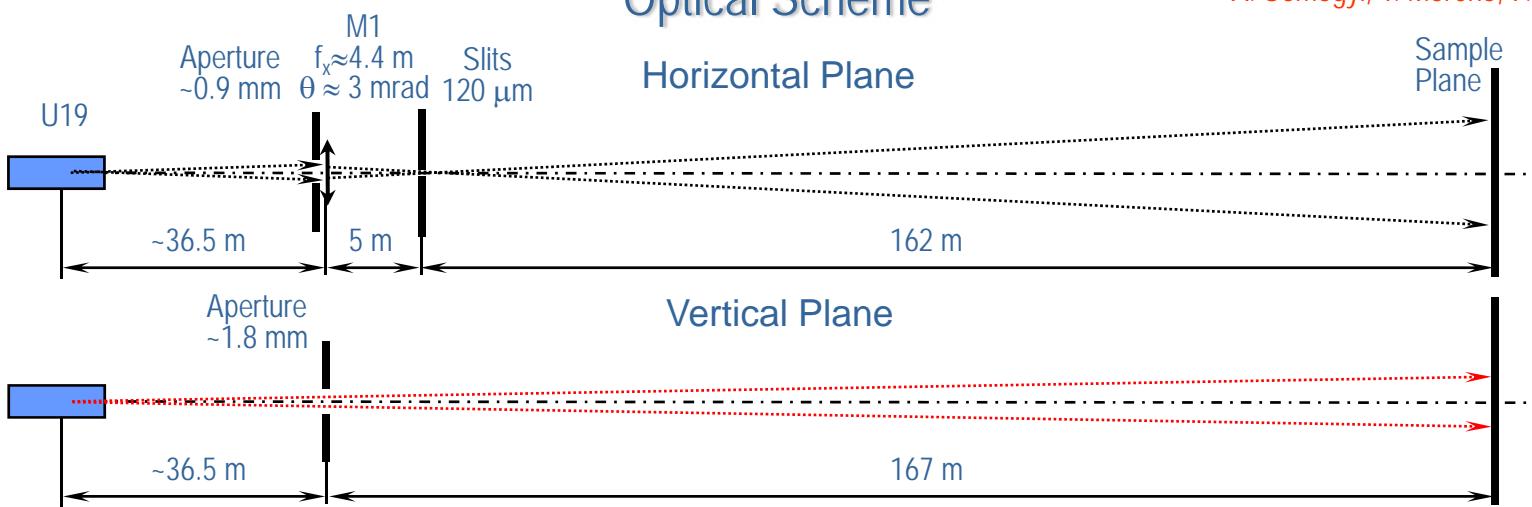


Intensity Distribution  
after Back-Propagation



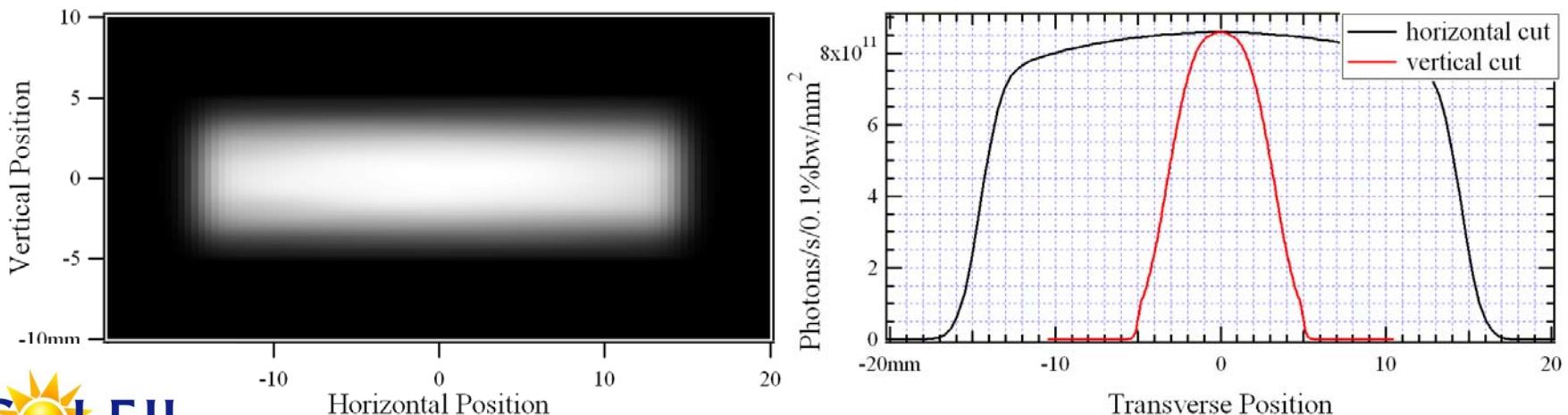
# Partially-Coherent Wavefront Propagation Simulations for Phase-Contrast Tomography BL: Approximate Scheme

## Optical Scheme



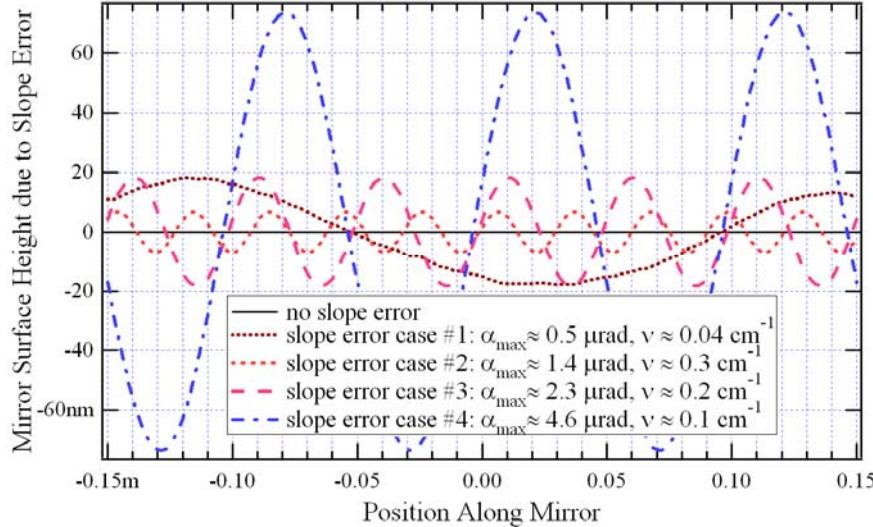
A. Somogyi, T. Moreno, F. Polack

## Intensity Distributions in Transverse Plane at Sample (no Slope Error, $\varepsilon \approx 10 \text{ keV}$ )

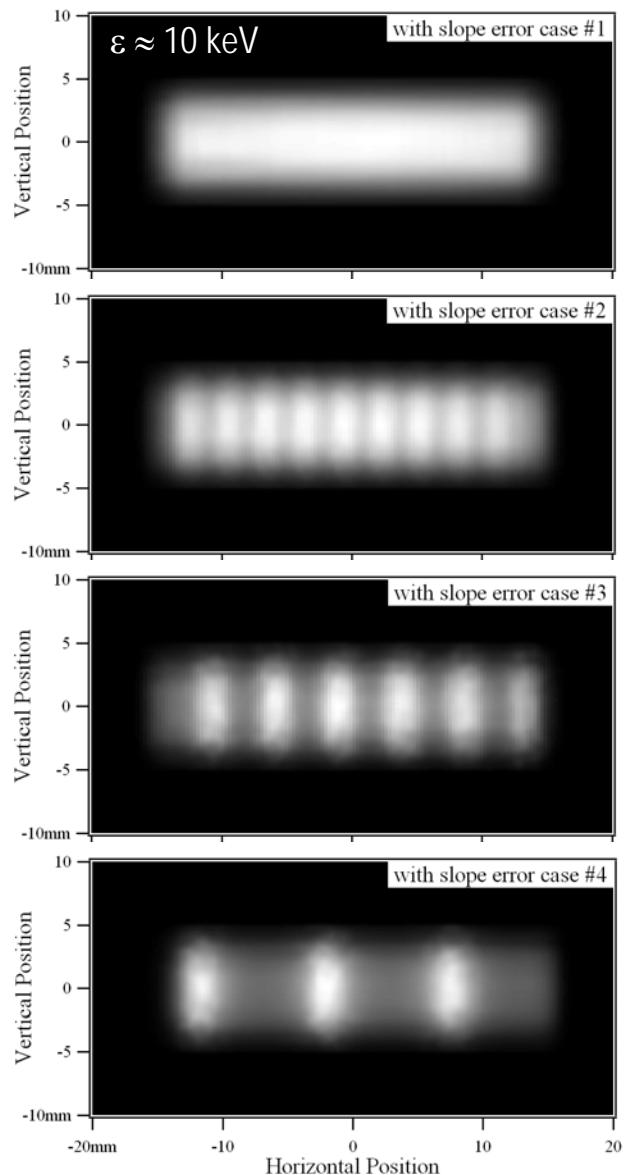
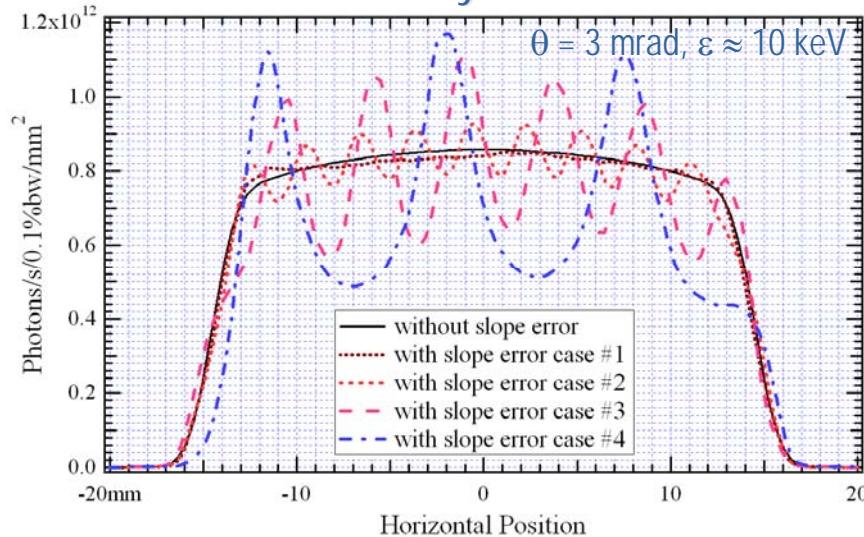


# Partially-Coherent Wavefront Propagation Simulations for Tomography BL: M1 Slope Error Effect

Modeling Surface Height Profile (due to Slope Error) Intensity Distributions at Sample of Horizontally-Focusing Mirror

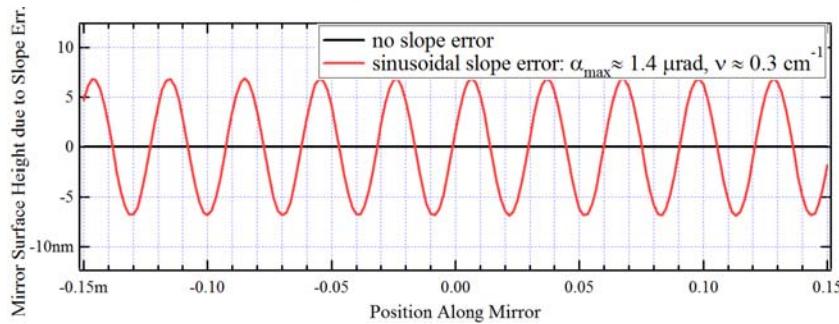


Horizontal Cuts of Intensity Distributions at Sample

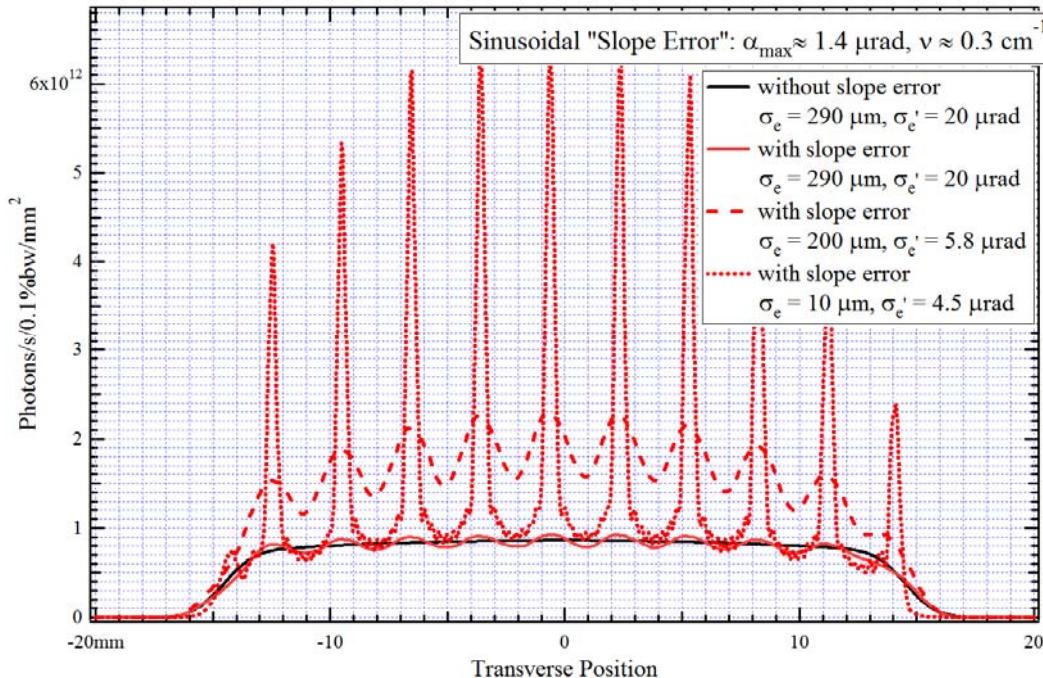


# M1 Slope Error Effects for Different E-Beam Parameters

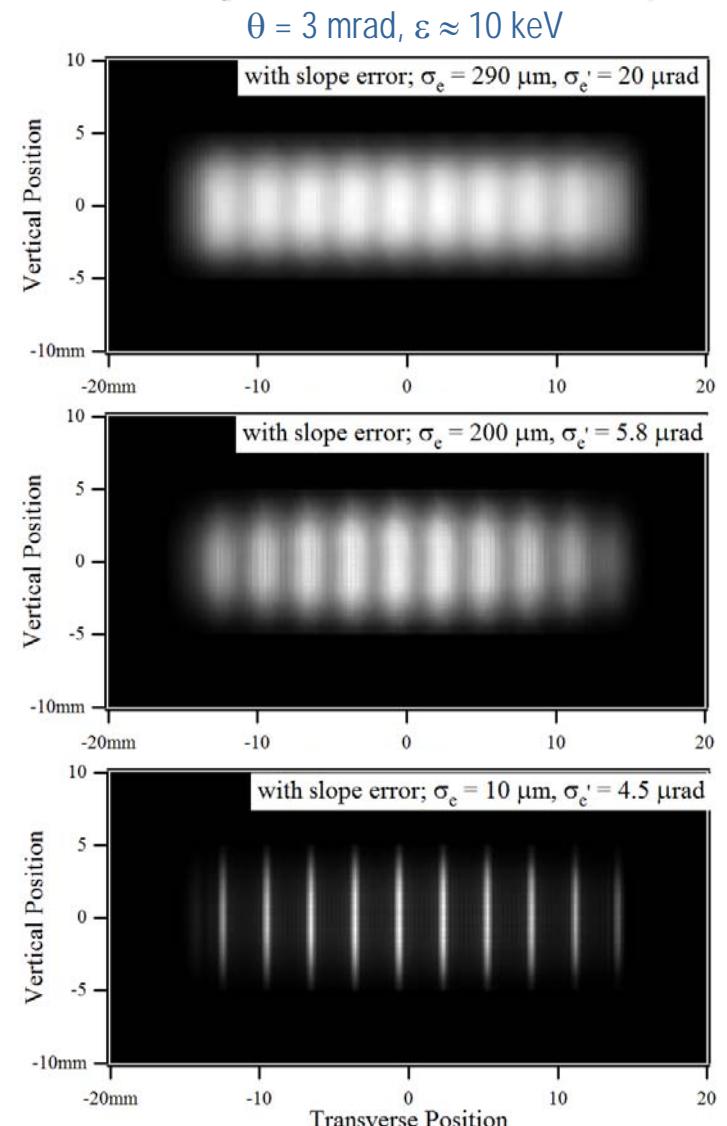
## Modeling Surface Height Profile (due to Slope Error)



