Numerical Propagation Simulations and Coherence Analysis of SASE Wavefronts

O. Chubar, F. Polack, M.-E. Couprie (SOLEIL)
M. Labat, G. Lambert, O. Tcherbakoff (CEA, DSM/SPAM)
91191 Gif-sur-Yvette, France

Existing Computer Codes
for (SR) Ray-Tracing and Wavefront Propagation

Ray-Tracing / Geometrical Optics

Free:	SHADOW (Univ. Wisconsin) XOP by S. del Rio (ESRF), R. Dejus (APS) RAY by A. Erko et. al. (BESSY) ...
Commercial:	OSLO CODE V ZEMAX ...

Wavefront Propagation / Physical Optics

Free:	PHASE by J. Bahrdt (BESSY) – Stationary Phase Method SRW (ESRF/SOLEIL) – Fourier Optics ...
Commercial:	ZEMAX GLAD MICROWAVE Studio ...

Self-Amplified Spontaneous Emission Described by Paraxial FEL Equations

SOLEIL SYNCHROTRON

Approximation of Slowly Varying Amplitude of Radiation Field

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

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

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

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

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

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

Paraxial wave equation
with current:

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

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

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

← Popular TD 3D FEL computer code: **GENESIS** (S.Reiche)

Time-Domain Electric Field in transverse plane at FEL exit: $E(x, y, z_{exit}, t)$

Wavefront Propagation

Electric Field in Frequency and Time domains:

$$\vec{\tilde{E}}(\vec{r},\omega) \equiv \int_{-\infty}^{\infty} \vec{E}(\vec{r},t)\exp(i\omega t)dt$$

$$\vec{E}(\vec{r},t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} \vec{\tilde{E}}(\vec{r},\omega)\exp(-i\omega t)d\omega$$

Huygens-Fresnel Principle:
(paraxial approximation)

$$\vec{\tilde{E}}_{\perp}(\vec{r}_2,\omega) \approx \frac{-i\omega}{2\pi c}\iint_{\Sigma_1} \vec{\tilde{E}}_{\perp}(\vec{r}_1,\omega)\frac{\exp[i\omega|\vec{r}_2-\vec{r}_1|/c]}{|\vec{r}_2-\vec{r}_1|}d\Sigma_1$$

Fourier Optics

Propagation through **Free Space**:

$\vec{r}_1$ and $\vec{r}_2$ belong to parallel planes perpendicular to optical axis (Z)

$$|\vec{r}_2-\vec{r}_1| = [\Delta z^2 + (x_2-x_1)^2 + (y_2-y_1)]^{1/2} \qquad d\Sigma_1 = dx_1 dy_1$$

Huygens-Fresnel Principle is **Convolution**-type integral, can be calculated using 2D FFT

"Thin" Optical Element:

$$\vec{\tilde{E}}_{\perp after}(x,y,\omega) \approx \mathbf{T}(x,y,\omega)\,\vec{\tilde{E}}_{\perp before}(x,y,\omega)$$

More Generally:

$$\vec{\tilde{E}}_{\perp after}(x_2,y_2,\omega) \approx \mathbf{G}(x_2,y_2,\omega)\exp[i\omega L(x_2,y_2)/c]\,\vec{\tilde{E}}_{\perp before}(x_1(x_2,y_2),y_1(x_2,y_2),\omega)$$

An “Economic” Version of Free-Space Propagator

Huygens-Fresnel Principle:
(paraxial approximation)

$$\tilde{\vec{E}}_{\perp}(\vec{r}_2,\omega) \approx \frac{-i\omega}{2\pi c}\iint_{\Sigma_1} \tilde{\vec{E}}_{\perp}(\vec{r}_1,\omega)\frac{\exp[i\omega|\vec{r}_2-\vec{r}_1|/c]}{|\vec{r}_2-\vec{r}_1|}d\Sigma_1$$

Analytical Treatment of Quadratic Phase Term:

Before Propagation:

$$E_1(x_1,y_1) = F_1(x_1,y_1)\exp\left[ik\frac{(x_1-x_0)^2}{2R_x}+ik\frac{(y_1-y_0)^2}{2R_y}\right]$$

After Propagation:

$$E_2(x_2,y_2) \approx \frac{-ik}{2\pi L}\exp(ikL)\iint_{\Sigma} F_1(x_1,y_1)\exp\left[ik\frac{(x_1-x_0)^2}{2R_x}+ik\frac{(y_1-y_0)^2}{2R_y}+ik\frac{(x_2-x_1)^2+(y_2-y_1)^2}{2L}\right]dx_1dy_1$$

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

$$\times\iint_{\Sigma} F_1(x_1,y_1)\exp\left[ik\frac{R_x+L}{2R_xL}\left(x_1-\frac{R_xx_2+Lx_0}{R_x+L}\right)^2+ik\frac{R_y+L}{2R_yL}\left(y_1-\frac{R_yy_2+Ly_0}{R_y+L}\right)^2\right]dx_1dy_1$$

$$= F_2(x_2,y_2)\exp\left[ik\frac{(x_2-x_0)^2}{2(R_x+L)}+ik\frac{(y_2-y_0)^2}{2(R_y+L)}\right]$$

Wavefront Characterization

Easy Measurable Quantities:

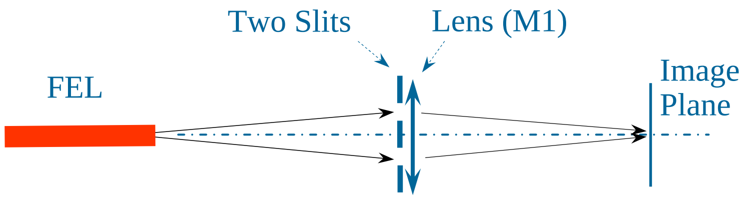
Intensity in Time and Frequency domains (or Power Density and Spectral Fluence) ~ $|\vec{E}(x,y,z_{obs},t)|^2, \quad |\tilde{\vec{E}}(x,y,z_{obs},\omega)|^2$

