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

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Outline

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  • Existing Computer Codes

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    ▪ Frequency Domain Electric Field from Liénard-Wiechert Potentials
  • Wavefront Propagation:
    ▪ Kirchhoff Theorem for Single-Electron SR
    ▪ Fourier Optics

• Computation Examples
  • Radiation from Insertion Devices:
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    ▪ 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)
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)**

<table>
<thead>
<tr>
<th>Approved Beamlines (December 2008)</th>
<th>Requires Physical Optics Simulations?</th>
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</thead>
<tbody>
<tr>
<td>Inelastic Scattering Beamline (0.1 – 1 meV spectral resolution)</td>
<td>yes</td>
</tr>
<tr>
<td>Nanoprobe Beamline</td>
<td>yes</td>
</tr>
<tr>
<td>Coherent Hard X-ray Beamline</td>
<td>yes</td>
</tr>
<tr>
<td>Coherent Soft X-ray Beamline</td>
<td>yes</td>
</tr>
<tr>
<td>X-ray Absorption Spectroscopy Beamline</td>
<td>?</td>
</tr>
<tr>
<td>Powder Diffraction Beamline</td>
<td>yes</td>
</tr>
</tbody>
</table>
Spontaneous Emission by One Relativistic Electron
Moving in Free Space

Lienard-Wiechert Potentials for One Electron:

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

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

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

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

Equivalence of the two expressions can be shown by integration by parts.
Spontaneous Emission by One Relativistic Electron

Electric Field in Frequency Domain:

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

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

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

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

Asymptotic Expansion to accelerate computation and “improve” numerical convergence:

\[ \int_{-\infty}^{+\infty} F \exp(i\Phi)ds = \int_{r_1}^{r_2} F \exp(i\Phi)ds + \int_{-\infty}^{r_1} F \exp(i\Phi)ds + \int_{r_2}^{+\infty} F \exp(i\Phi)ds \]

\[ \int_{-\infty}^{r_1} F \exp(i\Phi)ds + \int_{r_2}^{+\infty} F \exp(i\Phi)ds \approx \left[ \frac{F}{i\Phi'} + \frac{F'\Phi - F''\Phi''}{\Phi'^3} + ... \right] \exp(i\Phi) \]
Incoherent and Coherent Emission by Many Electrons

Electron Dynamics:

\[
\begin{pmatrix}
    x_e \\
    y_e \\
    z_e \\
    \beta_{xe} \\
    \beta_{ye} \\
    \delta\gamma_e
\end{pmatrix} = A(\tau) \begin{pmatrix}
    x_e^0 \\
    y_e^0 \\
    z_e^0 \\
    \beta_{xe}^0 \\
    \beta_{ye}^0 \\
    \delta\gamma_e^0
\end{pmatrix} + B(\tau)
\]

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

\[
\left\langle \left| \vec{E}_\omega \right|^2 \right\rangle = \int \int \vec{E}_{\omega 0}(\vec{r}; x_e^0, y_e^0, z_e^0, x_e', y_e', \delta\gamma_e^0) \left| f(x_e^0, y_e^0, z_e^0, x_e', y_e', \delta\gamma_e^0) dx_e^0 dy_e^0 d\gamma_e^0 \right|^2 + \left| \left( N_e - 1 \right) \vec{E}_{\omega 0}(\vec{r}; x_e^0, y_e^0, z_e^0, x_e', y_e', \delta\gamma_e^0) \right|^2
\]

"Coherent" SR

Common Approximation for CSR: “Thin” Electron Beam:

\[
\left\langle \left| \vec{E}_{\omega 0} \right|^2 \right\rangle_{CSR} \approx N_e \left| \int_{-\infty}^{\infty} f(z_e^0) \exp(ikz_e^0) dz_e^0 \right|^2 \left| \vec{E}_{\omega 0} \right|^2
\]

For Gaussian Longitudinal Bunch Profile:

\[
\left\langle \left| \vec{E}_{\omega 0} \right|^2 \right\rangle_{CSR} \approx N_e \exp(-k^2\sigma^2) \left| \vec{E}_{\omega 0} \right|^2
\]

However, if \( f(x_e^0, y_e^0, z_e^0, x_e', y_e', \delta\gamma_e^0) \) is Gaussian, the 6-fold integration can be done analytically (!)

