



1ST **OASYS** SCHOOL:

THE SRW PROPAGATORS

R. Celestre

rafael.celestre@esrf.eu

X-ray optics group

Instrumentation Services and Development Division

ESRF – The European Synchrotron

“SYNCHROTRON RADIATION WORKSHOP” – ELECTRODYNAMICS SIMULATION CODE FOR SR EMISSION AND PROPAGATION

First official version of SRW was developed at ESRF in 1997-98 (written in C++, interfaced to IGOR Pro); PASCAL ELLAUME and OLEG CHUBAR, "Accurate and efficient computation of synchrotron radiation in the near field region", Proc. EPAC-98, 1177-1179 (1998).

SRW was **released to Open Source** in 2012 under BSD type license.



U.S. DEPARTMENT OF
ENERGY

BROOKHAVEN
NATIONAL LABORATORY

The **main Open Source repository**, containing all C/C++ sources, C API, all interfaces and project development files, is on GitHub:

<https://github.com/ochubar/SRW>

SRW for Python (2.7.x & 3.x; 32- & 64-bit) cross-platform versions were released in 2012.

SRW development is partially supported by **US DOE SBIR**.



PHYSICAL OPTICS: FREE SPACE PROPAGATION

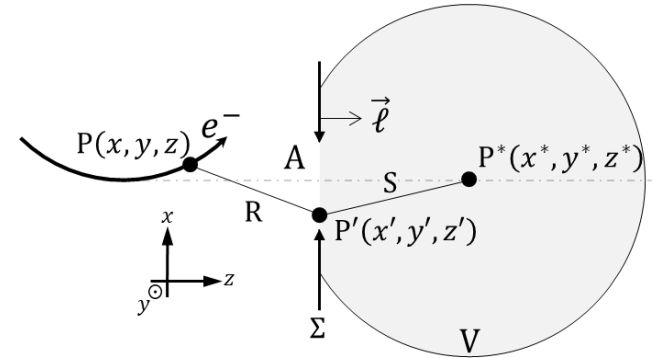
Problem: propagate an arbitrary electric field over a distance in free space.

Assumptions: “fields are propagating in a medium that is uniform, uncharged and non-conducting.”

If: the propagation distance is several times larger than the wavelength λ :

The Huygens-Fresnel principle:

$$U(P^*) = \frac{1}{i\lambda} \iint_A U(P') \frac{\exp(ikS)}{S} \cos \theta \, ds$$



PHYSICAL OPTICS: FREE SPACE PROPAGATION

Problem: propagate an arbitrary electric field over a distance in free space.

Assumptions: “fields are propagating in a medium that is uniform, uncharged and non-conducting.”

If: the propagation distance is several times larger than the wavelength λ :

The Huygens-Fresnel principle:

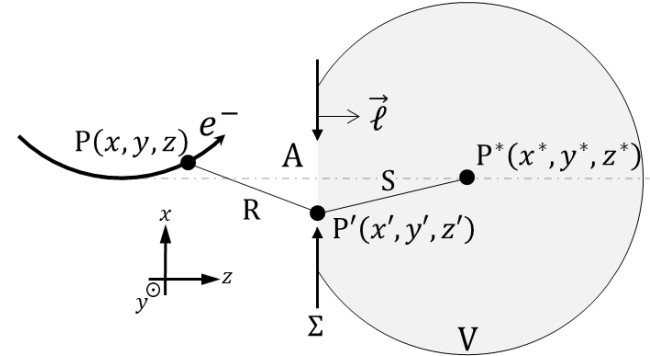
$$U(P^*) = \frac{1}{i\lambda} \iint_A U(P') \frac{\exp(ikS)}{S} \cos \theta \, ds$$

The Fresnel approximation:

a) $z^2 \gg (x^* - x')^2 + (y^* - y')^2$;

b) binomial expansion of the square root:

$$U(P^*) = \frac{e^{ikz}}{i\lambda z} \iint_{-\infty}^{\infty} U(P') \exp \left\{ i \frac{k}{2z} [(x^* - x')^2 + (y^* - y')^2] \right\} dx' dy'$$



PHYSICAL OPTICS: FREE SPACE PROPAGATION

Problem: propagate an arbitrary electric field over a distance in free space.