Fluence ~ $\int |\vec{E}(x,y,z_{obs},t)|^2\, dt = (const)\int |\tilde{\vec{E}}(x,y,z_{obs},\omega)|^2\, d\omega$

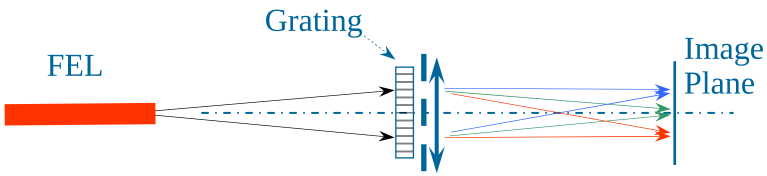
Power and Spectral Energy ~ $\iint |\vec{E}(x,y,z_{obs},t)|^2\, dxdy, \quad \iint |\tilde{\vec{E}}(x,y,z_{obs},\omega)|^2\, dxdy$

Simple Optical Schemes:

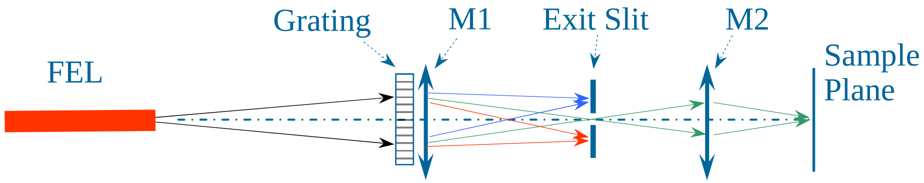
Young's Double-Slit Interference Scheme
- to test Special Coherence



Double-Slit Interference Scheme with Grating
- to test Temporal Coherence



Monochromator + Refocusing Scheme
- often used in VUV / Soft X-Ray Beamlines



Simulation Examples

SASE Pulse Profiles and Spectra at FEL Exit

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

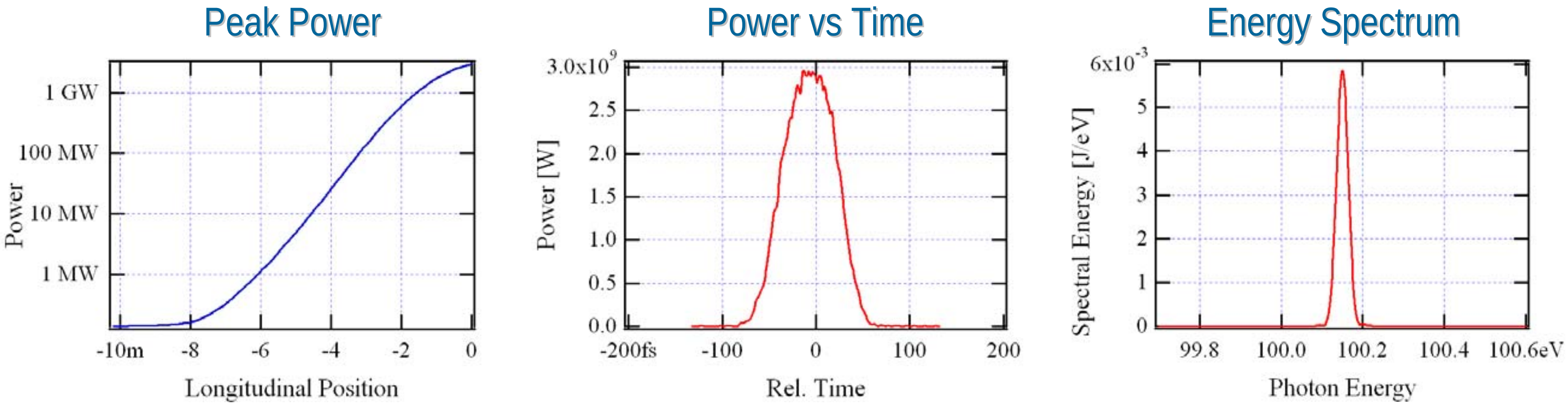
Undulator: $K \sim 2.06$
$\lambda_u = 30$ mm
$L_{tot} \sim 5 \times 2$ m
$\hbar\omega_0 = 100.15$ eV

~ ArcEnCiel (phase II)

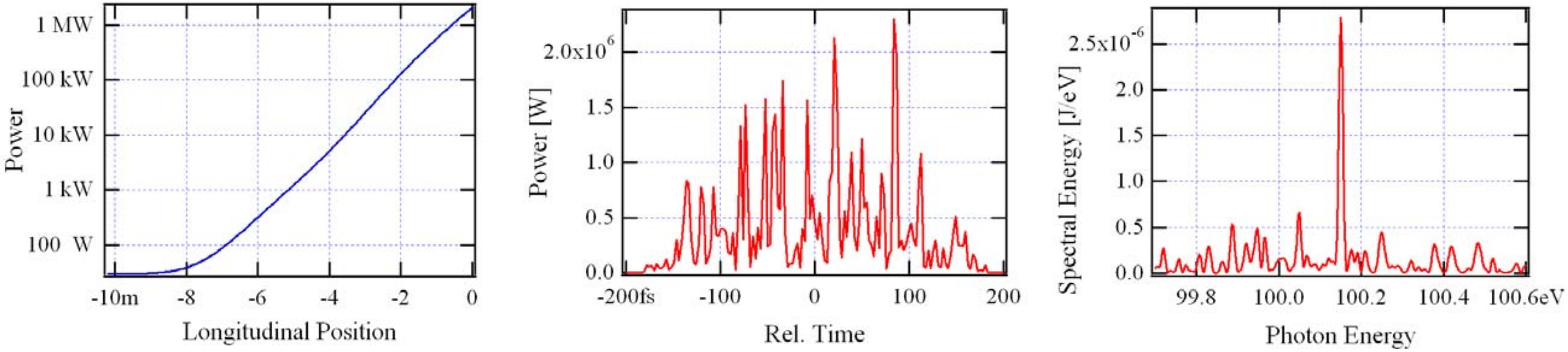
A: Seeded SASE (~ saturated)