\[
\Rightarrow \text{Efficient method for CSR computation taking into account 6D phase space distribution of electrons}
\]
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):

\[
\frac{d\theta}{dz} = k_u - k_r \left( 1 + p_\perp^2 + a_u^2 - 2a_r a_u \cos(\theta + \phi_r) \right) \frac{1}{2\gamma^2}
\]
\[
\frac{d\gamma}{dz} = -\frac{k_r f_r a_u a_r}{\gamma} \sin(\theta + \phi_r)
\]
\[
\frac{d\vec{p}_\perp}{dz} = -\frac{1}{2\gamma} \frac{\partial a_u^2}{\partial r_\perp} + \mathbf{k}_{\text{foc}} \vec{r}_\perp
\]
\[
\frac{d\vec{r}_\perp}{dz} = \frac{\vec{p}_\perp}{\gamma}
\]

Paraxial wave equation with current:

\[
\left[ 2ik_r \frac{\partial}{\partial z} + \nabla_\perp^2 \right] a_r \exp(i\phi_r) = -\frac{e\varepsilon_0 f_r a_u}{mc} \left\{ \frac{\exp(-i\theta)}{\gamma} \right\}
\]

Solving this system gives Electric Field at the FEL exit for one “Slice”:

\[
E_{\text{slice}}|_{z=z_{\text{exit}}} \sim a_r \exp(i\phi_r)|_{z=z_{\text{exit}}}
\]

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:

\[
E(x, y, z_{\text{exit}}, t) \leftrightarrow E_\omega(x, y, z_{\text{exit}})
\]

- 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

\[
\begin{aligned}
\vec{E}_{\omega 2 \perp}(P_2) &\approx \frac{k^2 e^2}{4\pi^2} \int_{-\infty}^{\infty} \int_{A} \vec{B}_{\perp} \cdot \vec{n}_{\perp} + \frac{k^2 e^2}{4\pi^2} \int_{A} \exp[ik(c \tau + R + S)] \cdot (\vec{\ell} \cdot \vec{n}_{p_1} + \vec{\ell} \cdot \vec{n}_{p_2}) d\Sigma \\
&= \frac{k}{\omega^2/c}
\end{aligned}
\]

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

Huygens-Fresnel Principle

\[
\begin{aligned}
\vec{E}_{\omega 2 \perp}(P_2) &\approx \frac{k}{4\pi i} \int_{A} \vec{E}_{\omega 1 \perp}(P_1) \frac{\exp(ikS)}{S} (\vec{\ell} \cdot \vec{n} + \vec{\ell} \cdot \vec{n}_{p_2}) d\Sigma \\
&= \frac{k}{\omega^2/c}
\end{aligned}
\]

Fourier Optics

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

\[
\begin{aligned}
\vec{E}_{\omega 2 \perp}(x_2, y_2) &\approx \frac{k}{2\pi i L} \int_{x_1, y_1} \exp[ik(L^2 + (x_2 - x_1)^2 + (y_2 - y_1)^2)]^2] dx_1 dy_1 \\
&= \frac{k}{\omega^2/c}
\end{aligned}
\]

Assumption of small angles

"Thin" Optical Element:

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

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

\[
\begin{aligned}
\vec{E}_{\omega 2 \perp}(x_2, y_2) &\approx G(x_2, y_2, \omega) \exp[ik\Lambda(x_2, y_2, k)] \vec{E}_{\omega 1 \perp}(x_1(x_2, y_2), y_1(x_2, y_2)) \\
&= \frac{k}{\omega^2/c}
\end{aligned}
\]

E.g. from Stationary Phase method
“Economic” Version of Free-Space Fourier-Optics Propagator

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

\[
\tilde{E}_{o2\perp}(\vec{r}_2) \approx \frac{k}{2\pi i} \iint_{\Sigma_i} \tilde{E}_{o1\perp}(\vec{r}_1) \frac{\exp[ik|\vec{r}_2 - \vec{r}_1|]}{|\vec{r}_2 - \vec{r}_1|} d\Sigma_i
\]

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

**Analytical Treatment of Quadratic Phase Term:**

Before Propagation:

\[
\tilde{E}_{o1\perp}(x_1, y_1) = \tilde{F}_{o1}(x_1, y_1) \exp \left[ ik \frac{(x_1 - x_0)^2}{2R_x} + ik \frac{(y_1 - y_0)^2}{2R_y} \right]
\]