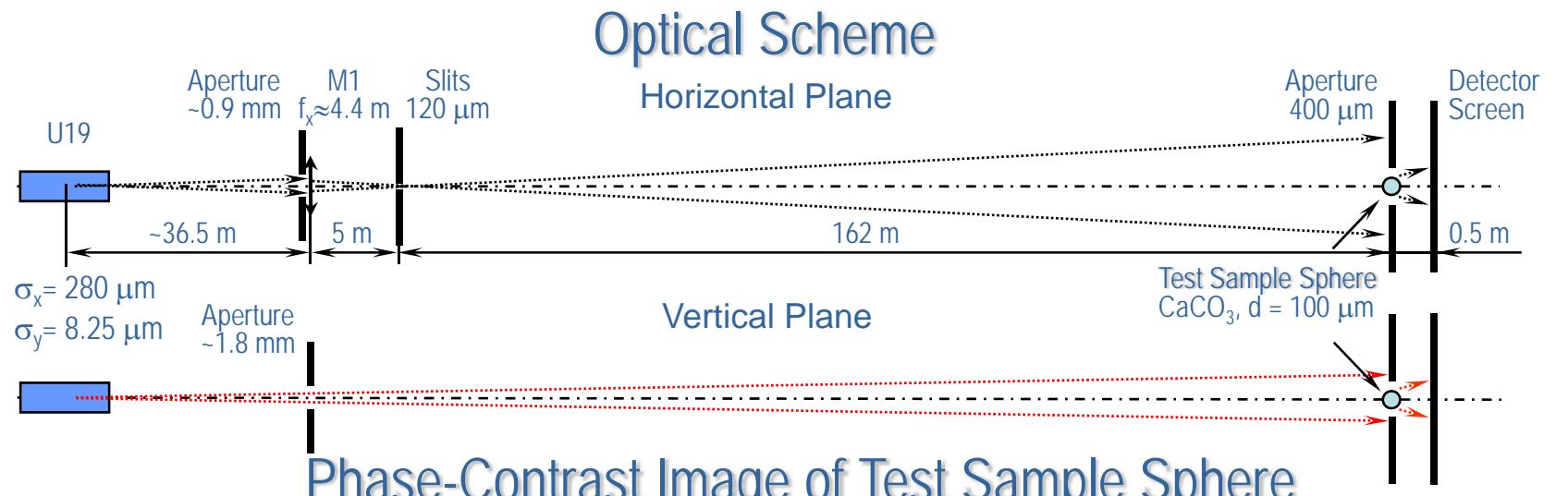
## Cuts of Intensity Distributions at Sample



## Intensity Distributions at Sample

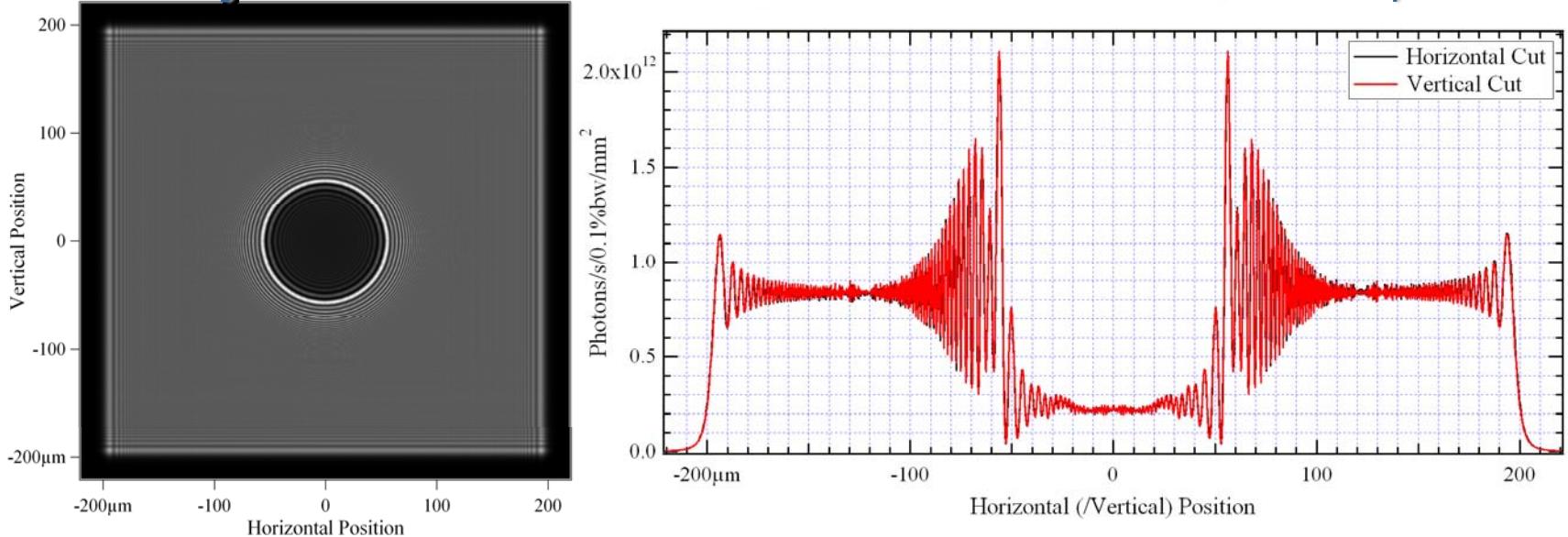


# Partially-Coherent Wavefront Propagation Simulations for Phase-Contrast Tomography BL: Image of Sample Sphere



**Phase-Contrast Image of Test Sample Sphere**

**Intensity Distribution at Detector Screen at  $\varepsilon \approx 10$  keV, M1 Slope Error**

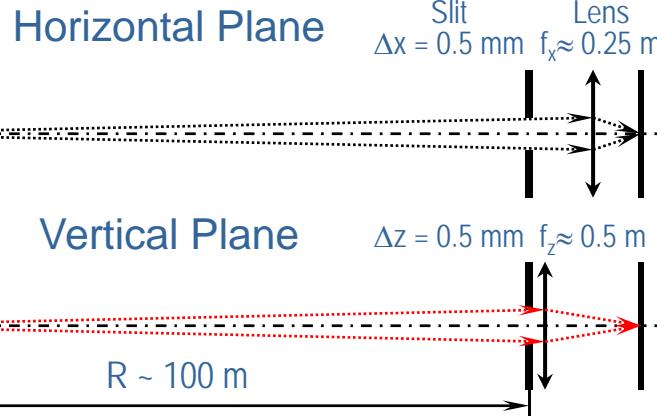


# Preliminary Wavefront Propagation Calculations for MICROSCOPIUM: Standard Long Straight Section (A)

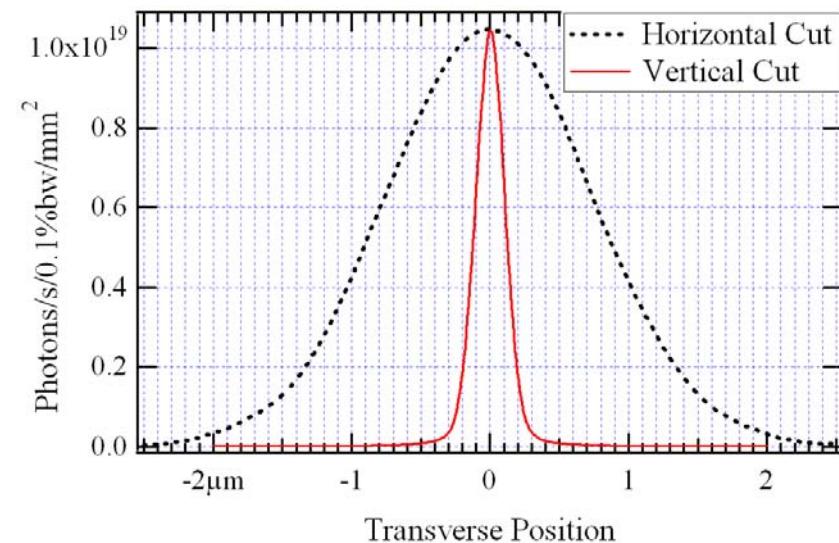
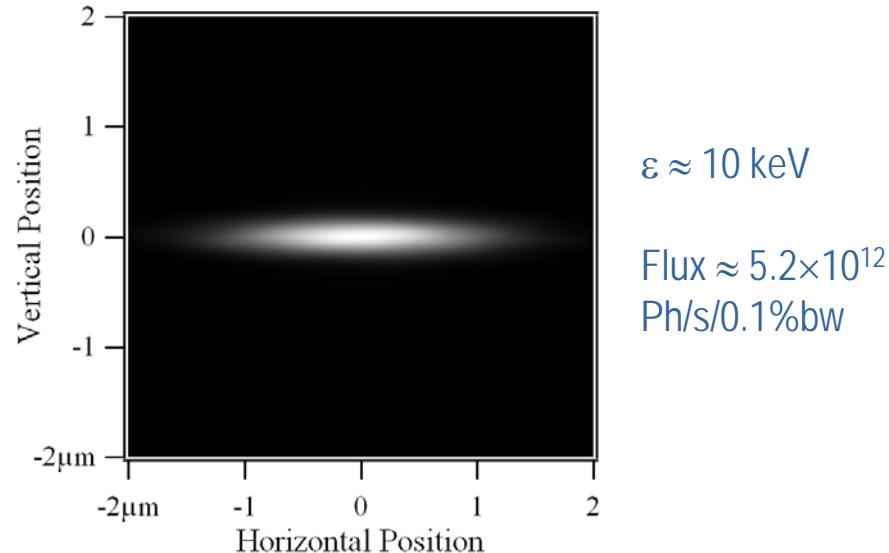
## Lattice Functions (Long Straight Section)



## Optical Scheme (A)

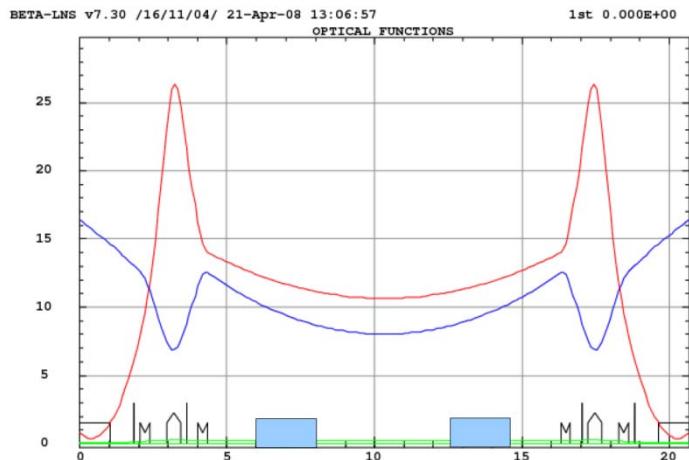


## Intensity @ Sample

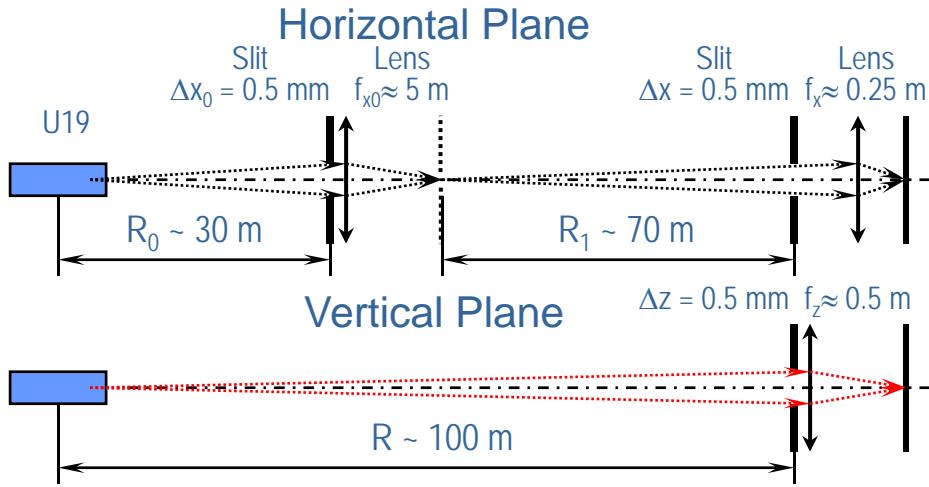


# Preliminary Wavefront Propagation Calculations for MICROSCOPIUM: Standard Long Straight Section (B)

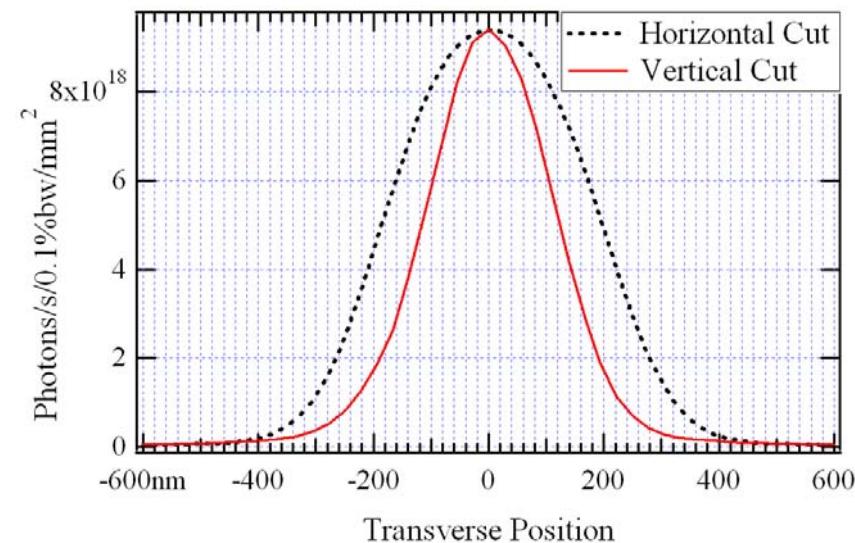
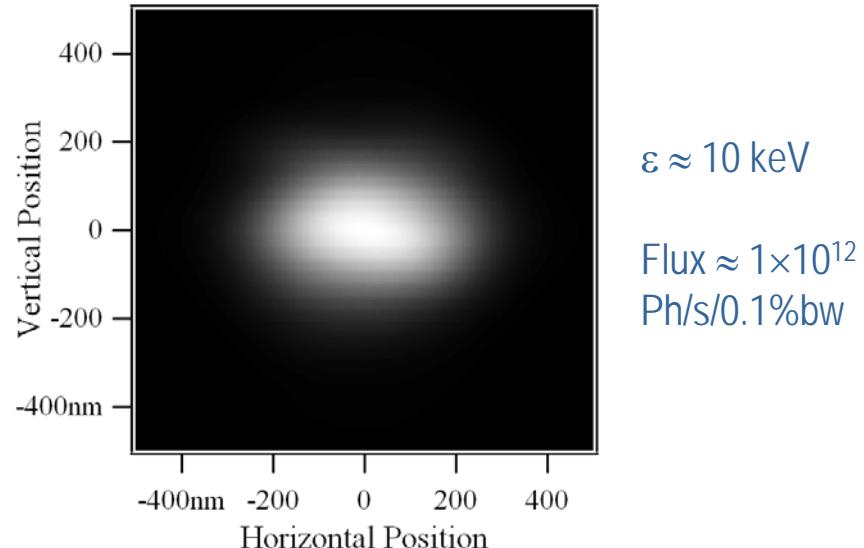
## Lattice Functions (Long Straight Section)