$P_{max\ ssed} \sim 50$ kW
$\sigma_{t\ seed} \sim 25$ fs

GENESIS



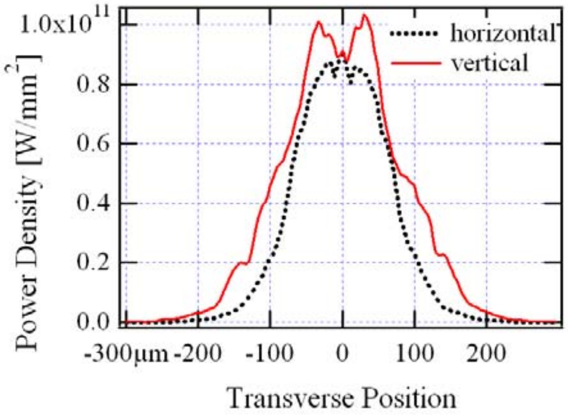
B: SASE Started-Up from Noise (not saturated)



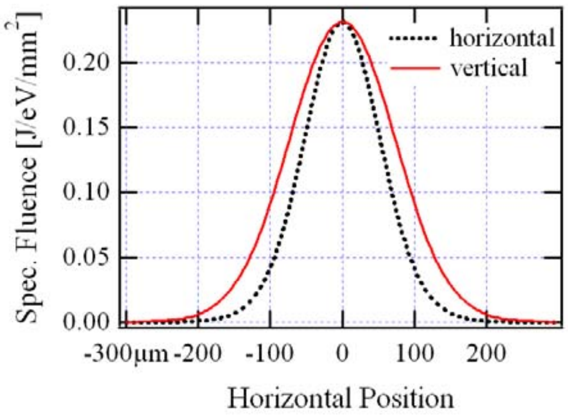
Intensity Distributions at FEL Exit

A: Seeded SASE (~ saturated)

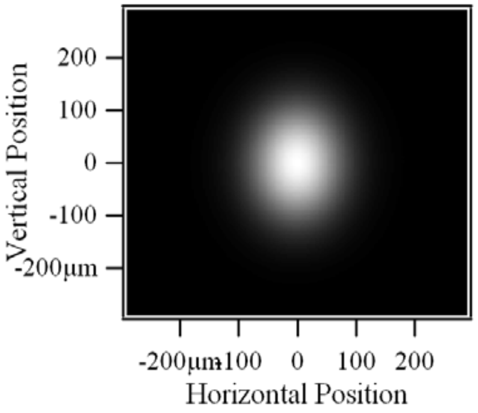
Power Density Cuts at Pulse Center



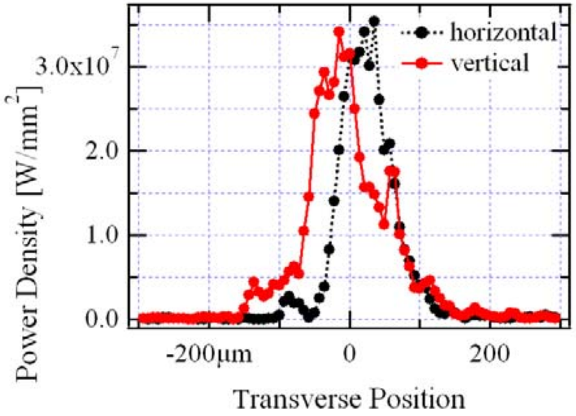
Peak Spectral Fluence Transverse Cuts

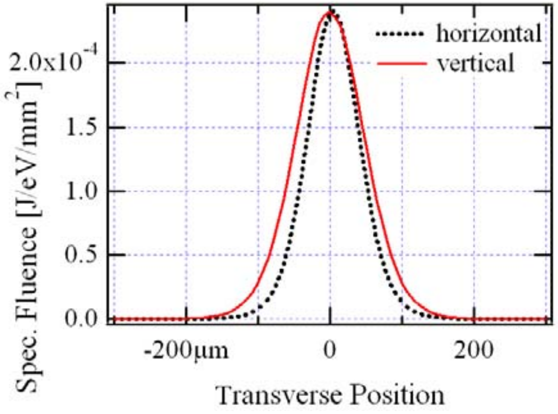


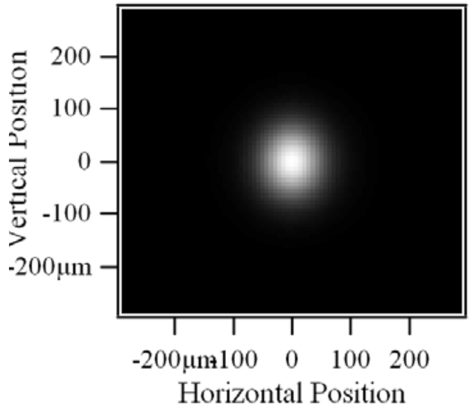
Fluence



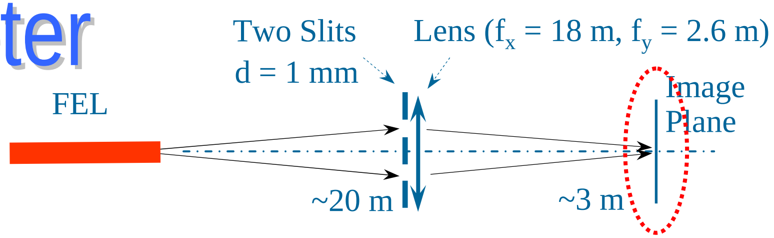
B: SASE Started-Up from Noise (not saturated)







Wavefront Characteristics in the Image Plane of Young's 2-Slit Interferometer



Two Slits
d = 1 mm

Lens (f_x = 18 m, f_y = 2.6 m)