After Propagation:

\[
\tilde{E}_{o2\perp}(x_2, y_2) \approx \frac{k}{2\pi i} \exp(ikL) \iint_{\Sigma} \tilde{F}_{o1}(x_1, y_1) \exp \left[ ik \frac{(x_1 - x_0)^2}{2R_x} + ik \frac{(y_1 - y_0)^2}{2R_y} + ik \frac{(x_2 - x_1)^2 + (y_2 - y_1)^2}{2L} \right] dx dy_1
\]

\[
= \frac{k}{2\pi i L} \exp \left[ ikL + ik \frac{(x_2 - x_0)^2}{2(R_x + L)} + ik \frac{(y_2 - y_0)^2}{2(R_y + L)} \right] \times
\]

\[
\times \iint_{\Sigma} \tilde{F}_{o1}(x_1, y_1) \exp \left[ ik \frac{R_x + L}{2R_x L} \left( x_1 - \frac{R_x x_2 + Lx_0}{R_x + L} \right)^2 + ik \frac{R_y + L}{2R_y L} \left( y_1 - \frac{R_y y_2 + Ly_0}{R_y + L} \right)^2 \right] dx dy_1
\]

\[
= \tilde{F}_{o2}(x_2, y_2) \exp \left[ ik \frac{(x_2 - x_0)^2}{2(R_x + L)} + ik \frac{(y_2 - y_0)^2}{2(R_y + L)} \right]
\]
Wavefront Propagation:
Taking Into Account Partial Coherence

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

\[
I_\omega(x, y) = \int I_{\omega0}(x, y; x_{e0}, y_{e0}, x'_{e0}, y'_{e0}, \delta_{\gamma e0})
\times f(x_{e0}, y_{e0}, x'_{e0}, y'_{e0}, \delta_{\gamma e0})
\times dx_{e0}dy_{e0}dx'_{e0}dy'_{e0}d\delta_{\gamma e0}
\]

Convolution is valid in many cases:

\[
I_\omega(x, y) \approx \int \int \tilde{I}_{\omega0}(x - \tilde{x}_e, y - \tilde{y}_e)
\times f(\tilde{x}_e, \tilde{y}_e) 
\times d\tilde{x}_e d\tilde{y}_e
\]

OR:

**Propagation of Mutual Intensity**

Mutual Intensity:

\[
M_\omega(x, y; \tilde{x}, \tilde{y}) = \int \tilde{E}_{\omega0\perp}(x, y; x_{e0}, y_{e0}, x'_{e0}, y'_{e0}, \delta_{\gamma e0})
\times \tilde{E}_{\omega0\perp}^*(\tilde{x}, \tilde{y}; x_{e0}, y_{e0}, x'_{e0}, y'_{e0}, \delta_{\gamma e0})
\times f(x_{e0}, y_{e0}, x'_{e0}, y'_{e0}, \delta_{\gamma e0})
\times dx_{e0}dy_{e0}dx'_{e0}dy'_{e0}d\delta_{\gamma e0}
\]

Wigner Distribution (or mathematical Brightness):

\[
B_\omega(x, y; \theta_x, \theta_y) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} M_\omega(x, y; \tilde{x}, \tilde{y}) \exp[ik(\theta_x \tilde{x} + \theta_y \tilde{y})] d\tilde{x} d\tilde{y}
\]
On-Axis Spectrum (taking into account e-beam Emittance)

**Undulator:**
- $\lambda_u = 35 \text{ mm}$
- $K = 2.2$

**e-Beam:**
- $E = 6 \text{ GeV}$
- $\sigma_{x_{eff}} / R = 16.2 \mu r$
- $\sigma_{z_{eff}} / R = 3.96 \mu r$
- $\sigma_E / E = 10^{-3}$
- $R = 30 \text{ m}$

**Spectral Flux / Surface**

Examples: Undulator Radiation

**Spectral Flux / Surface (vertical cuts)**
Examples: Undulator Radiation
U20 (SOLEIL) Spectra and Intensity Distributions @ H3

Spectral Flux

3rd Harmonic, Gap ~9 mm, Apertures:
- 1.5 mm x 0.74 mm @ 17.4 m
- 0.7 mm x 0.2 mm @ 17.4 m

Spectral Flux / Surface (vertical cuts)

Spectral Flux / Surface @ 17.4 m

E = 0.981 Ep
E = 0.994 Ep
E = Ep

Vertical Position

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

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

Evolution of 11th Harmonic of Single-Electron Spectrum

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

RMS Radiation Phase Error after Shimming $\sim 2.5^\circ$

$\varepsilon_x = 3.7 \text{ nm}, \sigma_E/E = 10^{-3}$
APPLE-II Undulator HU80-PLEIADES: Quasi-Periodic Field, Trajectory, Spectra