## Optical Scheme (B)

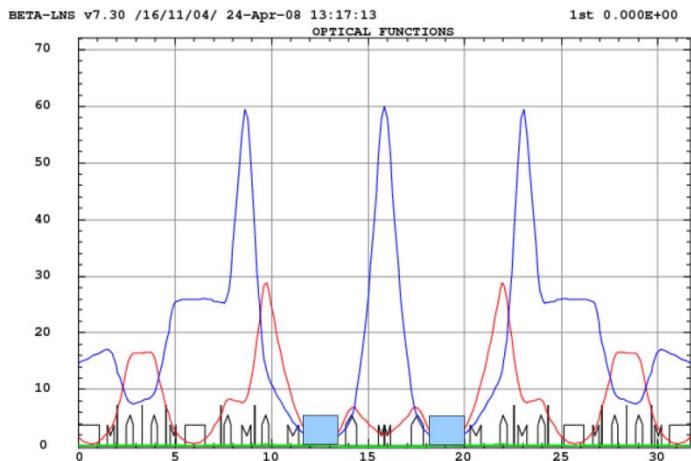


## Intensity @ Sample

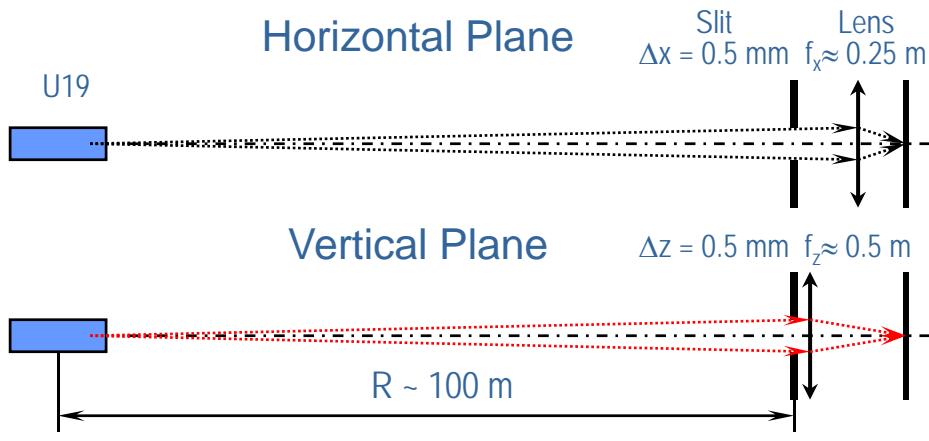


# Preliminary Wavefront Propagation Calculations for MICROSCOPIUM: Modified Long Straight Section

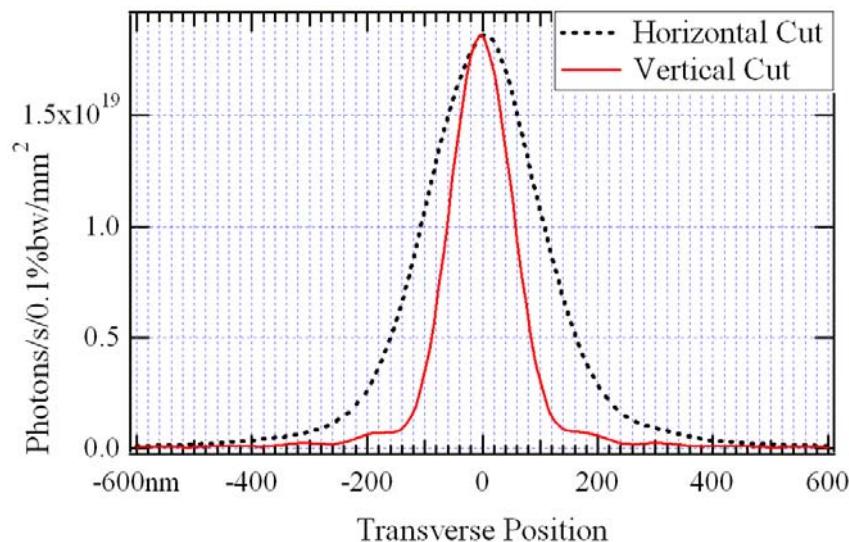
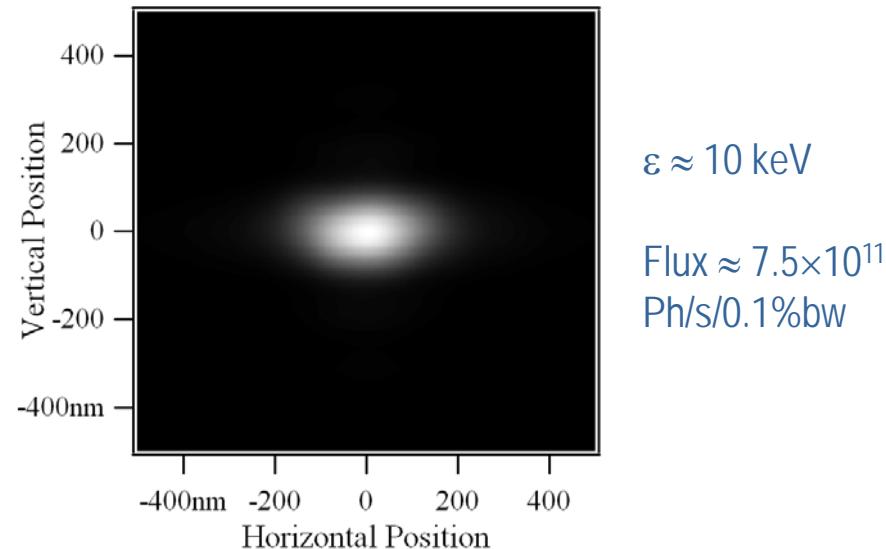
## Lattice Functions (Modified Long Straight Section)



## Optical Scheme (A)

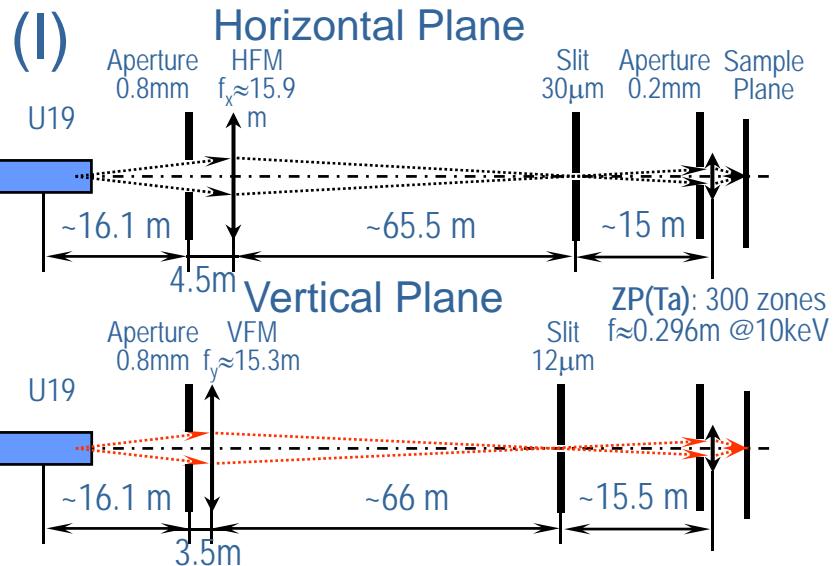


## Intensity @ Sample



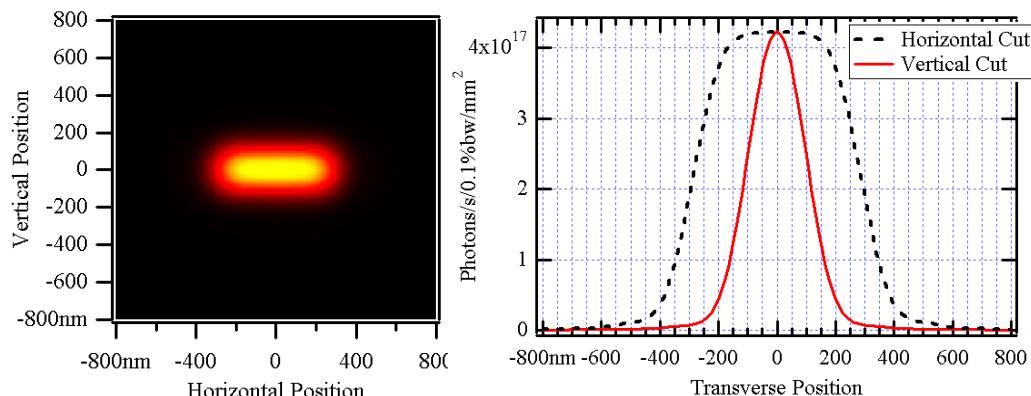
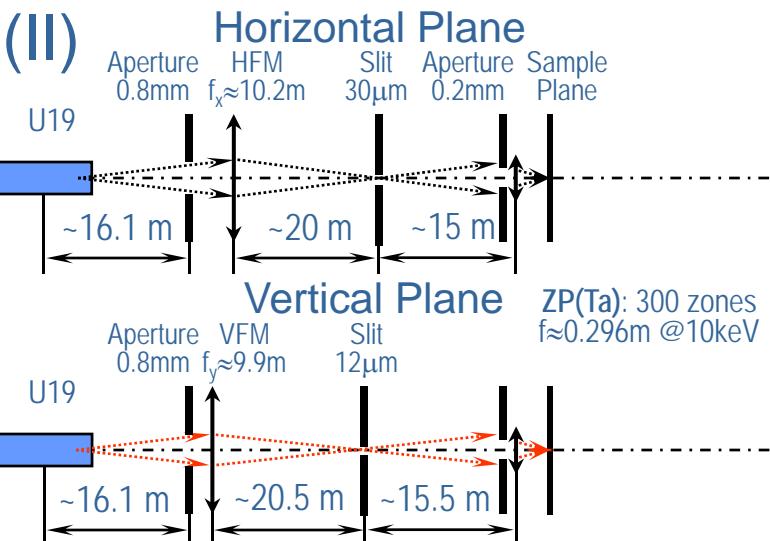
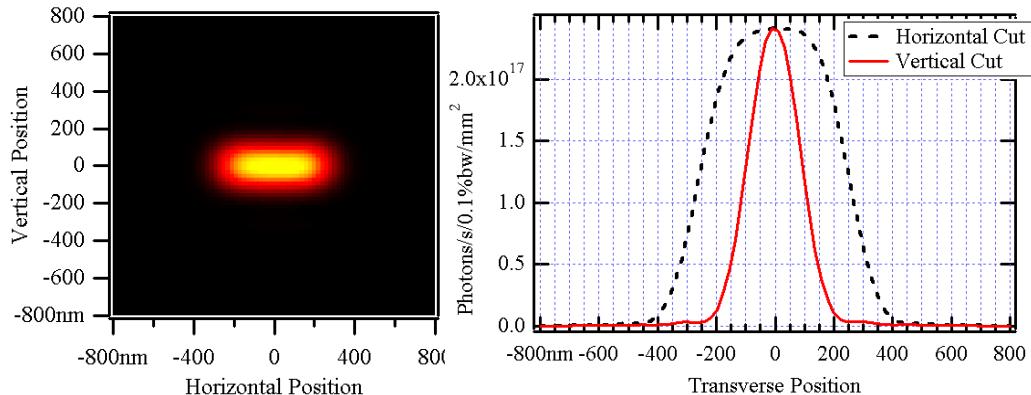
# Wavefront Propagation Calculations for MICROSCOPIUM: Comparison of Optical Schemes with Zone Plates

## Optical Schemes



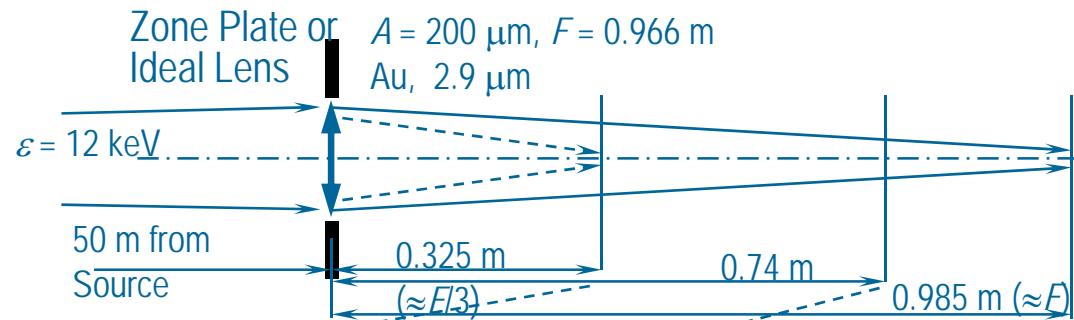
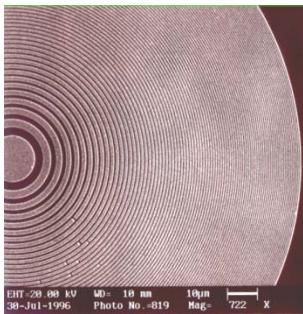
## Intensity and Flux at Sample

Photon Energy: 10 keV

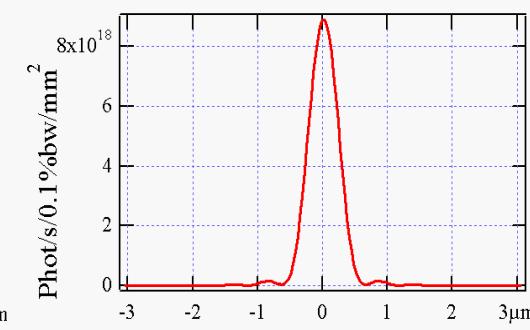
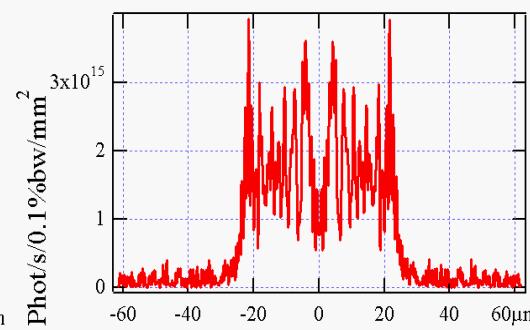
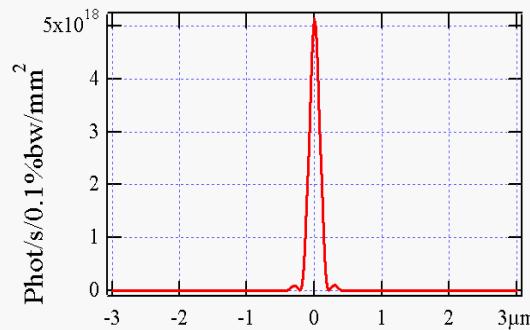


# Examples: Wavefront Propagation

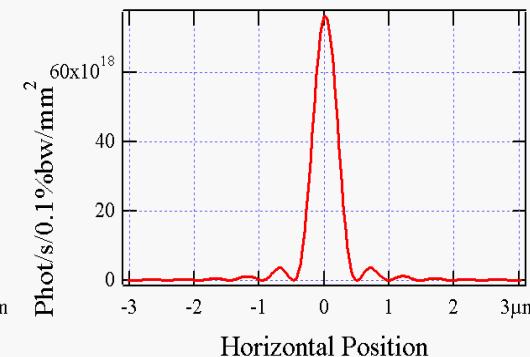
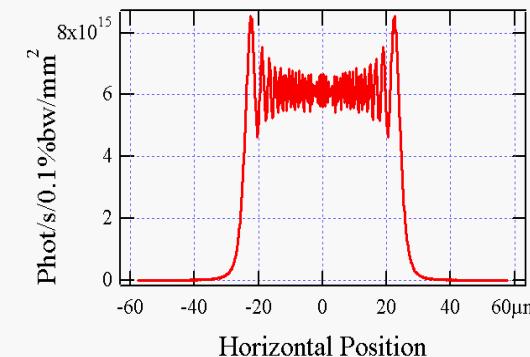
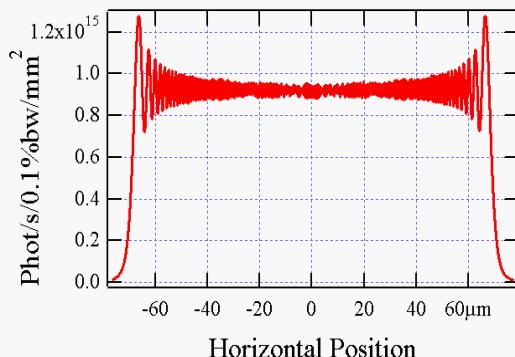
## X-Ray Focusing Using a Zone Plate (Full Transverse Coherence)