FEL

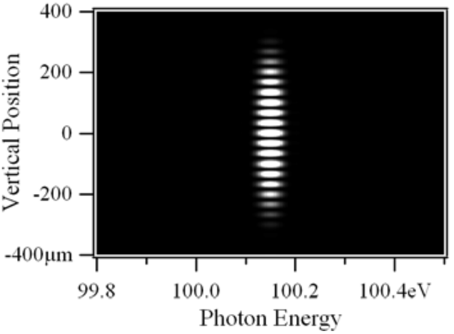
Image Plane

~20 m

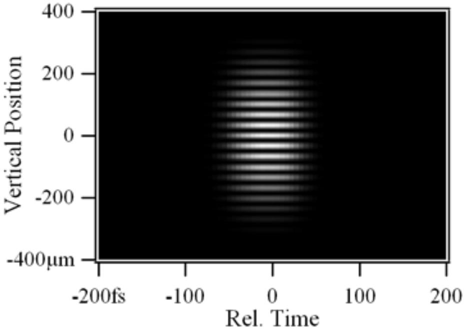
~3 m

A: Seeded SASE (~ saturated)

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

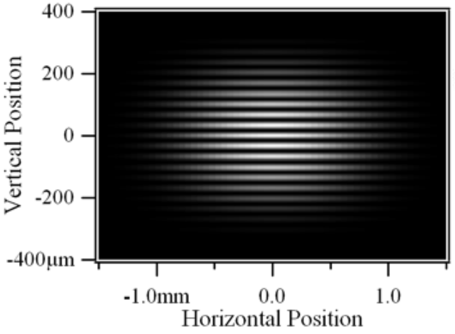


Power Density
vs Time
and Vertical Position (at *x* = 0)

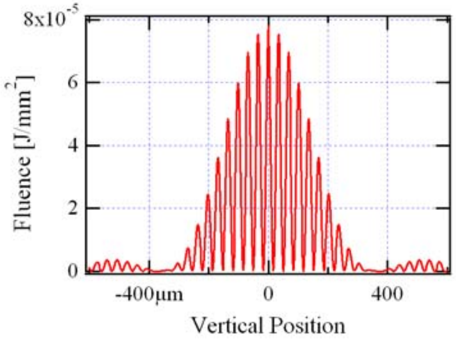


Fluence (/Time-Integrated Intensity)

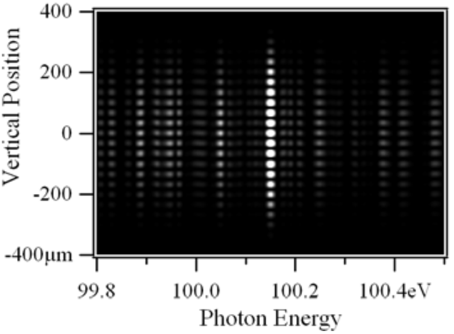
vs Horiz. and Vert. Positions

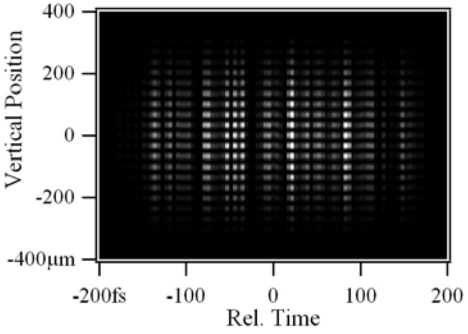


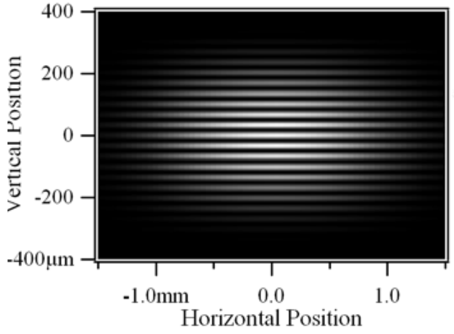
vs Vert. Position (at *x* = 0)

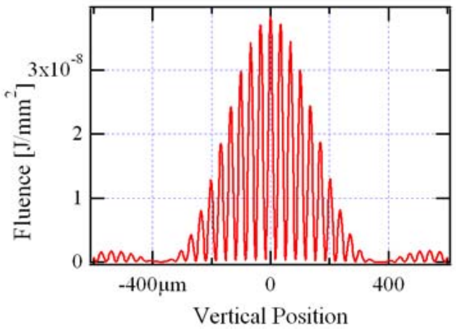


B: SASE Started-Up from Noise (not saturated)





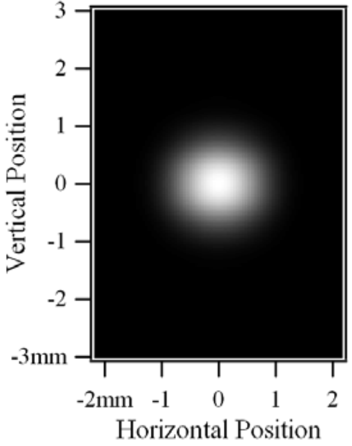




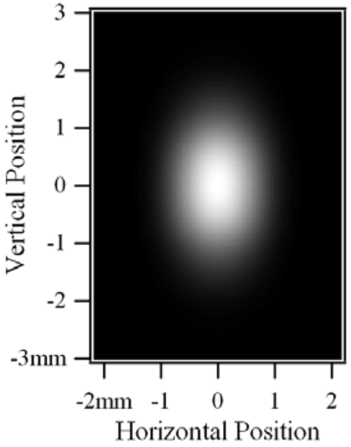
Effect of Grating: Seeded SASE Wavefront Before and Immediately After Grating