Measured Vertical Magnetic Field

Horizontal Trajectory

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

Spectra Through Finite Apertures

\[(F_2 + F_3)/F_1 \sim 0.1\]
RADIA-SRW Examples:
Electromagnetic Elliptical Undulator HU256

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

Magnetic Fields at Max. Currents (RADIA)

I_z max = 180 A, I_x max = 250 A

Specifications:

Circular Polarization: \( \varepsilon_{1\text{min}} < 10 \text{ eV} \)
Linear Horiz. Polarization: \( \varepsilon_{1\text{min}} < 10 \text{ eV} \)
Linear Vertical Polarization: \( \varepsilon_{1\text{min}} < 20 \text{ eV} \)

Calculated Spectra at Maximal Currents (SRW)
Examples: Undulator Radiation
Maximal Spectral Flux at Various Polarizations

Undulator: U20 (hybrid, in-vacuum)
Minimal Gap: 5.5 mm
Aperture: 0.15 mr hor. x 0.05 mr vert.

Circular (Left), \( F_{\text{cl}} / F_{\text{tot}} > 0.9 \)
Linear Horizontal, \( F_{\text{lh}} / F_{\text{tot}} > 0.9 \)
Linear Vertical, \( F_{\text{lv}} / F_{\text{tot}} > 0.9 \)

Undulator: HU256 (electromagnet)
Aperture: 0.7 mr x 0.7 mr

Circular (Left), \( F_{\text{cl}} / F_{\text{tot}} > 0.9 \)
Linear Horizontal, \( F_{\text{lh}} / F_{\text{tot}} > 0.9 \)
Linear Vertical, \( F_{\text{lv}} / F_{\text{tot}} > 0.9 \)

Undulator: HU80 (APPLE-II)
Magnets: 28 mm x 28 mm, \( M_r = 1.2 \) T
Min. Gap: 15 mm
Aperture: 0.4 mr x 0.4 mr

Undulator: HU640 (electromagnet)
Aperture: 0.7 mr x 0.7 mr

SOLEIL SYNCHROTRON
Examples: Wavefront Propagation
Focusing of Undulator Radiation


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

NIM-A, 1999
Examples: Wavefront Propagation

Peculiarities of UR Wavefronts

Planar Undulator, Even Harmonics

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

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**

- a: no correction
- b: \(\pi\)-correction at \(x > 0\)
- c: full phase correction
Examples: Wavefront Propagation

Peculiarities of UR Wavefronts

Helical Undulator, Harmonics $n > 1$

$E = 6 \text{ GeV}; B_{\text{max}} = B_{\text{z max}} = 0.3 \text{ T}; 28 \times 52 \text{ mm}; \varepsilon = 4.20 \text{ keV (2$^{\text{nd}}$ harmonic)}$

$1:1$ imaging; $30 \text{ m}$ from middle of Undulator to Thin Lens & Phase Correction

Examples: Wavefront Propagation

Peculiarities of UR Wavefronts

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

$E = 6 \text{ GeV}; B_{x_{\text{max}}} = B_{z_{\text{max}}} = 0.3 \text{ T}; 28 \times 52 \text{ mm}; \varepsilon = 4.20 \text{ keV (2}\text{-}\text{nd harmonic})$

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)

**Vertical Plane**
- Electron Trajectories from Measured Magnetic Field
- Gap: 30 mm
- Phase: -20 mm

**Intensity Distribution at M1**
- Photon Energy: 163 eV

**Horizontal Cuts**
- Distance from Und. to M1: 20 m
- Aperture @ M1: 5 mm (H) x 4 mm (V)

**Intensity Distribution after Back-Propagation**
- Vertical Cuts
- Horizontal Cuts

**Notes**
- SOLEIL SYNCHROTRON
Partially-Coherent Wavefront Propagation Simulations for Phase-Contrast Tomography BL: Approximate Scheme

Optical Scheme

Horizontal Plane
- M1
- Aperture f≈4.4 m, θ≈3 mrad
- Slits 120 μm

Vertical Plane
- Aperture ~1.8 mm

Intensity Distributions in Transverse Plane at Sample (no Slope Error, ε≈10 keV)

A. Somogyi, T. Moreno, F. Polack
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

\( \theta = 3 \text{ mrad}, \varepsilon \approx 10 \text{ keV} \)
M1 Slope Error Effects for Different E-Beam Parameters