Zone Plate

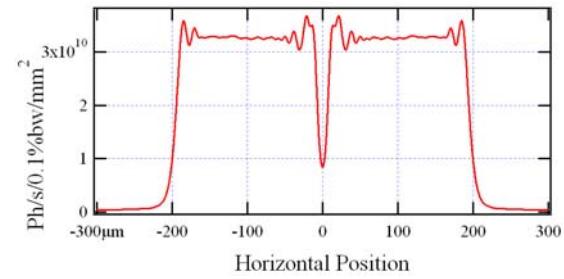
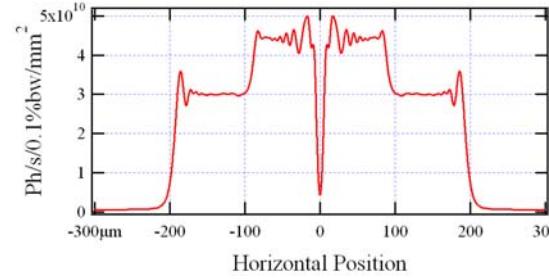
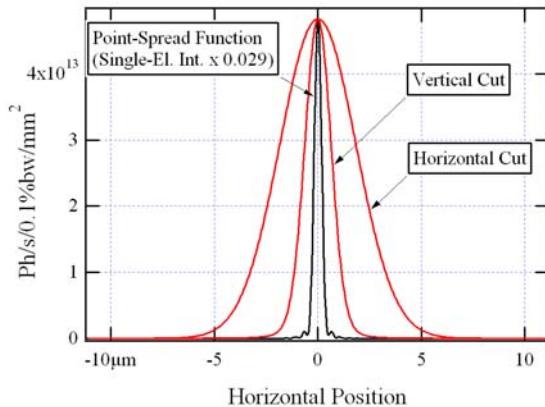
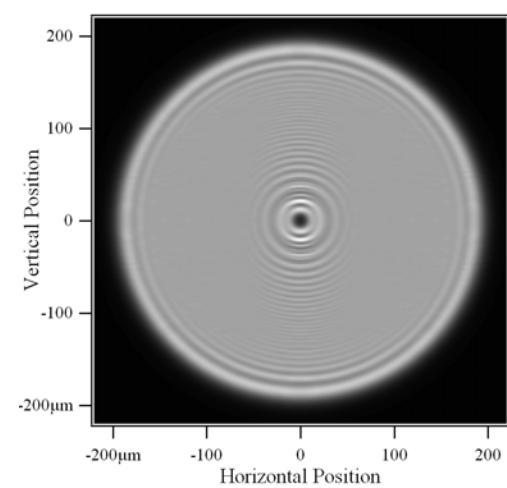
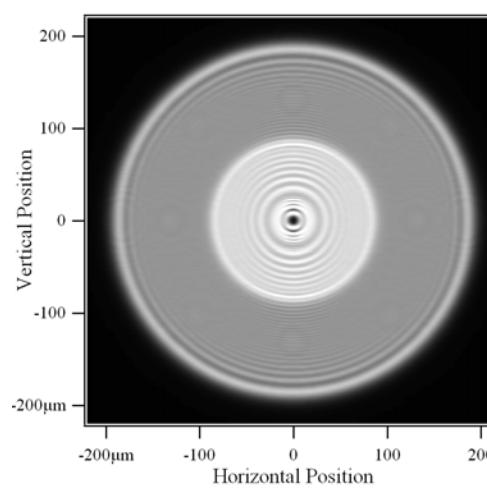
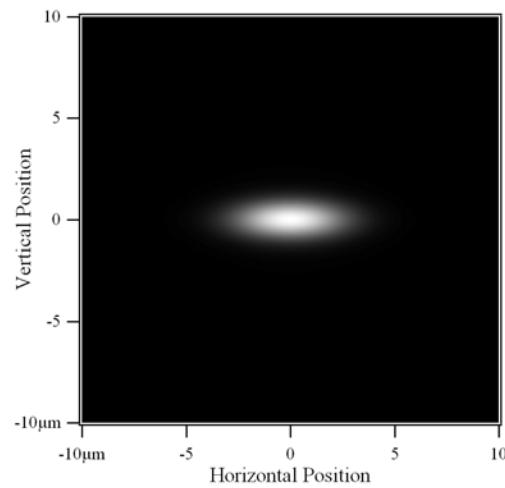
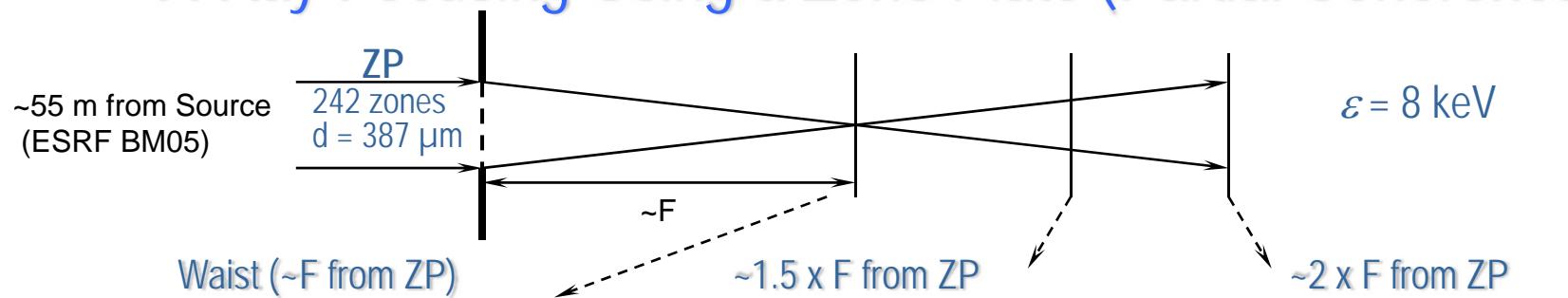


Ideal Lens



# Examples: Wavefront Propagation

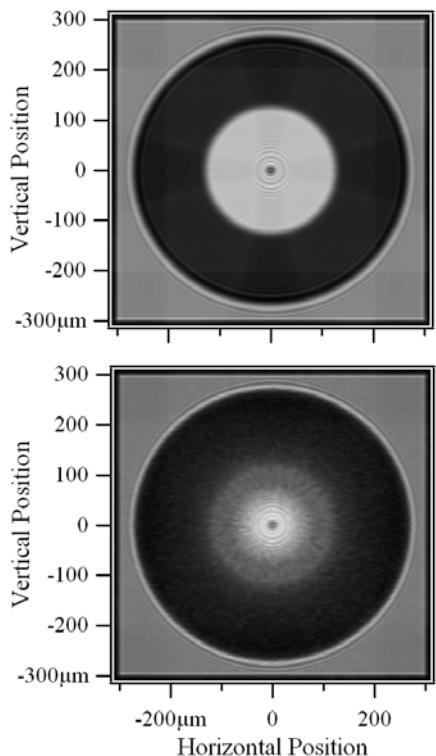
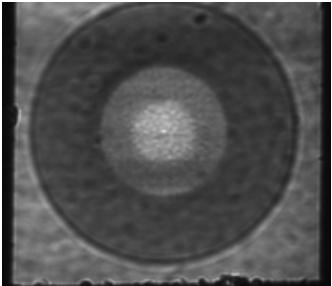
## X-Ray Focusing Using a Zone Plate (Partial Coherence)



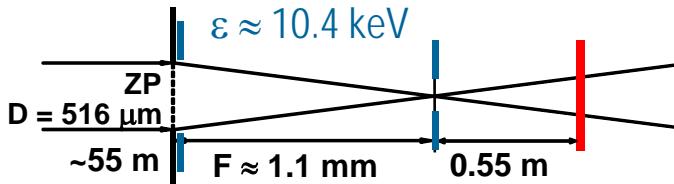
# Examples: Wavefront Propagation / Analysis

## Partially Coherent X-Rays Observed Out of Focus of a Zone Plate

Aperture at Waist:  
600  $\mu\text{m} \times 600 \mu\text{m}$



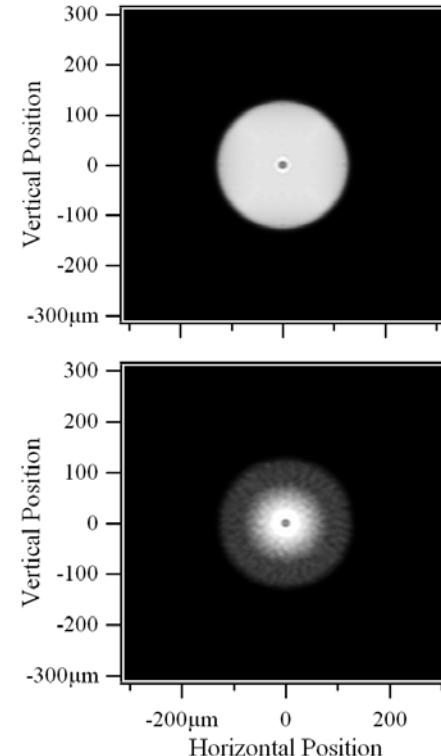
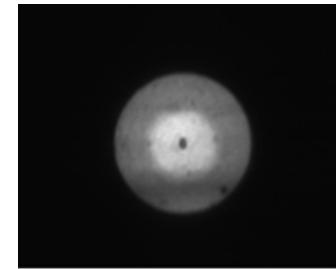
Intensity Distributions  
at 0.55 m after Waist



Measurements (ESRF BM5)

M.Idir, A.Snigirev et. al.

Aperture at Waist:  
10  $\mu\text{m} \times 10 \mu\text{m}$

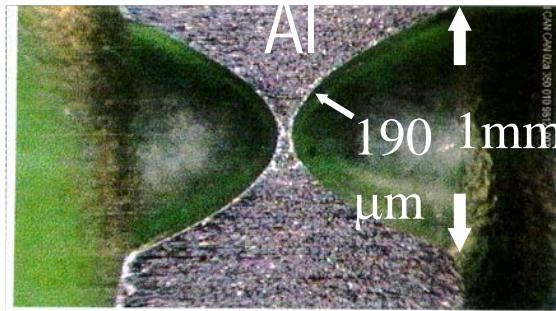


Calculation for Perfect ZP

Calculation for ZP  
with non-perfect outer zones

# Examples: Wavefront Propagation

## Point-Spread Function Computation for Parabolic X-Ray CRL



A.Snígirev, B.Lengeler, et. al., 1998

$$\epsilon = 8.9 \text{ keV}$$

$$\delta = 6.9 \times 10^6$$

$$L_{\text{atten}} = 0.106 \text{ mm}$$

$$N = 1$$

$$F = 13.6 \text{ m}$$

$$\Delta_{\text{FWHM}} = 7.3 \mu\text{m}$$

$$\epsilon = 23 \text{ keV}$$

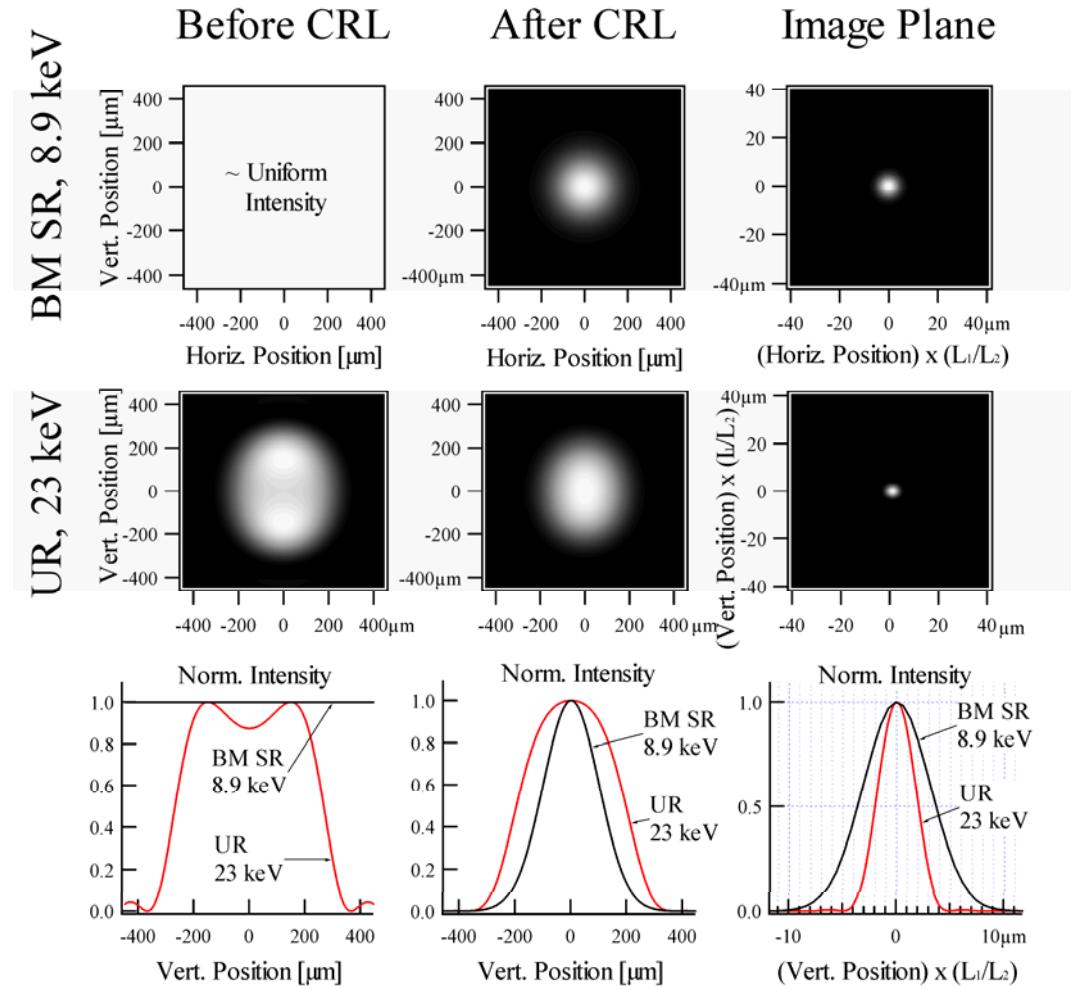
$$\delta = 1. \times 10^6$$

$$L_{\text{atten}} = 1.89 \text{ mm}$$

$$N = 7$$

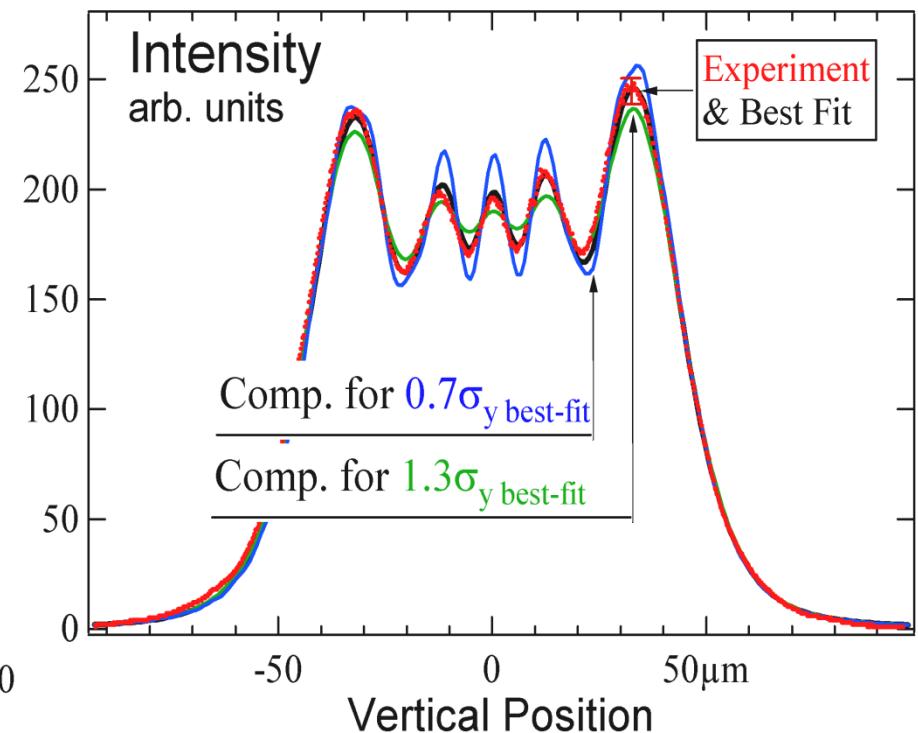
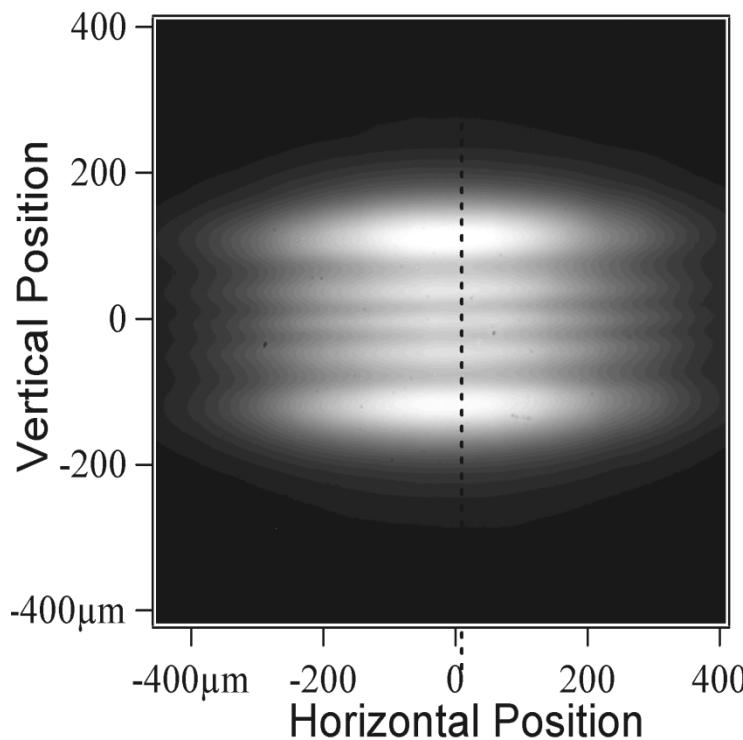
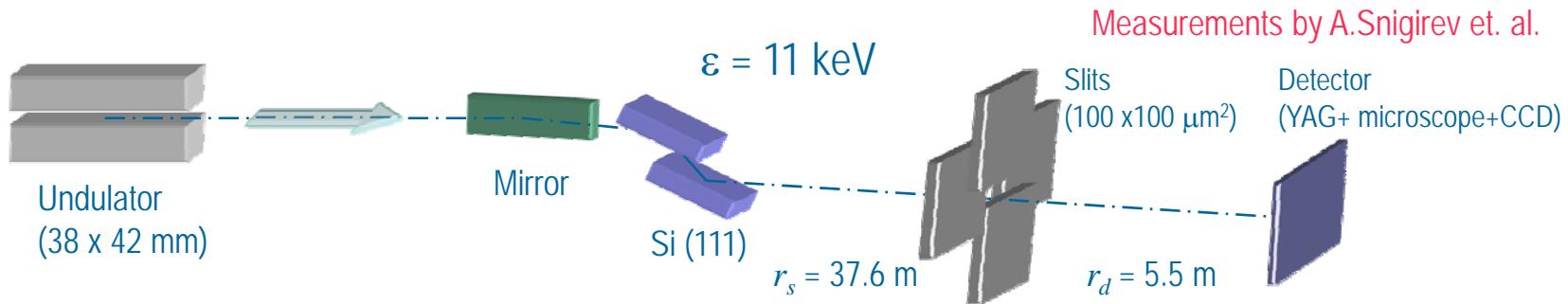
$$F = 13.1 \text{ m}$$