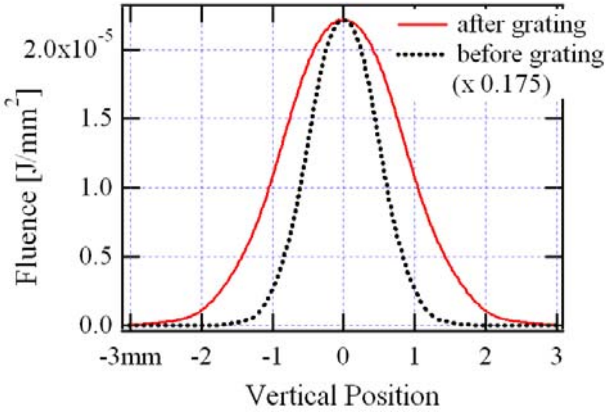
Fluence in Transverse Planes Perpendicular to Optical Axis

Before Grating

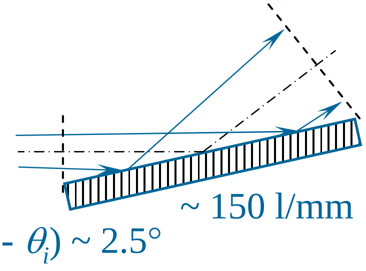


After Grating





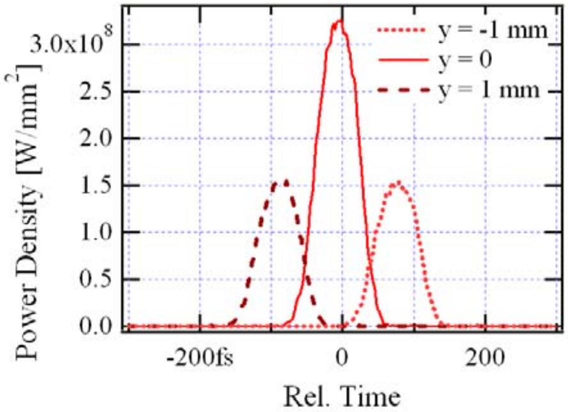
Plane Grating



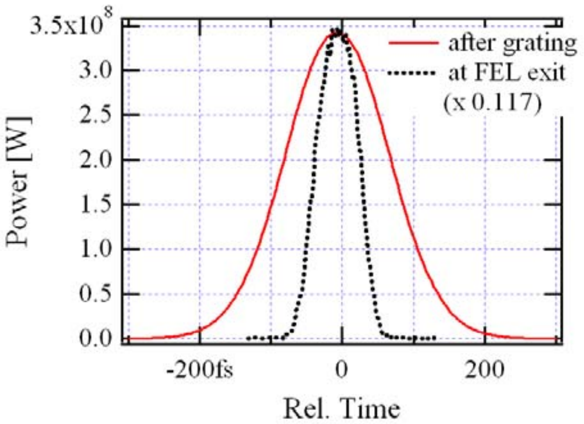
$$m\lambda = d[\sin\theta_m + \sin(\theta_i)]$$

Power Density After Grating

at Different Vertical Positions

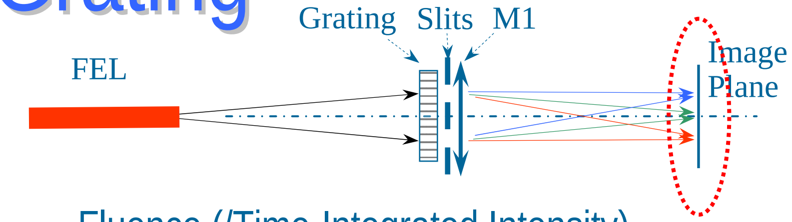


Power vs Time



Simulation Examples

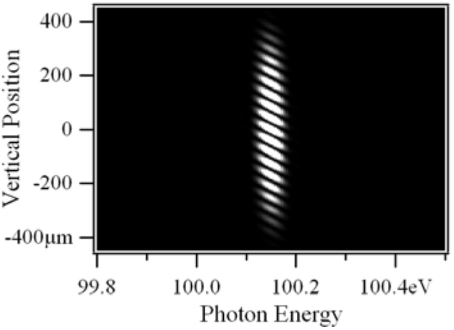
Wavefront Characteristics in the Image Plane of a 2-Slit Interferometer with Grating



A: Seeded

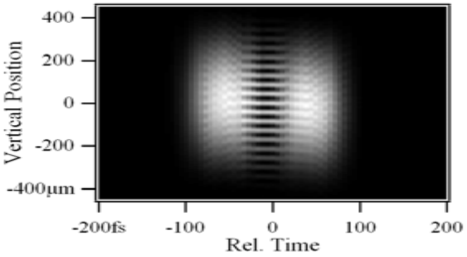
Spectral Fluence

vs Photon Energy
and Vertical Position (at *x* = 0)

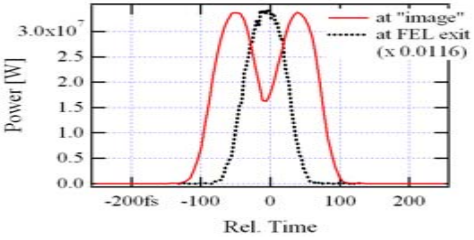


Power Density

vs Time and Vert. Pos. (at *x* = 0)



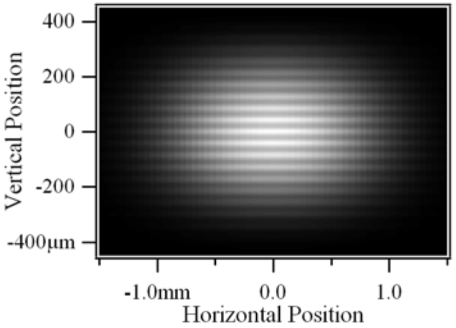
Power vs Time

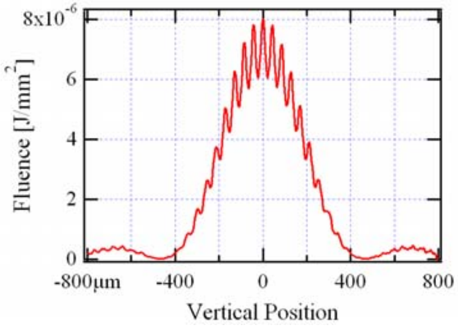


Fluence (/Time-Integrated Intensity)