Assumptions: “fields are propagating in a medium that is uniform, uncharged and non-conducting.”

If: the propagation distance is several times larger than the wavelength λ :

The Huygens-Fresnel principle:

$$U(P^*) = \frac{1}{i\lambda} \iint_A U(P') \frac{\exp(ikS)}{S} \cos \theta \, ds$$

The Fresnel approximation:

a) $z^2 \gg (x^* - x')^2 + (y^* - y')^2$;

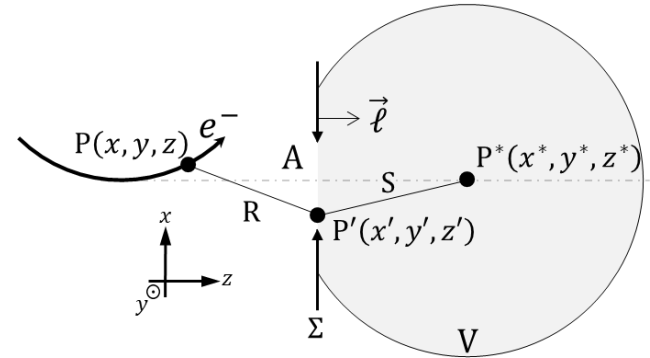
b) binomial expansion of the square root:

$$U(P^*) = \frac{e^{ikz}}{i\lambda z} \iint_{-\infty}^{\infty} U(P') \exp \left\{ i \frac{k}{2z} [(x^* - x')^2 + (y^* - y')^2] \right\} dx' dy'$$

The Fraunhofer approximation:

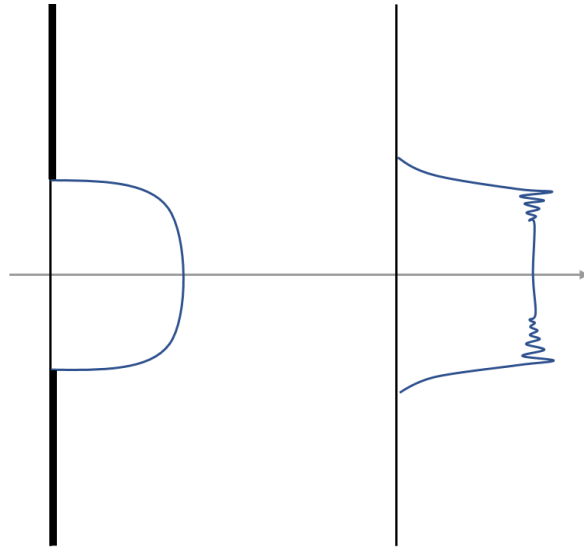
a) $z \gg \frac{k(x'^2 + y'^2)_{\max}}{2}$.

$$U(P^*) = \frac{e^{ikz} e^{i \frac{k}{2z} (x^{*2} + y^{*2})}}{i\lambda z} \iint_{-\infty}^{\infty} U(P') \exp \left[-i \frac{2\pi}{\lambda z} (x^* x' + y^* y') \right] dx' dy'$$