$$\Delta_{\text{FWHM}} = 4.1 \mu\text{m}$$



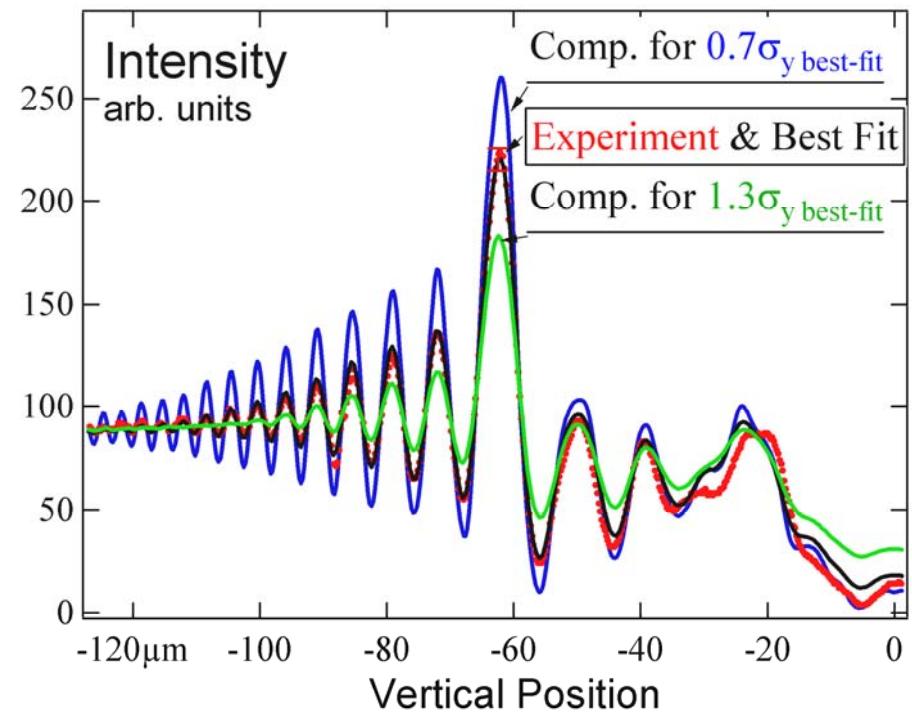
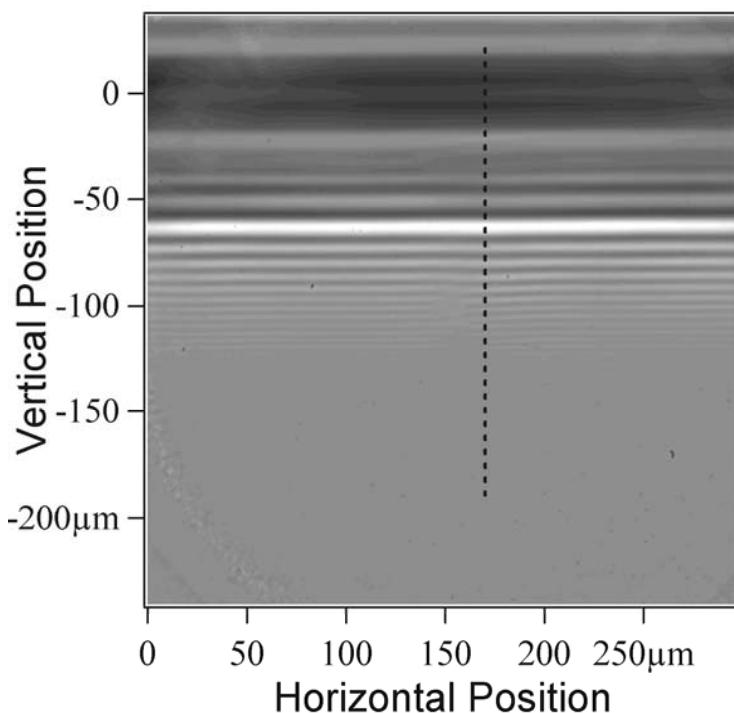
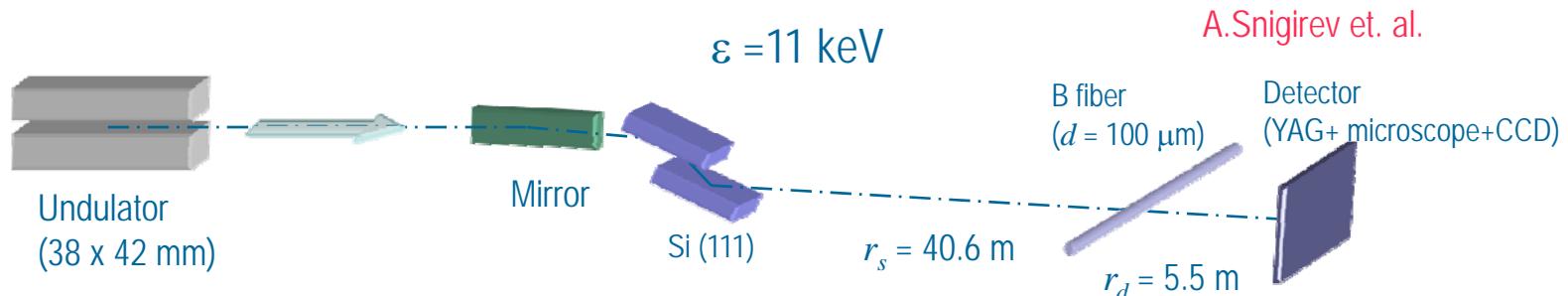
# Examples: Wavefront Propagation

## Fresnel Diffraction of Partially Coherent X-Rays

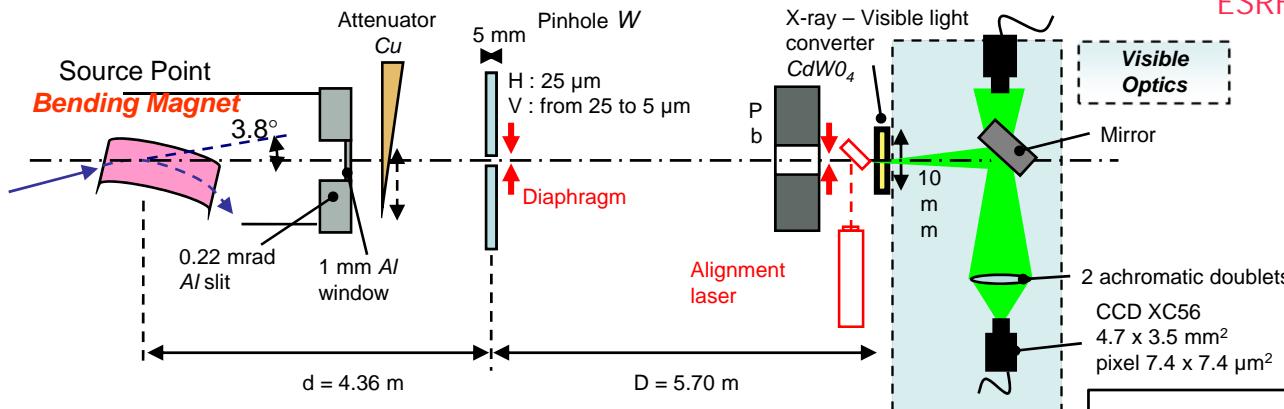


# Examples: Wavefront Propagation

## Interference of Partially Coherent X-Rays



# Resolution of the Well-Known X-ray Pinhole Camera

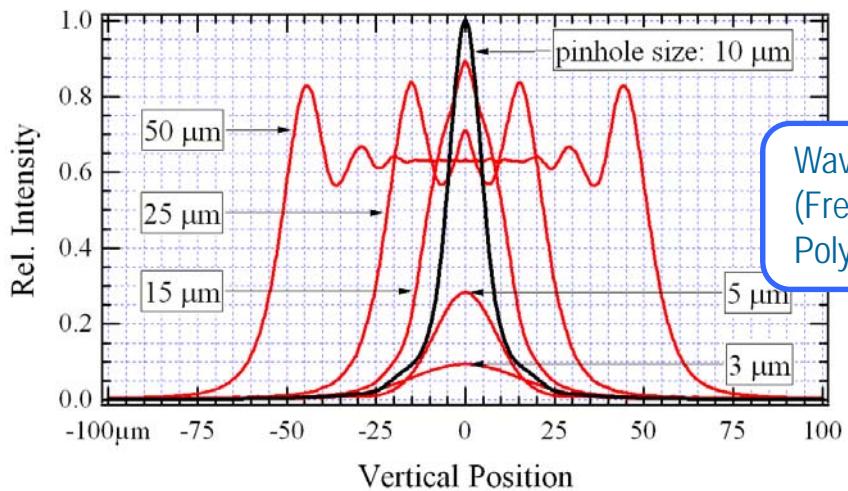


ESRF Pinhole Camera by P. Elleaume et. al. (1995)

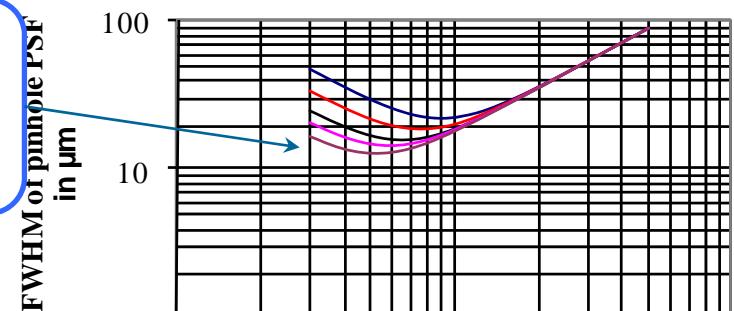
SOLEIL version by M.-A. Tordeux et. al.  
(DIPAC-2007)

Resolution  
vs Pinhole Size  
for Diff. Attenuator Thickness

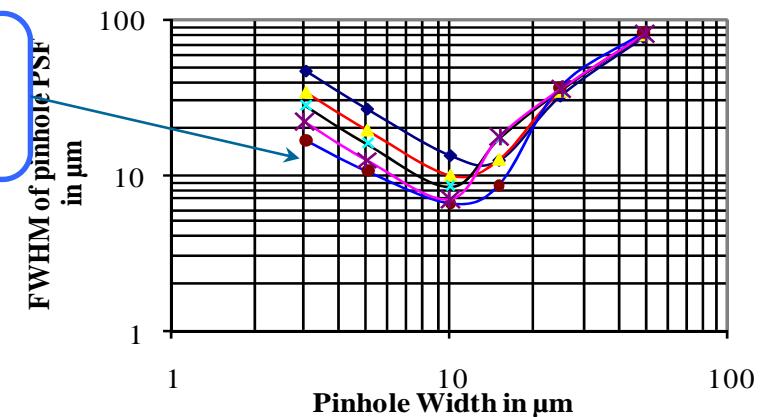
**PSF Calculations:**  
Intensity Distributions at Converter  
(White Beam after 1 mm Cu Attenuator)



Quadratic sum of the Geometry and Fraunhofer Diffraction contributions

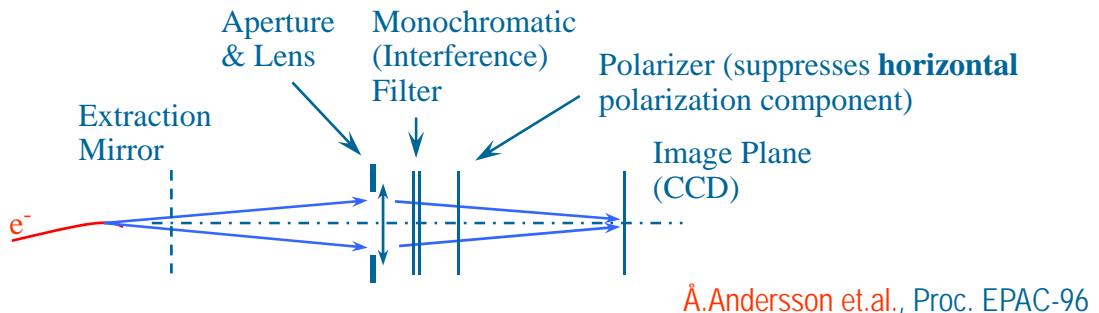


Wave-optics calculation  
(Fresnel Diffraction of Polychromatic SR)



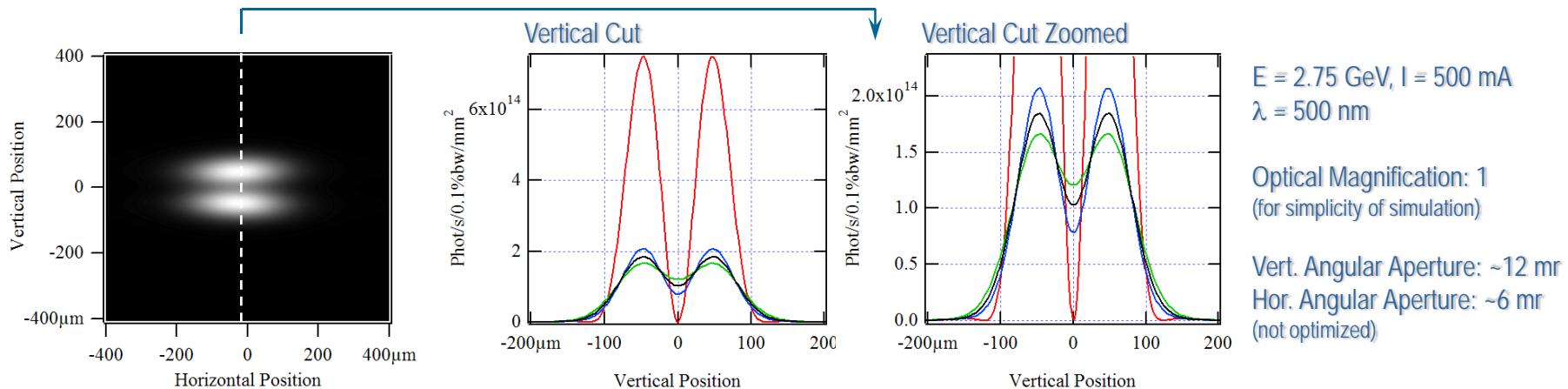
# E-Beam Imaging Using Vertically Polarized BM SR

## Simplified Optical Scheme (Top View)



Å.Andersson et.al., Proc. EPAC-96

## SR Intensity Distribution in the Image Plane (Vertical Polarization)



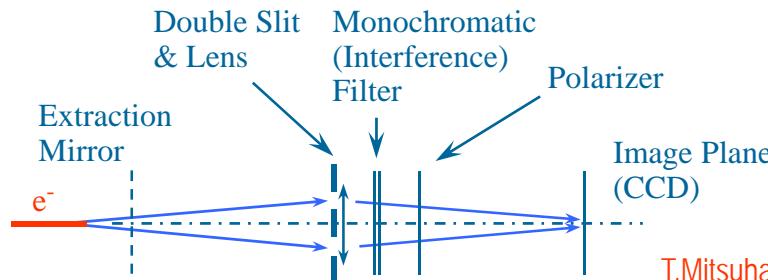
## RMS Vertical Size of the E-Beam and the Intensity Fluctuation in the Fringes:

red curve: filament e-beam ( $\sigma_{e_z} = 0$ ),  
blue:  $\sigma_{e_z} = 18.3 \mu\text{m}$ ,  
black:  $\sigma_{e_z} = 23.3 \mu\text{m}$  (expected),  
green:  $\sigma_{e_z} = 28.3 \mu\text{m}$ ,