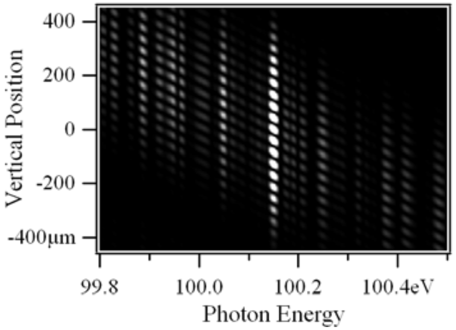
vs Horiz. and Vert. Positions

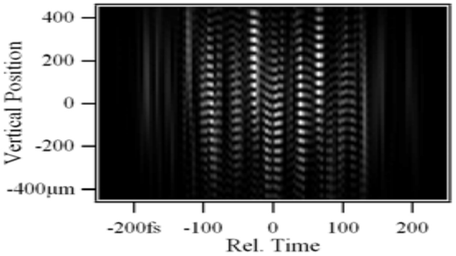
vs Vert. Position (at *x* = 0)

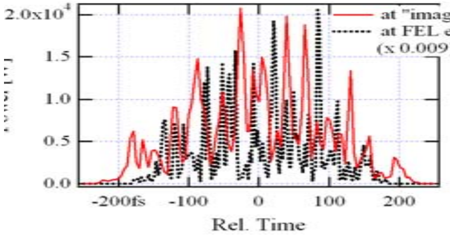


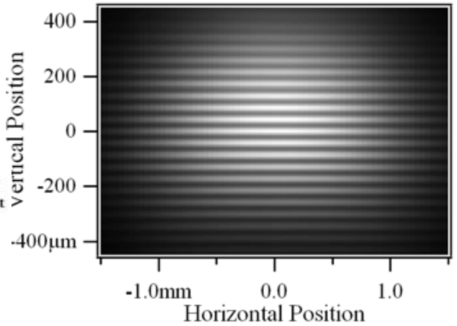


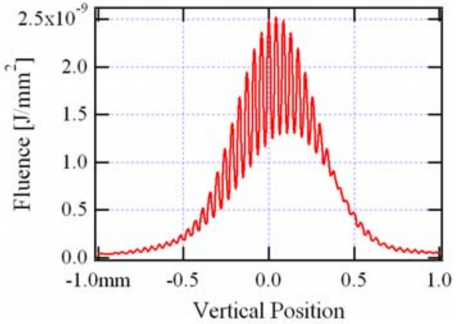
B: Started from Noise



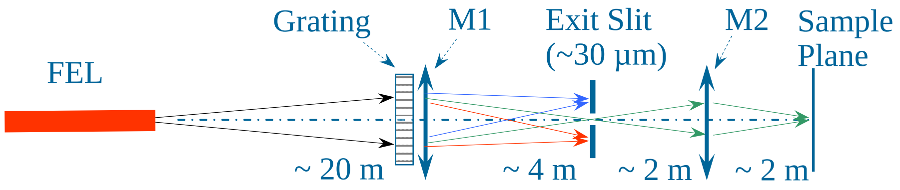




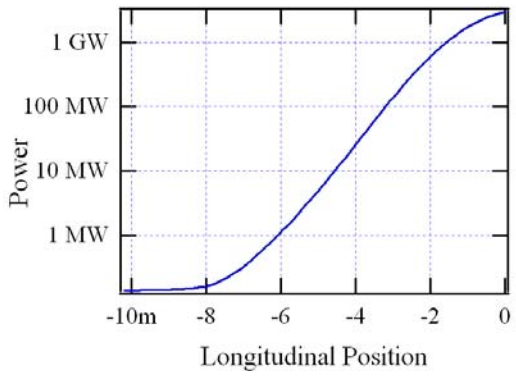


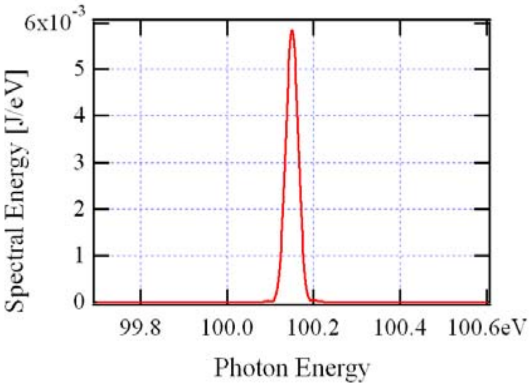


Wavefront Cases for Simulation of Propagation through a Monochromator

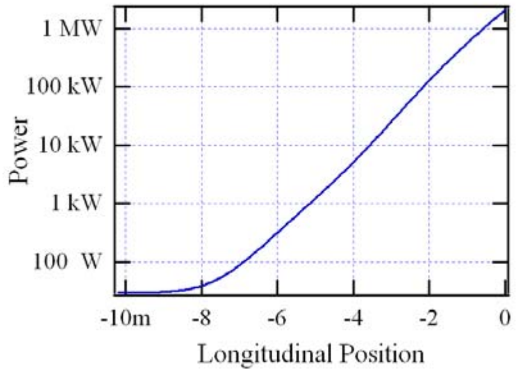


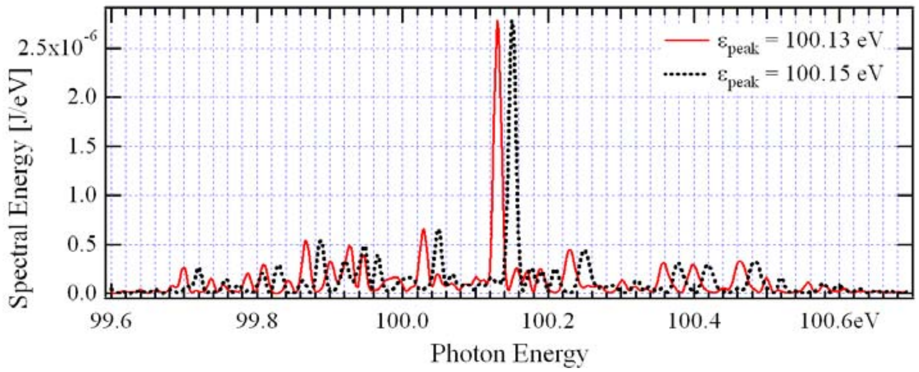
A: Seeded SASE (~ saturated)