Modeling Surface Height Profile (due to Slope Error)

- θ = 3 mrad, ε ≈ 10 keV

Intensity Distributions at Sample

θ = 3 mrad, ε ≈ 10 keV

Cuts of Intensity Distributions at Sample

- Sinusoidal "Slope Error": α_{max} ≈ 1.4 μrad, ν ≈ 0.3 cm⁻¹

- Intensity Distributions at Sample with slope error: σ_e = 290 μm, σ_e' = 20 μrad
- Intensity Distributions at Sample with slope error: σ_e = 200 μm, σ_e' = 5.8 μrad
- Intensity Distributions at Sample with slope error: σ_e = 10 μm, σ_e' = 4.5 μrad
Partially-Coherent Wavefront Propagation Simulations for Phase-Contrast Tomography BL: Image of Sample Sphere

Optical Scheme

Horizontal Plane

Vertical Plane

Phase-Contrast Image of Test Sample Sphere

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

U19

Aperture ~0.9 mm

M1 $f \approx 4.4$ m

Slits 120 $\mu$m

Aperture ~0.9 mm

M1 $f \approx 4.4$ m

Slits 120 $\mu$m

Aperture 400 $\mu$m

Detector Screen

$\sigma_x = 280 \, \mu$m

$\sigma_y = 8.25 \, \mu$m

Aperture ~1.8 mm

Test Sample Sphere CaCO$_3$, d = 100 $\mu$m

Detector Screen

Aperture ~0.9 mm

M1 $f \approx 4.4$ m

Slits 120 $\mu$m

Aperture 400 $\mu$m

Detector Screen

$\sigma_x = 280 \, \mu$m

$\sigma_y = 8.25 \, \mu$m

Aperture ~1.8 mm

Test Sample Sphere CaCO$_3$, d = 100 $\mu$m

Detector Screen

$\sigma_x = 280 \, \mu$m

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Aperture ~1.8 mm

Test Sample Sphere CaCO$_3$, d = 100 $\mu$m

Detector Screen

$\sigma_x = 280 \, \mu$m

$\sigma_y = 8.25 \, \mu$m

Aperture ~1.8 mm

Test Sample Sphere CaCO$_3$, d = 100 $\mu$m

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

Lattice Functions (Long Straight Section)

Horizontal Plane

Vertical Plane

R ~ 100 m

Slit \( \Delta x = 0.5 \text{ mm} \)

Lens \( f_x \approx 0.25 \text{ m} \)

\( \Delta z = 0.5 \text{ mm} \)

\( f_z \approx 0.5 \text{ m} \)

Optical Scheme (A)

U19

\( R \sim 100 \text{ m} \)

Vertical Plane

Intensity @ Sample

\( \varepsilon \approx 10 \text{ keV} \)

Flux \( \approx 5.2 \times 10^{12} \text{ Ph/s/0.1\%bw} \)

Horizontal Position

Vertical Position

Transverse Position

Photon/s/0.1\%bw/mm²

Horizontal Cut

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

Lattice Functions (Long Straight Section)

Optical Scheme (B)

Intensity @ Sample

\[ \varepsilon \approx 10 \text{ keV} \]

\[ \text{Flux} \approx 1 \times 10^{12} \text{ Ph/s/0.1\%bw} \]
Preliminary Wavefront Propagation Calculations for MICROSCOPIUM: Modified Long Straight Section

Lattice Functions
(Modified Long Straight Section)

Optical Scheme (A)

Horizontal Plane

Vertical Plane

Intensity @ Sample

\[ \varepsilon \approx 10 \text{ keV} \]

\[ \text{Flux} \approx 7.5 \times 10^{11} \text{ Ph/s/0.1\%bw} \]
Wavefront Propagation Calculations for MICROSCOPIUM: Comparison of Optical Schemes with Zone Plates

### Optical Schemes

#### (I) Horizontal Plane
- Aperture: 0.8mm
- HFM: f = 15.9 m
- Slit: 30 μm
- Aperture Sample Plane: 0.2 mm
- ZP(Ta): 300 zones
- f ≈ 0.296 m @ 10 keV
- Flux: ≈ 2.9 × 10^{10} Ph/s/0.1%bw
- U19: ~16.1 m
- Vertical Plane: ~66.5 m
- ~15 m