$I_{\min}/I_{\max} \approx 0$  ( $< 10^{-3}$ )  
 $I_{\min}/I_{\max} \approx 0.36$   
 $I_{\min}/I_{\max} \approx 0.56$   
 $I_{\min}/I_{\max} \approx 0.73$

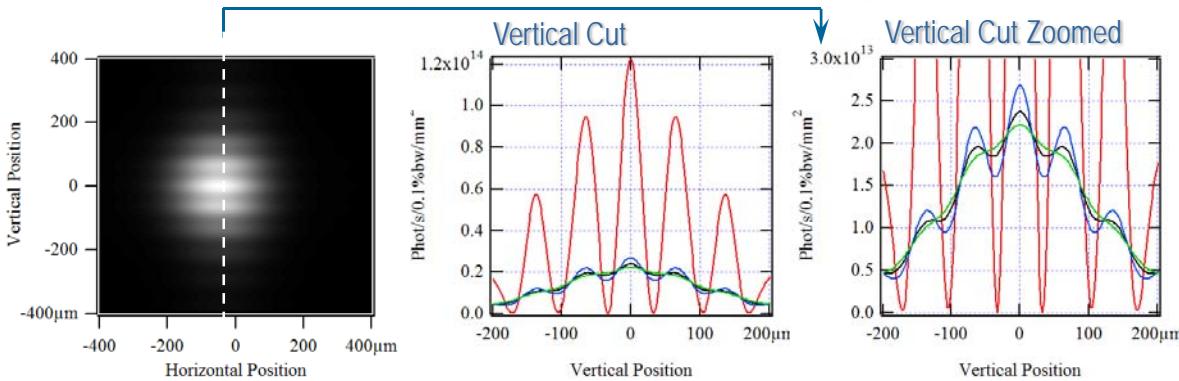
# E-Beam Imaging Using Double-Slit Interferometer

## Simplified Optical Scheme (Side View)



T.Mitsuhashi, Proc. PAC-97

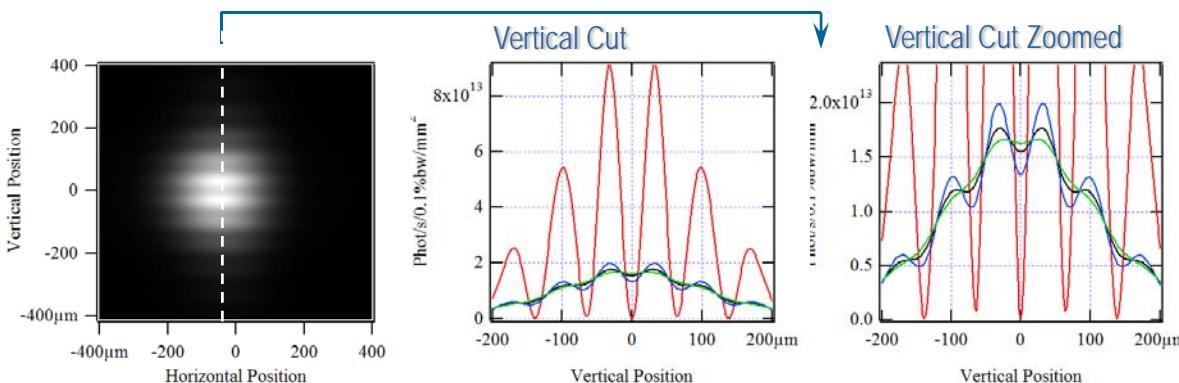
## SR Intensity Distribution in the Image Plane (Horizontal Polarization Component)



$E = 2.75 \text{ GeV}$ ,  $I = 500 \text{ mA}$ ,  $\lambda = 500 \text{ nm}$   
 Distance from Source to Slits: 5 m  
 Optical Magnification: 1 (for simplicity of simulation)  
 Vertical Distance between Slits: 30 mm (not optimized)

red: filament e-beam ( $\sigma_{e_z} = 0$ ),  $I_{\min}/I_{\max} \approx 0 < 10^{-3}$   
 blue:  $\sigma_{e_z} = 18.3 \mu\text{m}$ ,  $I_{\min}/I_{\max} \approx 0.59$   
 black:  $\sigma_{e_z} = 23.3 \mu\text{m}$ ,  $I_{\min}/I_{\max} \approx 0.78$   
 green:  $\sigma_{e_z} = 28.3 \mu\text{m}$ ,  $I_{\min}/I_{\max} \approx 0.88$  (no fringes)

## SR Intensity Distribution in the Image Plane (Vertical Polarization Component)



red: filament e-beam ( $\sigma_{e_z} = 0$ ),  $I_{\min}/I_{\max} \approx 0 < 10^{-5}$   
 blue:  $\sigma_{e_z} = 18.3 \mu\text{m}$ ,  $I_{\min}/I_{\max} \approx 0.67$   
 black:  $\sigma_{e_z} = 23.3 \mu\text{m}$ ,  $I_{\min}/I_{\max} \approx 0.88$   
 green:  $\sigma_{e_z} = 28.3 \mu\text{m}$ ,  $I_{\min}/I_{\max} \approx 0.99$  (no fringes)

# Angular Horizontal FS Slice Separation Scheme (SLS)

Idea of FS Slicing: A.Zholents (LBNL)

FS Slicing at SLS: G.Ingold et. al.

E-Beam, Modulation:

$$E_0 = 2.44 \text{ GeV}$$

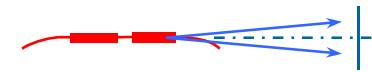
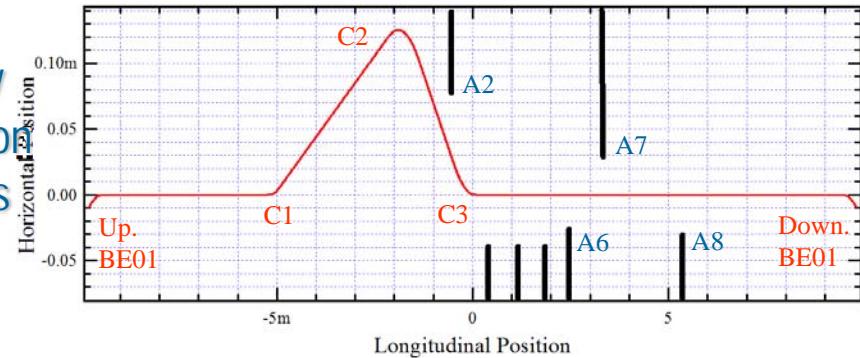
$$I_{\text{s.b.}} = 2 \text{ mA}$$

$$\sigma_b = 12 \text{ ps}$$

Radiator:

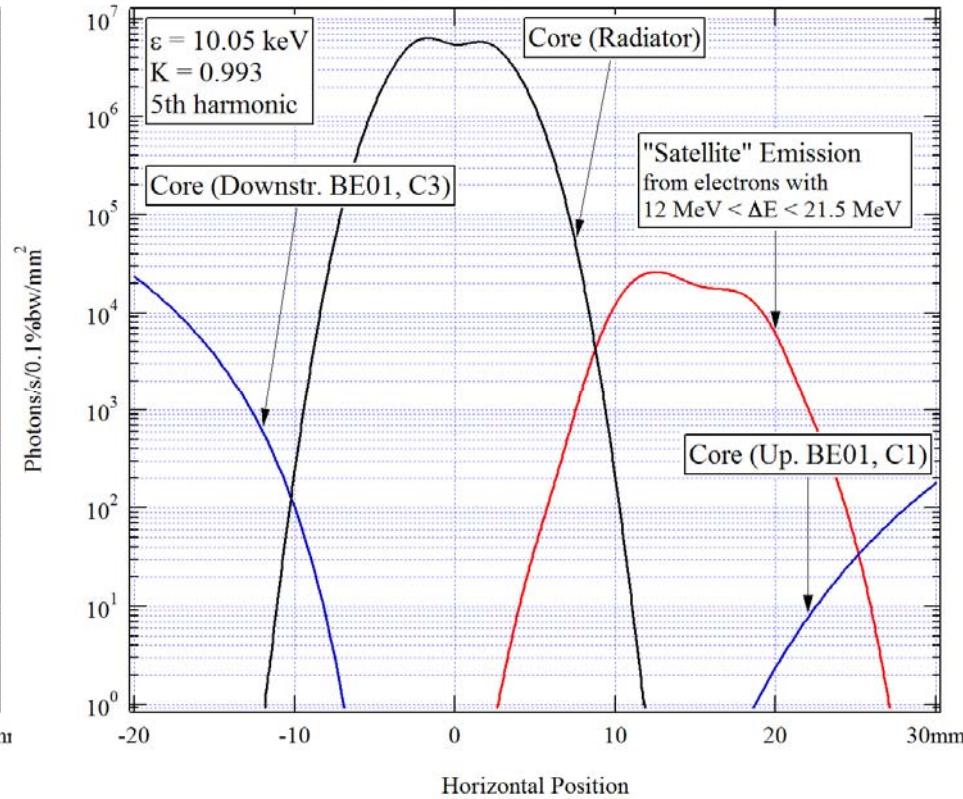
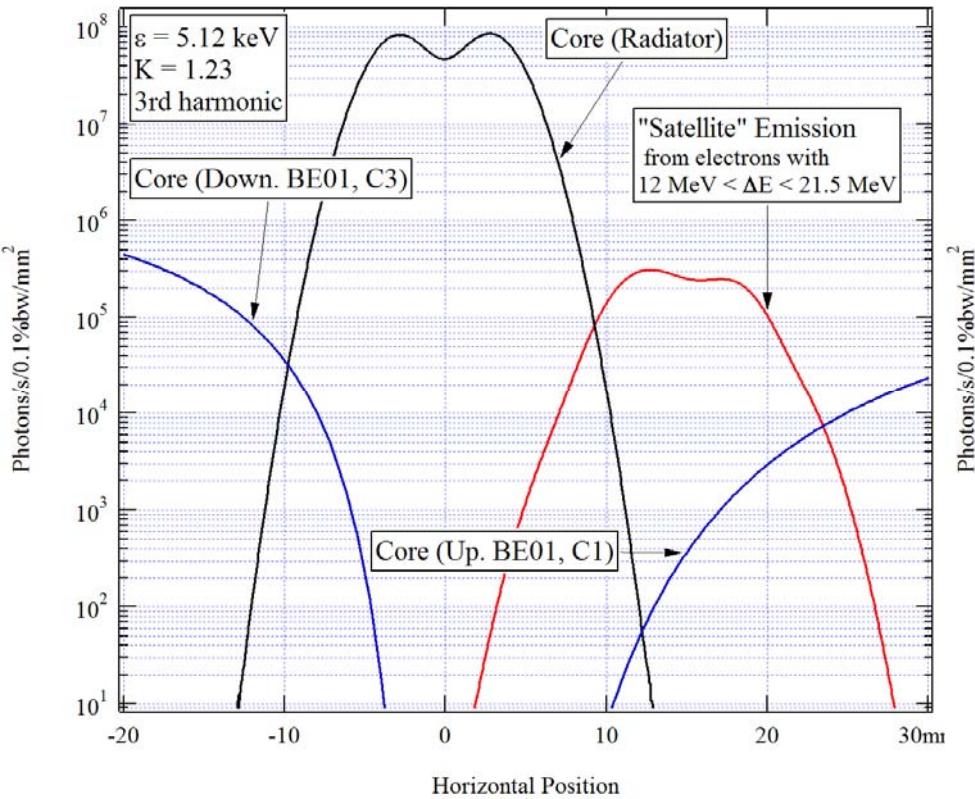
Undulator U19  
(in-vacuum)

Electron  
Trajectory  
and Photon  
Absorbers



Intensity Distributions in the Median Plane

~15.7 m from Radiator; Finite-Emittance Electron Beam



# FS Slice Separation Using SOLEIL "Native" Dispersion

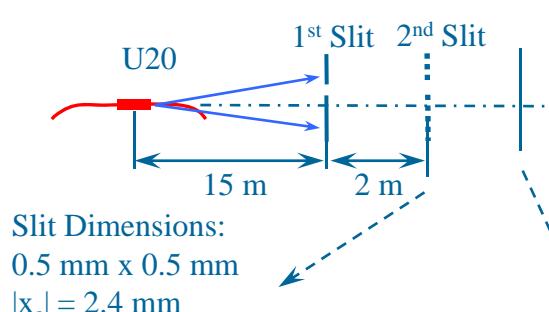
## Hard X-Rays: Slit- (Pinhole-) Based Spatial Horizontal Separation Scheme

E-Beam, Modulation:

$$\begin{aligned} E_0 &= 2.75 \text{ GeV} & \Delta E_{\max} &\approx 14 \text{ MeV} \text{ (pessimistic)} \\ I_{s.b.} &= 10 \text{ mA} & f_L &= 10 \text{ kHz} \\ \sigma_b &= 24 \text{ ps} & \sigma_L &= 50 \text{ fs} \end{aligned}$$

Hard X-Ray Radiator:

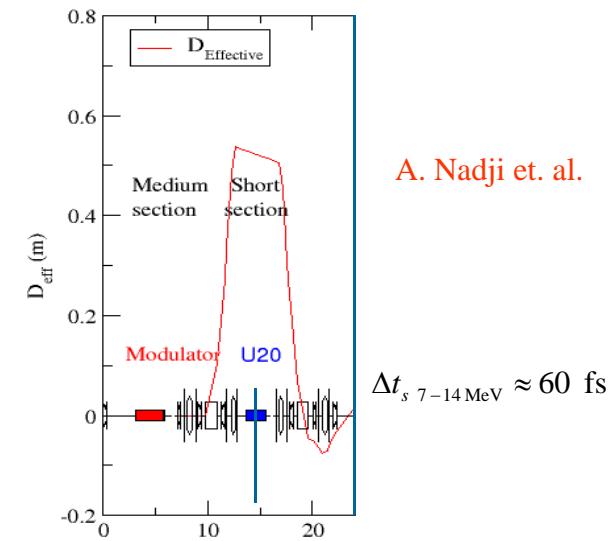
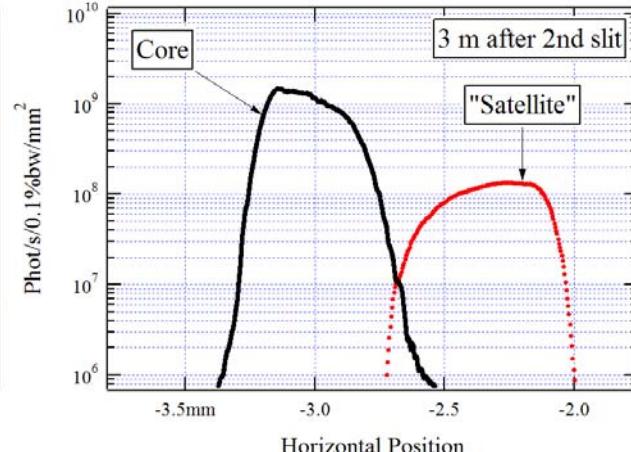
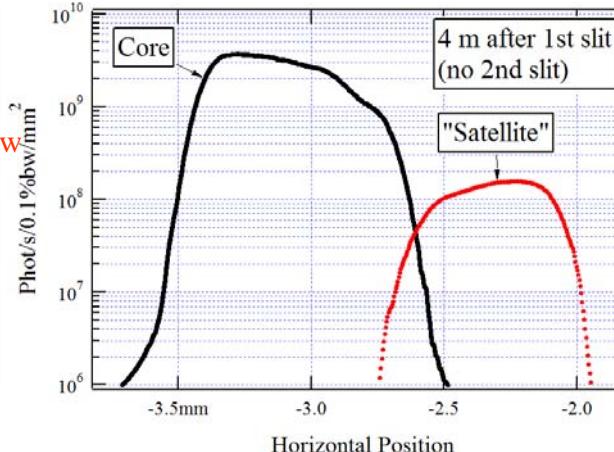
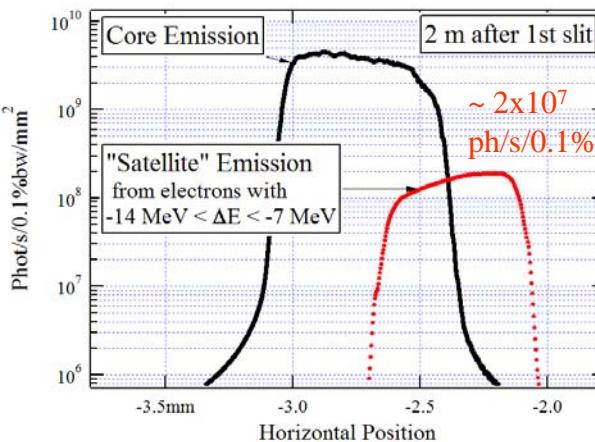
Undulator U20



T. Moreno  
M. Idir

$\varepsilon = 6.93 \text{ keV}$

Intensity in Transverse Planes After Slit(s)  
Cuts by Median Plane



Electron Beam Emittance,  
Peculiarities of Undulator Radiation,  
Slit Diffraction  
are taken into account