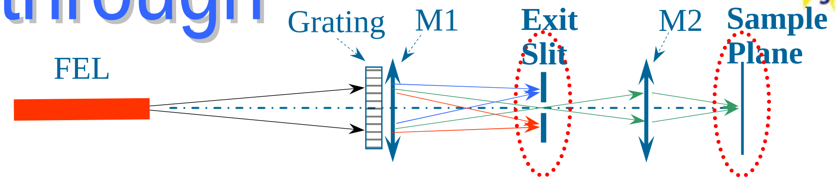
B, C: SASE Started-Up from Noise: 2 Cases with slightly shifted Spectra



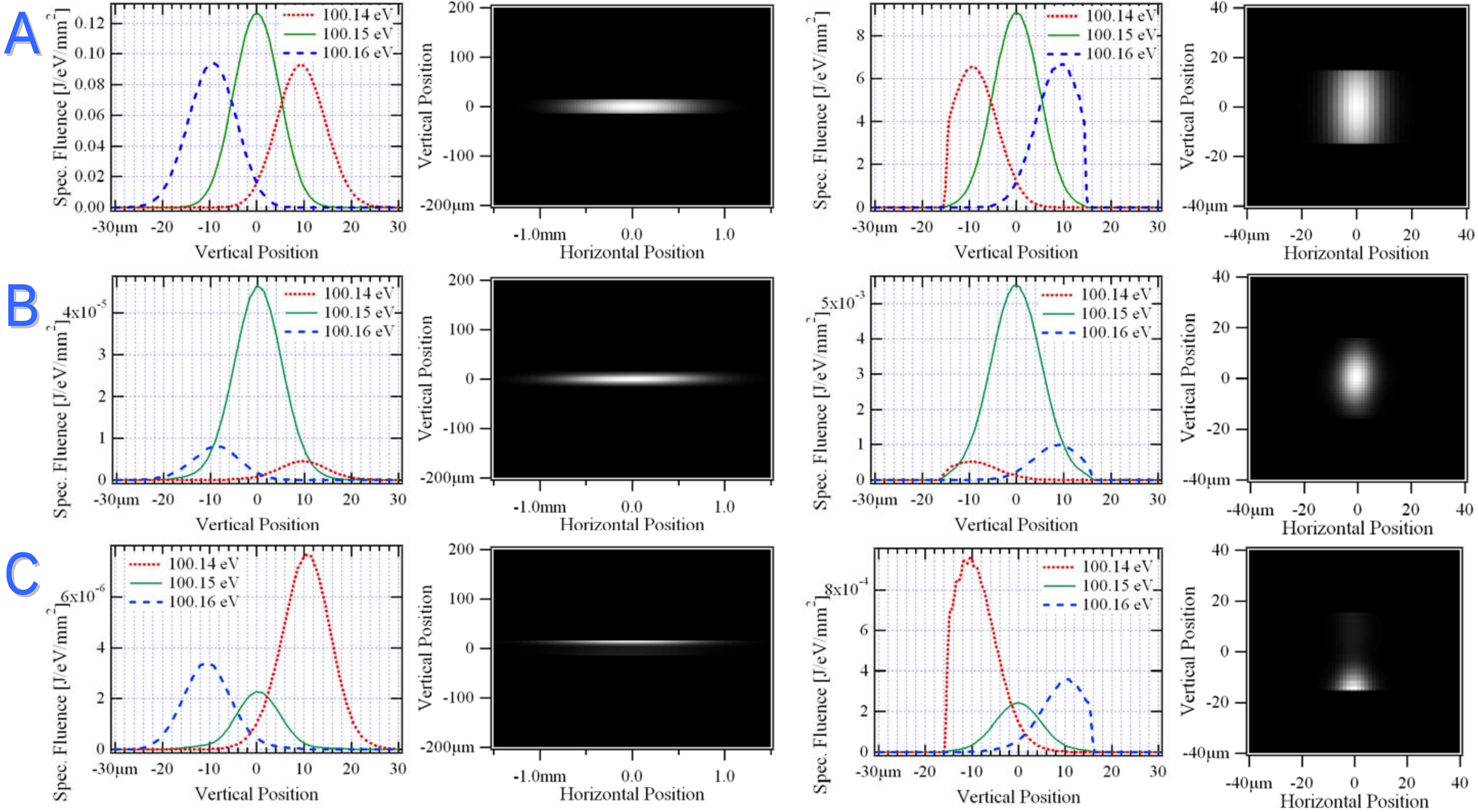


Simulation Examples

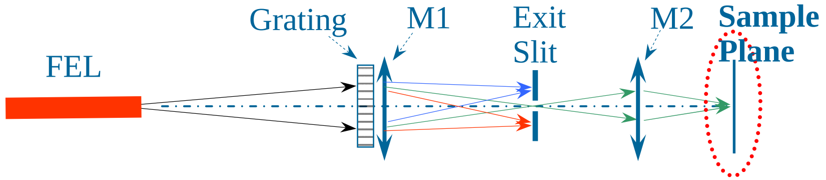
Wavefront Propagation through a Monochromator



Spectral Fluence Before Exit Slit (vert. cuts at x = 0) | Fluence After Exit Slit | Spectral Fluence at Sample (vert. cuts at x = 0) | Fluence at Sample