#### (II) Horizontal Plane
- Aperture: 0.8mm
- HFM: f = 10.2 m
- Slit: 30 μm
- Aperture Sample Plane: 0.2 mm
- ZP(Ta): 300 zones
- f ≈ 0.296 m @ 10 keV
- Flux: ≈ 6.6 × 10^{10} Ph/s/0.1%bw
- U19: ~16.1 m
- Vertical Plane: ~66 m
- ~15.5 m

### Intensity and Flux at Sample

- Photon Energy: 10 keV
- ZP Efficiency ~ 0.11
- Flux: ~2.9 × 10^{10} Ph/s/0.1%bw
- Flux: ~6.6 × 10^{10} Ph/s/0.1%bw

A. Somogyi, T. Moreno, F. Polack
Examples: Wavefront Propagation
X-Ray Focusing Using a Zone Plate (Full Transverse Coherence)

Zone Plate or Ideal Lens

\[ A = 200 \, \mu m, \quad F = 0.966 \, m \]
\[ \varepsilon = 12 \, keV \]

50 m from Source

0.325 m \((\approx F/3)\)

0.74 m

0.985 m \((\approx F)\)

Examples: Wavefront Propagation
X-Ray Focusing Using a Zone Plate (Full Transverse Coherence)
Examples: Wavefront Propagation
X-Ray Focusing Using a Zone Plate (Partial Coherence)

~55 m from Source (ESRF BM05)

ZP
242 zones
d = 387 µm

ε = 8 keV

Waist (~F from ZP)
~1.5 x F from ZP
~2 x F from ZP
Examples: Wavefront Propagation / Analysis
Partially Coherent X-Rays Observed Out of Focus of a Zone Plate

Aperture at Waist: 600 μm x 600 μm
Intensity Distributions at 0.55 m after Waist
Aperture at Waist: 10 μm x 10 μm

Measurements (ESRF BM5)
M. Idris, A. Snigirev et. al.

Calculation for Perfect ZP
Calculation for ZP with non-perfect outer zones
ε ≈ 10.4 keV
Examples: Wavefront Propagation
Point-Spread Function Computation for Parabolic X-Ray CRL

A. Snigirev, B. Lengeler, et. al., 1998

$\varepsilon = 8.9 \text{ keV}$
$\delta = 6.9 \times 10^6$
$L_{\text{atten}} = 0.106 \text{ mm}$
$N = 1$
$F = 13.6 \text{ m}$
$\Delta_{\text{FWHM}} = 7.3 \mu\text{m}$

$\varepsilon = 23 \text{ keV}$
$\delta = 1.0 \times 10^6$
$L_{\text{atten}} = 1.89 \text{ mm}$
$N = 7$
$F = 13.1 \text{ m}$
$\Delta_{\text{FWHM}} = 4.1 \mu\text{m}$
Examples: Wavefront Propagation
Fresnel Diffraction of Partially Coherent X-Rays

Measurements by A. Snigirev et. al.

Intensity
arb. units

Comp. for $0.7\sigma_y$ best-fit
Comp. for $1.3\sigma_y$ best-fit
Examples: Wavefront Propagation
Interference of Partially Coherent X-Rays

A. Snigirev et. al.

Undulator (38 x 42 mm)
Mirror
Si (111)
B fiber ($d = 100 \mu m$)
Detector (YAG+ microscope+CCD)

$\varepsilon = 11$ keV
$r_s = 40.6$ m
$r_d = 5.5$ m

Intensity
arb. units

Experiment & Best Fit
Comp. for 0.7$\sigma_{y_{best-fit}}$
Comp. for 1.3$\sigma_{y_{best-fit}}$

vertical position
horizontal position
vertical position
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)

Wave-optics calculation
(Fresnel Diffraction of Polychromatic SR)

Quadratic sum of the Geometry and Fraunhofer Diffraction contributions
E-Beam Imaging Using Vertically Polarized BM SR

Simplified Optical Scheme (Top View)

SR Intensity Distribution in the Image Plane (Vertical Polarization)

Vertical Cut

- red curve: filament e-beam ($\sigma_{ez} = 0$), $I_{min}/I_{max} \approx 0 \ (< 10^{-3})$
- blue: $\sigma_{ez} = 18.3$ $\mu$m, $I_{min}/I_{max} \approx 0.36$
- black: $\sigma_{ez} = 23.3$ $\mu$m (expected), $I_{min}/I_{max} \approx 0.56$
- green: $\sigma_{ez} = 28.3$ $\mu$m, $I_{min}/I_{max} \approx 0.73$