# FS Slice Separation Using SOLEIL "Native" Dispersion

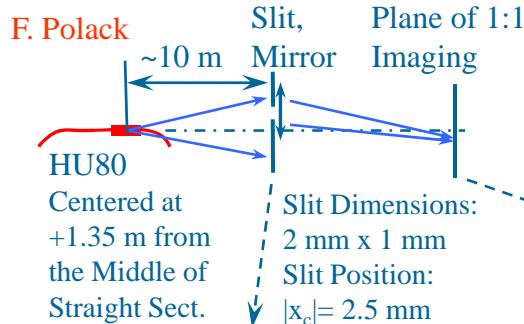
## Soft X-Rays: Mixed Angular-Spatial Horizontal Separation Scheme

E-Beam, Modulation:

$$\begin{aligned} E_0 &= 2.75 \text{ GeV} & \Delta E_{\max} &\approx 20 \text{ MeV} \\ I_{s.b.} &= 10 \text{ mA} & f_L &= 10 \text{ kHz} \\ \sigma_b &= 24 \text{ ps} & \sigma_L &= 50 \text{ fs} \end{aligned}$$

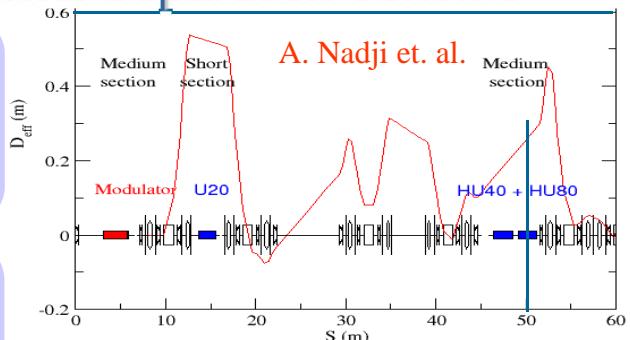
Soft X-Ray Radiator:

Undulator HU80  
(Apple-II)



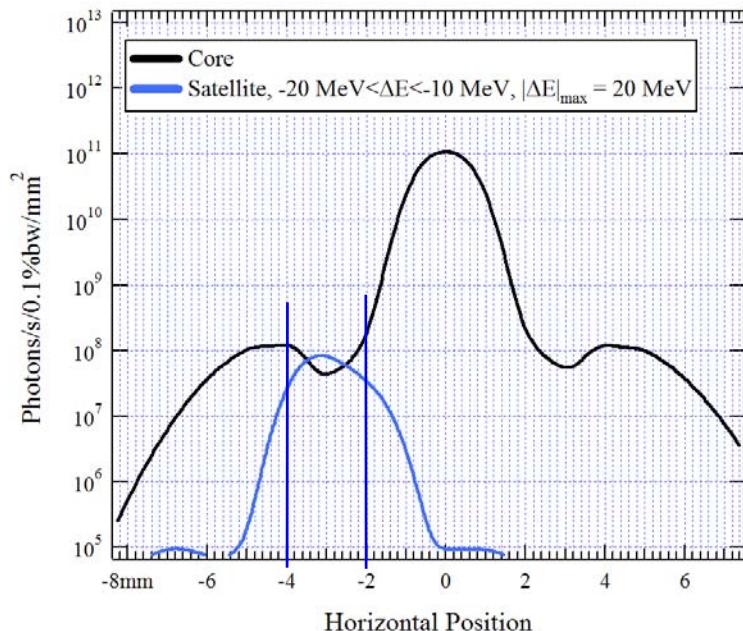
Mirror Surface Assumptions:

- Average Slope Error:  $\sim 1.5 \mu\text{rad}$ ,
- Average Roughness:  $\sim 2.5 \text{\AA}$ ,
- Incidence Angle:  $\sim 1^\circ$
- Error Distribution: Random  
(Density to be studied)



- Peculiarities of Undulator Radiation,
- Electron Beam Emittance,
- Slit Diffraction,
- Scattering from Mirror Surface
- are taken into account

Intensity in Transverse Plane Before Mirror

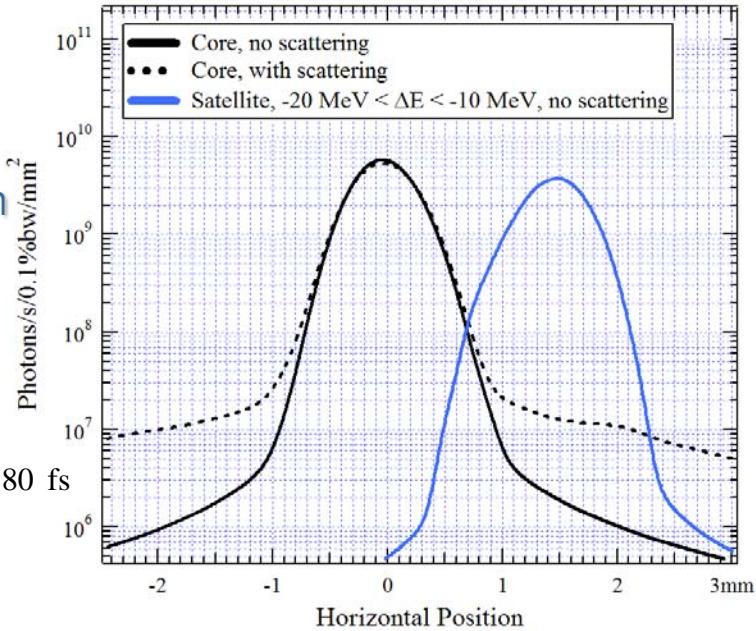


$\epsilon = 415 \text{ eV}$

Linear-  
Horizontal  
Polarization

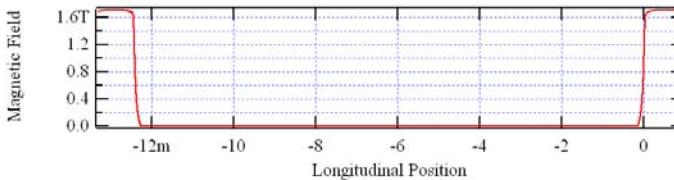
$$\Delta t_s |_{10-20 \text{ MeV}} = 180 \text{ fs}$$

Intensity in the Plane of 1:1 Imaging

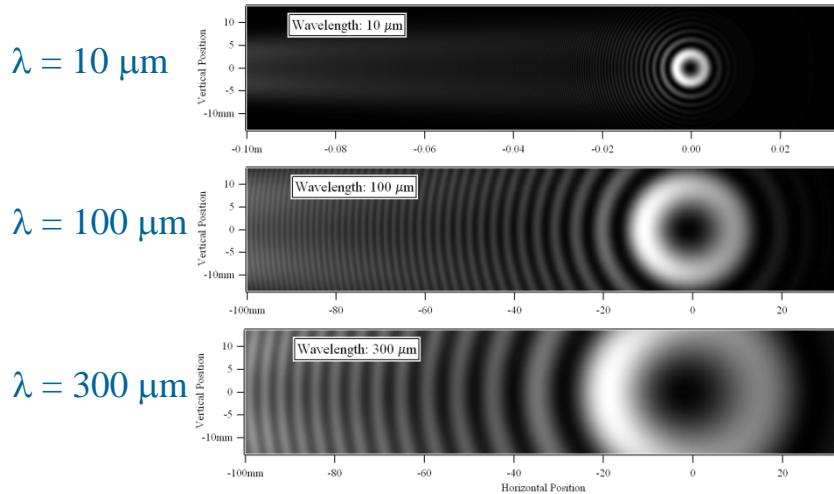


# Examples: Infrared Edge Radiation Emission at Different Wavelengths (SOLEIL)

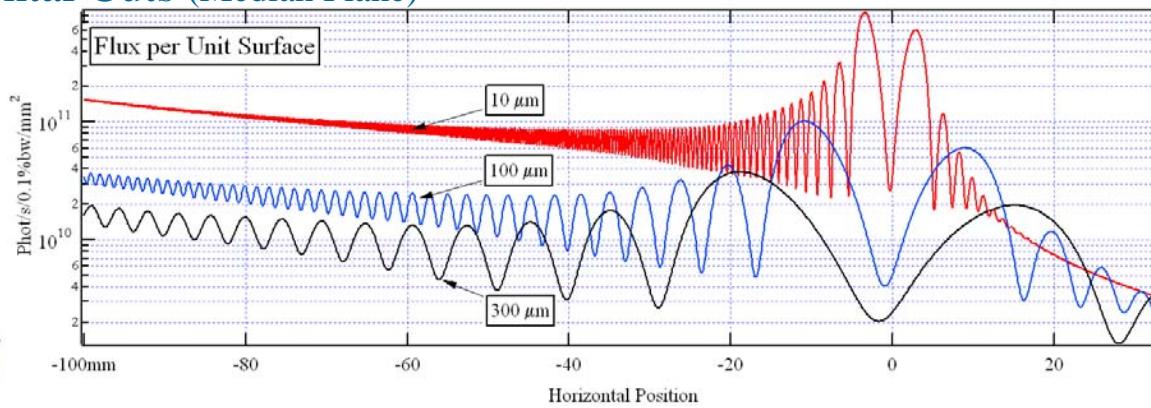
## Magnetic Field (Medium-Size Straight Section)



## Spectral Flux / Surface (Distance from BM Edge: 1.27 m)

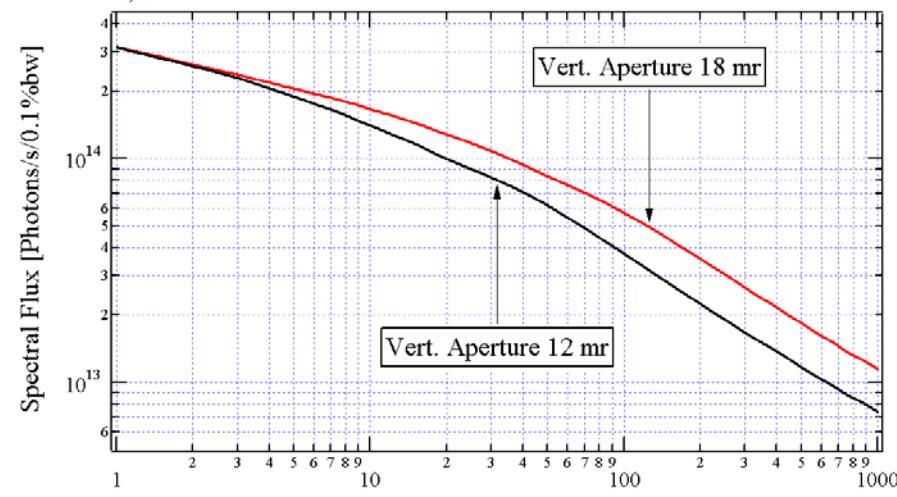


## Horizontal Cuts (Median Plane)



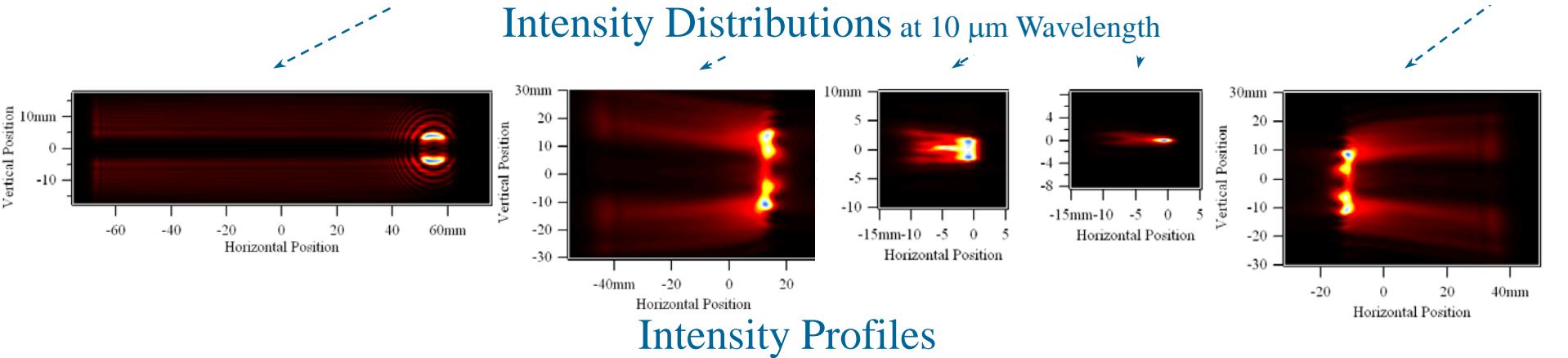
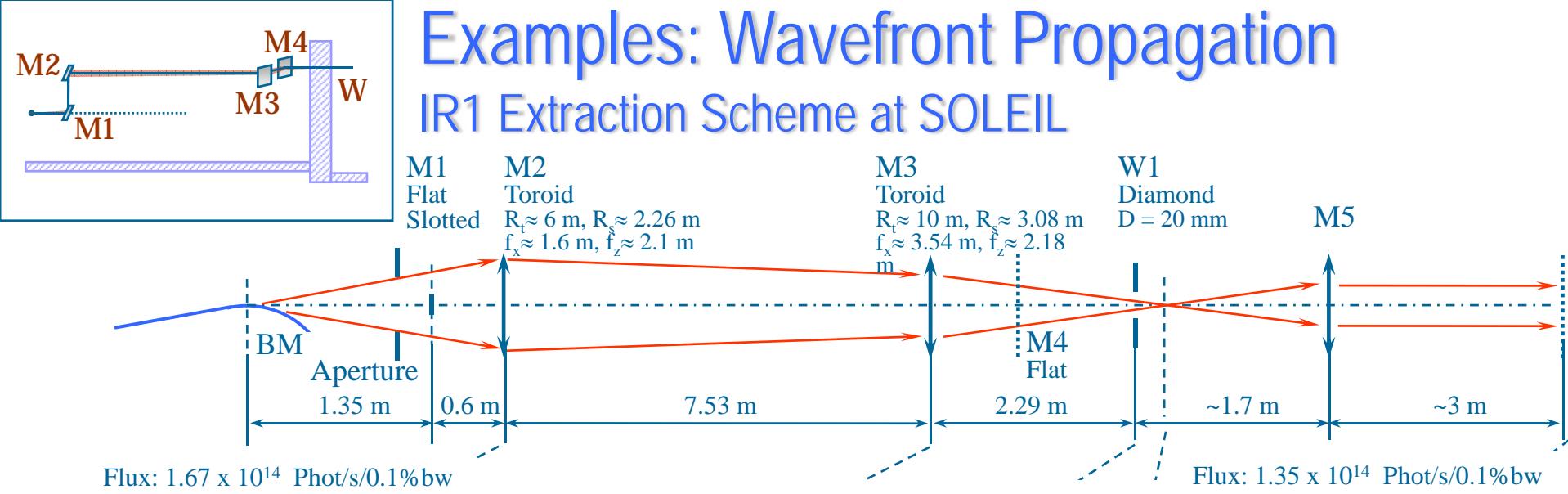
## Spectral Flux through Finite Aperture

66.2 mr (= 61 mr + 5.2 mr) Hor. x 18 mr Vert

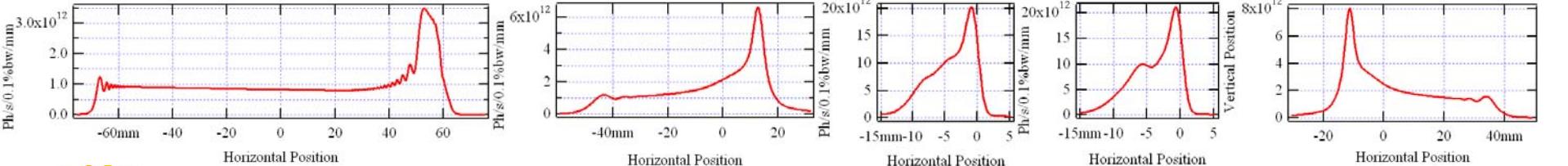


# Examples: Wavefront Propagation

## IR1 Extraction Scheme at SOLEIL



Intensity Profiles



# Examples: Time-Dependent Wavefront Propagation

## SASE Pulse Profiles and Spectra at FEL Exit

E-Beam:  $E = 1 \text{ GeV}$   $\sigma_{t,e} \sim 200 \text{ fs}$   
 $I_{peak} = 1.5 \text{ kA}$   $\varepsilon_x = \varepsilon_y = 1.2 \pi \text{ mm-mrad}$

Undulator:  $K \sim 2.06$   
 $\lambda_u = 30 \text{ mm}$   
 $L_{tot} \sim 5 \times 2 \text{ m}$