Wavefront Characteristics at “Sample” Plane of a Monochromator

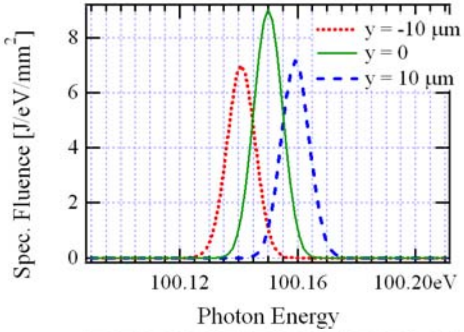


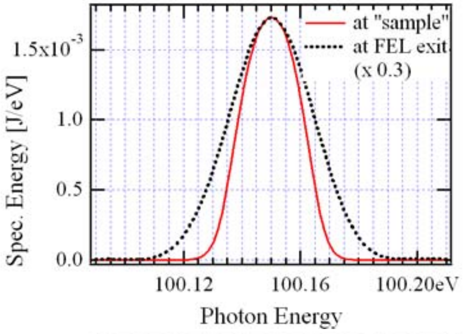
Spectral Fluence
(vs photon energy, at x = 0)

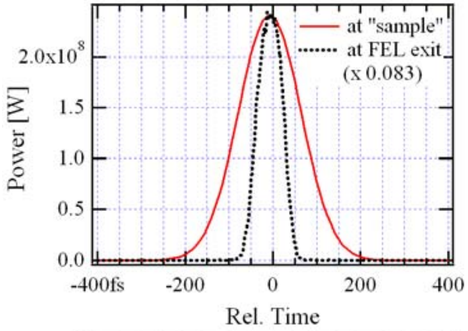
Energy Spectrum

Power

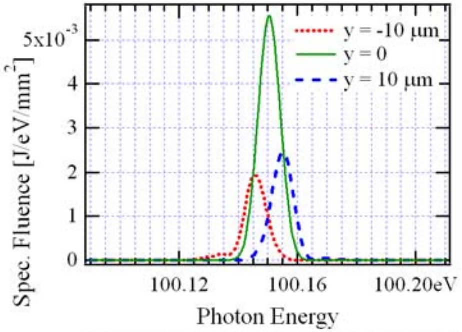
A

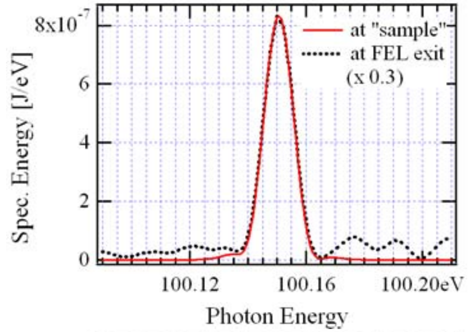


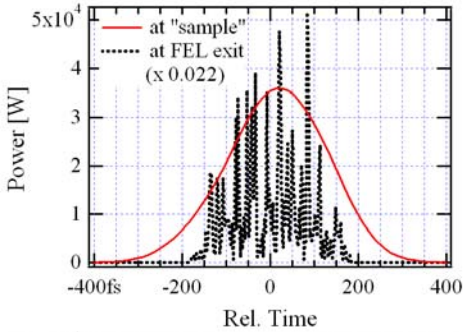




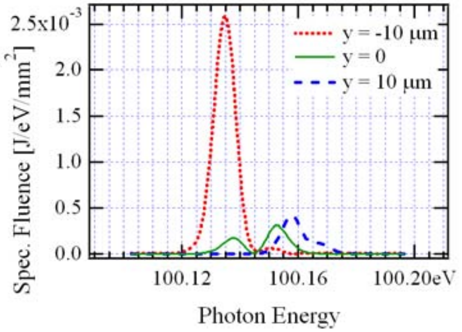
B

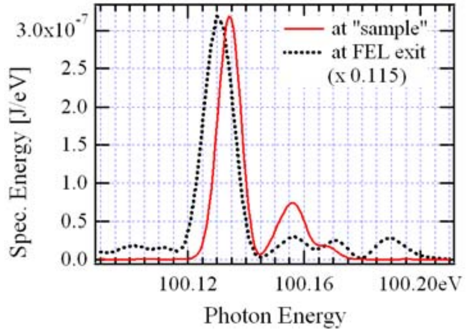


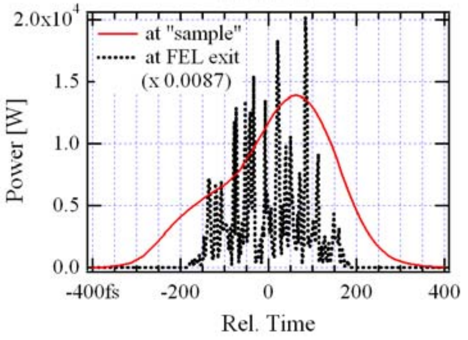




C







Practical Aspects of Simulations

- All examples were calculated on a **regular PC** with **1 GB** of RAM (32-bit Windows)

- An **entire wavefront** sampled vs Photon Energy (/Time), Horizontal and Vertical Positions (/Angles) was kept **in memory** during propagation

  - typical sampling: ~**300 (phot. en.)** x 400 (h. pos.) x 400 (v. pos)
  - extensive use of **Resizing / Resampling** at each step of propagation
  - propagation simulations took ~40 times less CPU time than calculation of original SASE wavefronts

- To facilitate data exchange and automation of simulations, **GENESIS** 1.3 has been **integrated into** Emission part of **SRW** (after conversion by “F2C”)

- Front-End used by SRW: **IGOR Pro**

  - powerful scripting environment (easy to sequence / automate simulations)
  - “instant” graphics / visualization

Acknowledgements

- J.-L. Laclare, P. Elleaume, A. Snigirev (ESRF)
- P. Dumas, P. Roy (SOLEIL)
- G. Williams (JLab)
- M. Bowler (4GLS)
- N. Vinokurov, O. Shevchenko (BINP)
- E. Saldin (DESY)

- EuroFEL
- All Users of SRW and RADIA