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

- Extraction Mirror
- Aperture & Lens
- Monochromatic (Interference) Filter
- Polarizer (suppresses horizontal polarization component)
- Image Plane (CCD)

A. Andersson et al., Proc. EPAC-96

Monochromatic (Interference) Filter Polarizer (suppresses horizontal polarization component)

Extraction Mirror

Aperture & Lens

Monochromatic (Interference) Filter

Polarizer (suppresses horizontal polarization component)

Image Plane (CCD)
E-Beam Imaging Using Double-Slit Interferometer

Simplified Optical Scheme
(Side View)

Double Slit & Lens
Monochromatic (Interference) Filter
Extraction Mirror
Image Plane (CCD)

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

E = 2.75 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 (\( \sigma_{e z} = 0 \)), \( I_{\text{min}}/I_{\text{max}} \approx 0 \ (< 10^{-5}) \)
blue: \( \sigma_{e z} = 18.3 \mu m \), \( I_{\text{min}}/I_{\text{max}} \approx 0.67 \)
black: \( \sigma_{e z} = 23.3 \mu m \), \( I_{\text{min}}/I_{\text{max}} \approx 0.88 \) (no fringes)
green: \( \sigma_{e z} = 28.3 \mu m \), \( I_{\text{min}}/I_{\text{max}} \approx 0.99 \) (no fringes)

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

T. Mitsuhashi, Proc. PAC-97
Angular Horizontal FS Slice Separation Scheme (SLS)

Idea of FS Slicing: A. Zholents (LBNL)
FS Slicing at SLS: G. Ingold et. al.

Electron Trajectory and Photon Absorbers

Intensity Distributions in the Median Plane

~15.7 m from Radiator; Finite-Emittance Electron Beam

E-Beam, Modulation:
- \( E_0 = 2.44 \text{ GeV} \)
- \( I_{b,s} = 2 \text{ mA} \)
- \( \sigma_b = 12 \text{ ps} \)
- \( \Delta E_{\text{max}} \approx 21.5 \text{ MeV} \)
- \( f_s = 1 \text{ kHz} \)
- \( \sigma_L = 21 \text{ fs} \)

Radiator:
- Undulator U19 (in-vacuum)

\( \Delta \text{E}_{\text{max}} \approx 21.5 \text{ MeV} \)

E0 = 2.44 GeV, \( f_s = 1 \text{ kHz} \)
\( \sigma_L = 21 \text{ fs} \)

Intensity Distributions in the Median Plane

Core (Radiator)
"Satellite" Emission from electrons with 12 MeV < \( \Delta E \) < 21.5 MeV
Core (Down. BE01, C3)
Core (Up. BE01, C1)

Core (Radiator)
"Satellite" Emission from electrons with 12 MeV < \( \Delta E \) < 21.5 MeV
Core (Downstr. BE01, C3)
Core (Up. BE01, C1)
FS Slice Separation Using SOLEIL “Native” Dispersion

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

E-Beam, Modulation:
- $E_0 = 2.75$ GeV
- $\Delta E_{\text{max}} \approx 14$ MeV (pessimistic)
- $I_{\text{e.b.}} = 10$ mA
- $\sigma_b = 24$ ps

Slit Dimensions:
- $0.5$ mm x $0.5$ mm
- $|x_c| = 2.4$ mm

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

Hard X-Ray Radiator:
- $\varepsilon = 6.93$ keV
- $\Delta t_x \approx 7 - 14$ MeV (pessimistic)
- $f_L = 10$ kHz
- $\sigma_L = 50$ fs
- $\Delta t_s \approx 60$ fs

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

A. Nadji et. al.
FS Slice Separation Using SOLEIL “Native” Dispersion

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

Intensity in Transverse Plane Before Mirror

\[ \Delta E_{\text{max}} \approx 20 \text{ MeV} \]

Soft X-Ray Radiator:

Unidulator HU80 (Apple-II)

\[ f_{\text{L}} = 10 \text{ kHz} \]

\[ \sigma_{\text{L}} = 50 \text{ fs} \]

E-Beam, Modulation:

\[ E_0 = 2.75 \text{ GeV} \]

\[ I_{\text{b,h}} = 10 \text{ mA} \]

\[ \sigma_{\text{b}} = 24 \text{ ps} \]

Intensity in the Plane of 1:1 Imaging

\[ E_0 = 2.75 \text{ GeV} \]

\[ I_{\text{b,h}} = 10 \text{ mA} \]

\[ \sigma_{\text{b}} = 24 \text{ ps} \]

\[ \sigma_{\text{L}} = 50 \text{ fs} \]

F. Polack

~10 m

Slit Dimensions:

2 mm x 1 mm

Slit Position:

| \( x_c | = 2.5 \text{ mm} \)

HU80

Centered at +1.35 m from the Middle of Straight Sect.