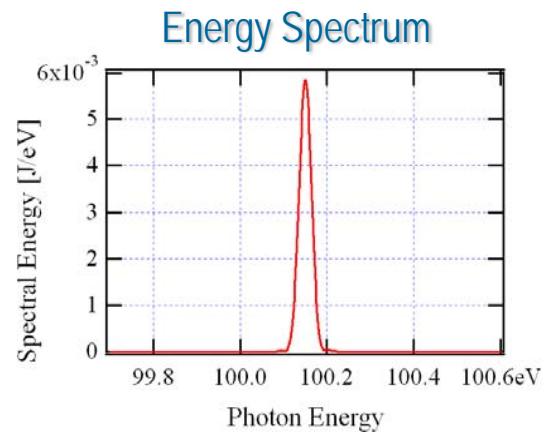
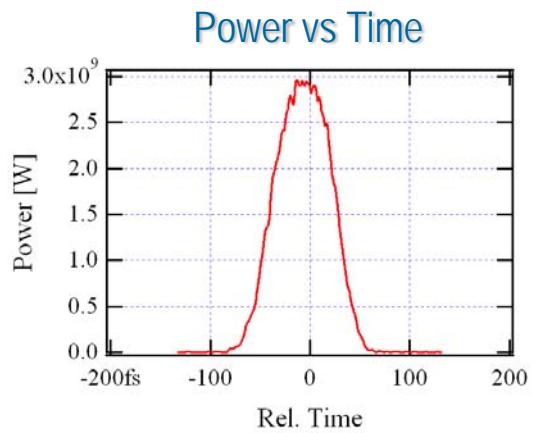
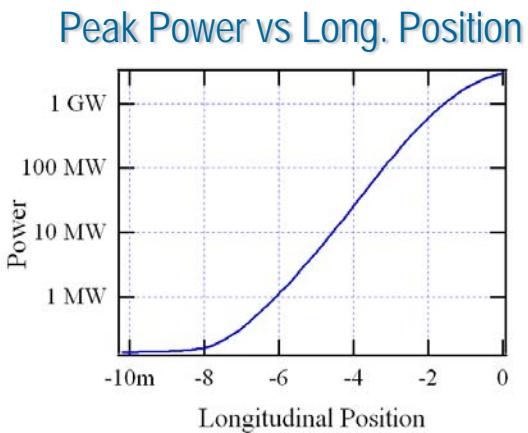
ArcEnCiel (phase 2)

$P_{max\ sseed} \sim 50 \text{ kW}$

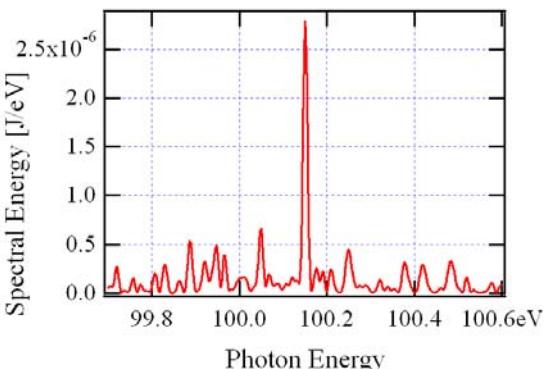
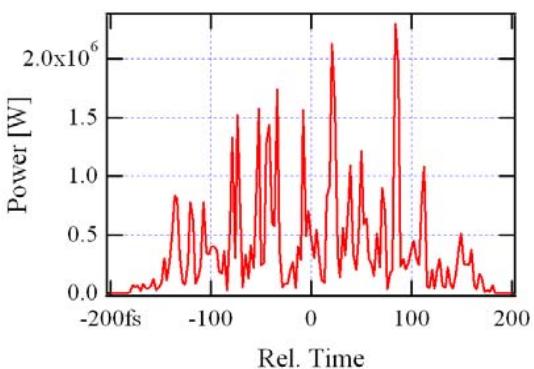
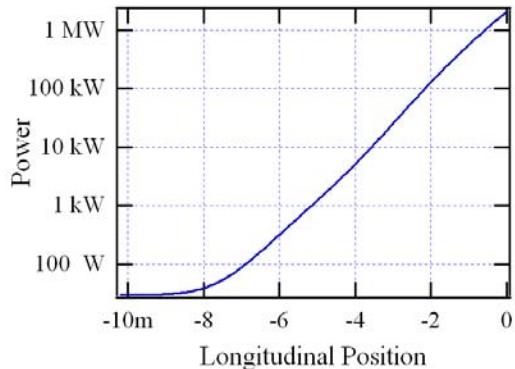
$\sigma_{t\ seed} \sim 25 \text{ fs}$

GENESIS

### A: Seeded FEL operation



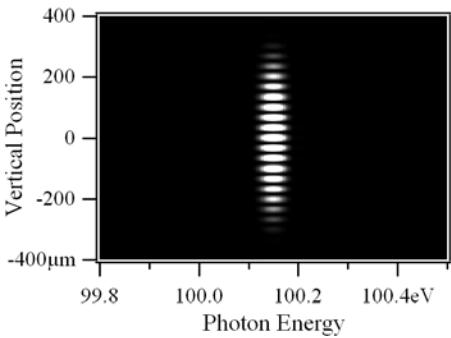
### B: SASE (not saturated)



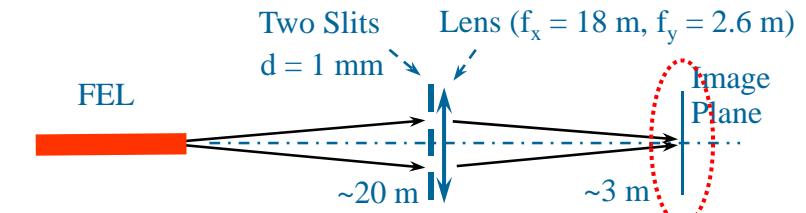
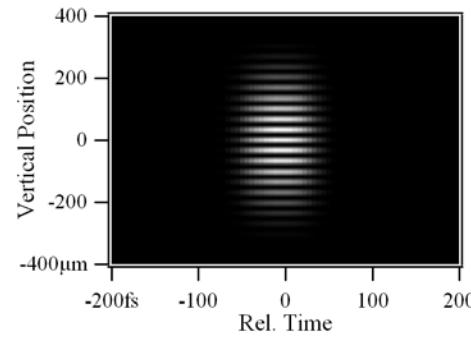
# Examples: Time-Dependent Wavefront Propagation Wavefront Characteristics in Image Plane of Young's 2-Slit Interferometer

## A: Seeded

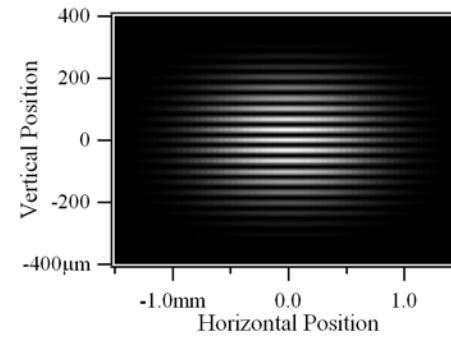
Spectral Fluence  
vs Photon Energy  
and Vertical Position (at  $x = 0$ )



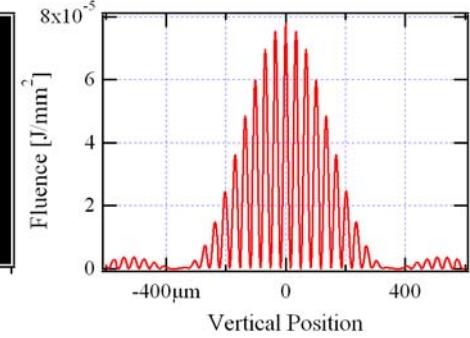
Power Density  
vs Time  
and Vertical Position (at  $x = 0$ )



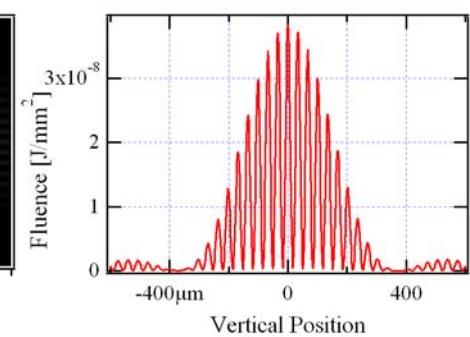
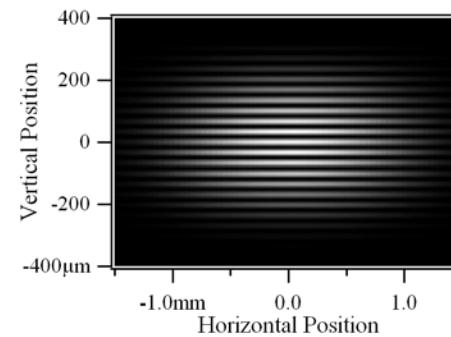
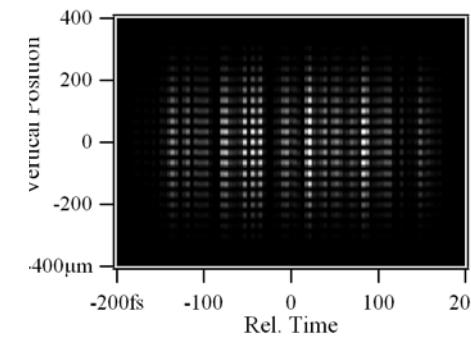
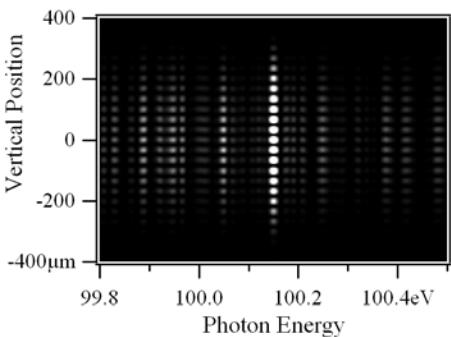
Fluence (/Time-Integrated Intensity)  
vs Horiz. and Vert. Positions



Fluence (/Time-Integrated Intensity)  
vs Vert. Position (at  $x = 0$ )



## B: Started from noise



# Examples: Time-Dependent Wavefront Propagation

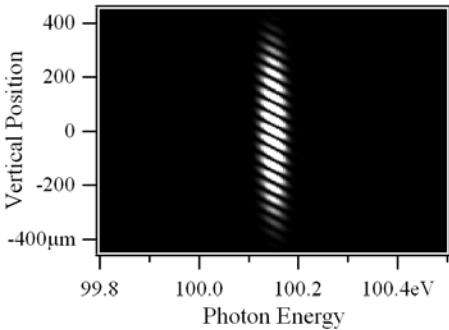
## Wavefront Characteristics in Image Plane

### of a 2-Slit Interferometer with Grating

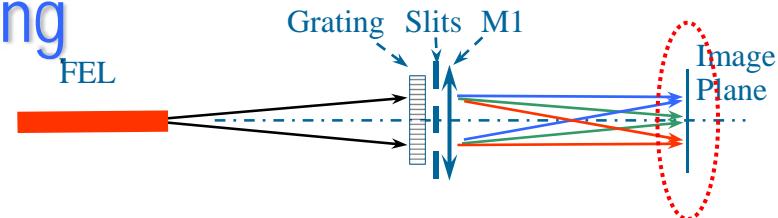
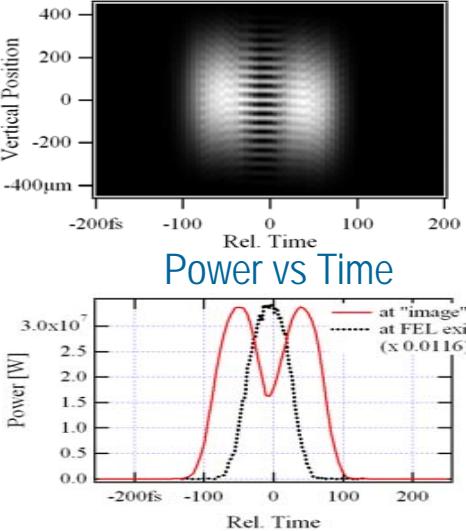
#### A: Seeded

Spectral Fluence  
vs Photon Energy

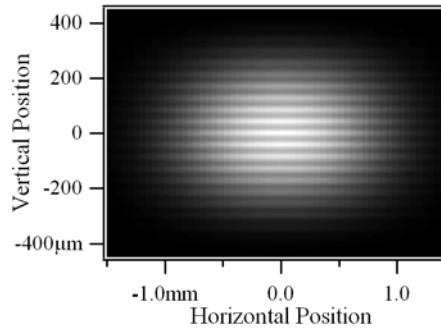
and Vertical Position (at  $x = 0$ )



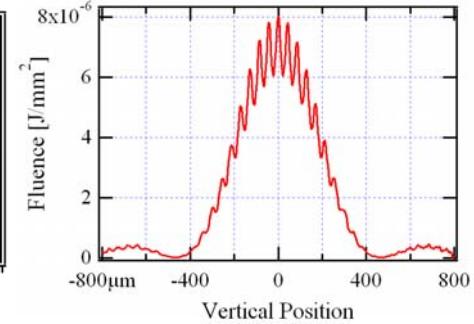
Power Density  
vs Time and Vert. Pos. (at  $x = 0$ )



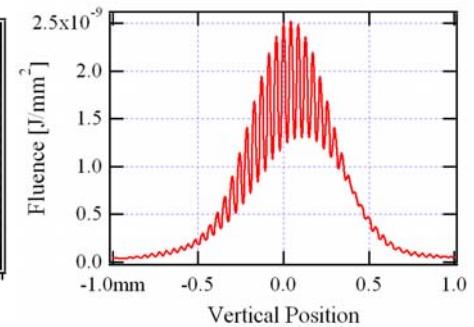
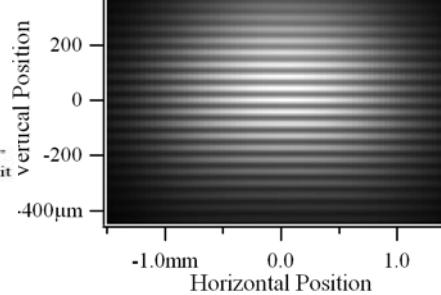
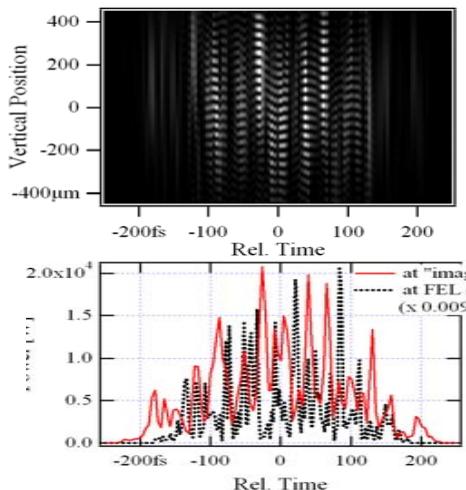
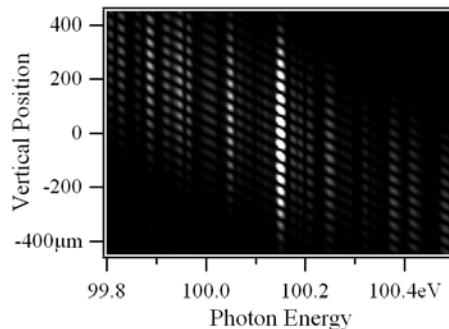
Fluence (/Time-Integrated Intensity)  
vs Horiz. and Vert. Positions



Fluence [J/mm<sup>2</sup>] vs Vert. Position (at  $x = 0$ )



#### B: Started from noise



# SRW and Others...

## RADIA

- Solver of 3D Magnetostatics problems;
- Very efficient for IDs, good for Accelerator Magnets;
- Extension to Eddy Currents is considered

## SRW

- Simulator for Spontaneous Synchrotron Emission and Wavefront Propagation;
- Applicable to large variety of problems of high importance for 3<sup>rd</sup> and 4<sup>th</sup> Generation Sources;
- ...However, it is not a "proven" tool for SR Beamline optimization... (yet ?)

## IDBuilder

- GA-based Optimizer for ID construction: magnet Sorting, Swapping, Shimming,...;
- Can be generalized to Magnet Design problems

- The codes are written in C++ as shared libraries (with documented API);
- Currently interfaced to IGOR Pro (all) and Mathematica (some);
- Can be interfaced to other Front-Ends / Scripting Environments, e.g. Python;
- Are easily "extendable" by users, thanks to Scripting Environments.

# Acknowledgements

- J.-L. Laclare P. Elleaume, J. Chavanne (ESRF)
- J.-M. Filhol, P. Dumas, P. Roy, O. Rudenko (SOLEIL)
- G.P. Williams (JLab), Y.-L. Mathis (ANKA)
- B. Diviacco (ELETTRA), R. Carr (LCLS)
- T. Tanabe, G. Rakowsky (BNL)
- All Users of SRW and RADIA