Mirror Surface Assumptions:

- Average Slope Error: ~1.5 μrad,
- Average Roughness: ~2.5 Å,
- Incidence Angle: ~1°
- Error Distribution: Random (Density to be studied)

Linear-Horizontal Polarization

\[ \varepsilon = 415 \text{ eV} \]

\[ \Delta\varepsilon = 20 \text{ MeV} \]

\[ \Delta t_{10-20\text{MeV}} = 180 \text{ fs} \]

F. Polack

Slit, Mirror Plane of 1:1 Imaging

Soft X-Ray Radiator:

Unidulator HU80 (Apple-II)

\[ f_{\text{L}} = 10 \text{ kHz} \]

\[ \sigma_{\text{L}} = 50 \text{ fs} \]

E-Beam, Modulation:

\[ E_0 = 2.75 \text{ GeV} \]

\[ I_{\text{b,h}} = 10 \text{ mA} \]

\[ \sigma_{\text{b}} = 24 \text{ ps} \]

\[ \sigma_{\text{L}} = 50 \text{ fs} \]

A. Nadji et al.

Peculiarities of Undulator Radiation,

- Electron Beam Emittance,
- Slit Diffraction,
- Scattering from Mirror Surface are taken into account

Intensity in the Plane of 1:1 Imaging

Core, no scattering

Core, with scattering

Satellite, -20 MeV < ΔE < -10 MeV, no scattering
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)

- $\lambda = 10 \, \mu m$
- $\lambda = 100 \, \mu m$
- $\lambda = 300 \, \mu m$

Horizontal Cuts (Median Plane)

Spectral Flux through Finite Aperture
$66.2 \, mr = 61 \, mr + 5.2 \, mr$ Hor. x $18 \, mr$ Vert

SOLEIL SYNCHROTRON
Examples: Wavefront Propagation

IR1 Extraction Scheme at SOLEIL

BM Aperture

M1 Flat Slotted

M2 Toroid
$R_t \approx 6 \text{ m}, R_s \approx 2.26 \text{ m}$
$f_x \approx 1.6 \text{ m}, f_z \approx 2.1 \text{ m}$

M3 Toroid
$R_t \approx 10 \text{ m}, R_s \approx 3.08 \text{ m}$
$f_x \approx 3.54 \text{ m}, f_z \approx 2.18 \text{ m}$

W1 Diamond
$D = 20 \text{ mm}$

M4 Flat

M5

Flux: $1.67 \times 10^{14} \text{ Phot/s/0.1\%bw}$

Flux: $1.35 \times 10^{14} \text{ Phot/s/0.1\%bw}$

Intensity Distributions at 10 μm Wavelength

Intensity Profiles

Optical scheme: F. Polack, P. Dumas
Examples: Time-Dependent Wavefront Propagation
SASE Pulse Profiles and Spectra at FEL Exit

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

**Undulator:** \[ K \sim 2.06 \quad \lambda_u = 30 \text{ mm} \]
\[ L_{\text{tot}} \sim 5 \times 2 \text{ m} \]
\[ \hbar \omega_0 = 100.15 \text{ eV} \]

**A: Seeded FEL operation**

- **Peak Power vs Long. Position**
- **Power vs Time**
- **Energy Spectrum**

**B: SASE (not saturated)**

- **Peak Power vs Long. Position**
- **Power vs Time**
- **Energy Spectrum**
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 vs Vert. Position (at $x = 0$)

B: Started from noise

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 vs Vert. Position (at $x = 0$)
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 $x = 0$)

B: Started from noise
Power Density vs Time and Vert. Pos. (at $x = 0$)

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

Power vs Time at "image" at FEL exit ($\approx 0.011s$)

Fluence [/Jum$^2$] vs Vert. Position (at $x = 0$)
SRW and Others...

**SRW**
- Simulator for Spontaneous Synchrotron Emission and Wavefront Propagation;
- Applicable to large variety of problems of high importance for 3rd and 4th 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

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

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

**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.
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