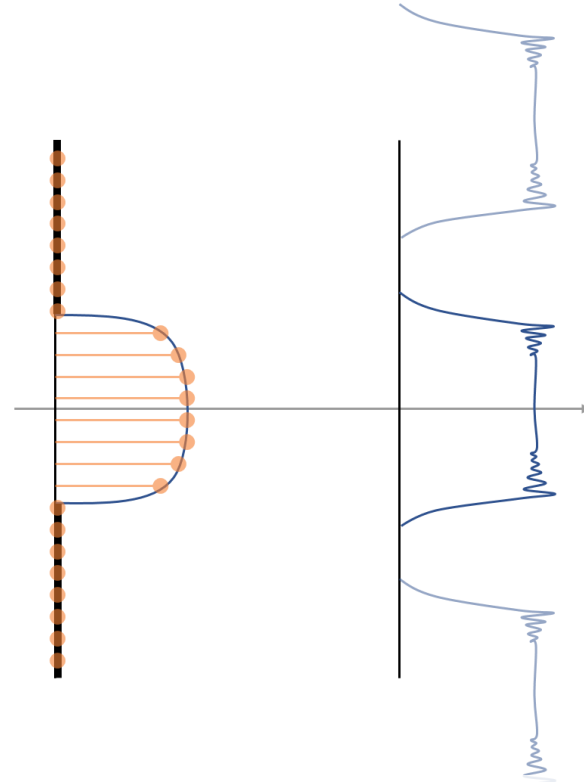


PHYSICAL OPTICS: FREE SPACE PROPAGATION

Issues: when calculating numerically the convolution-type or the Fourier transformation-type integrals **replicas** and **aliasing** occur:



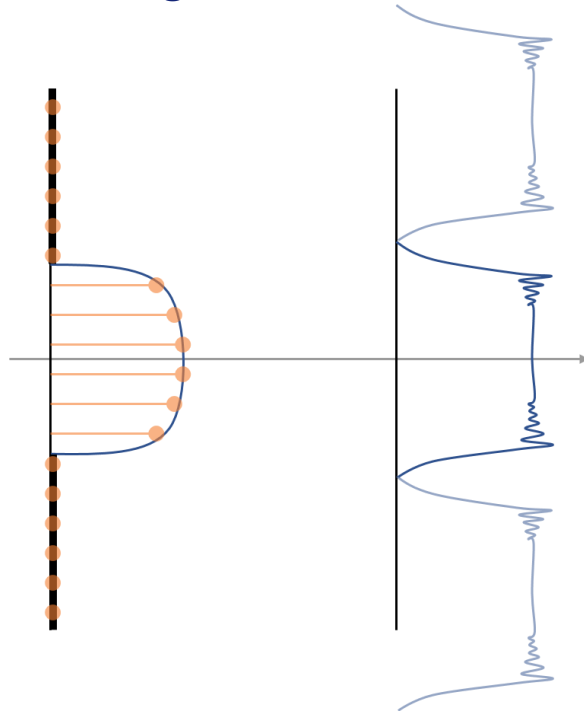
(a) analytical solution



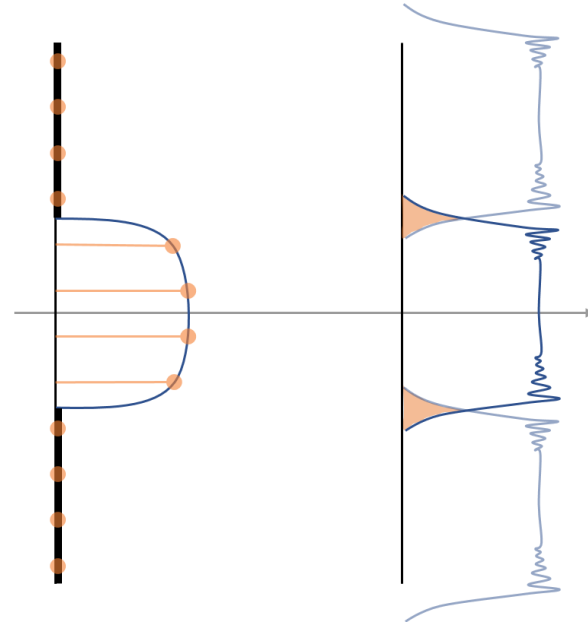
(b) sampling effect (replicas)

PHYSICAL OPTICS: FREE SPACE PROPAGATION

Issues: when calculating numerically the convolution-type or the Fourier transformation-type integrals **replicas** and **aliasing** occur:

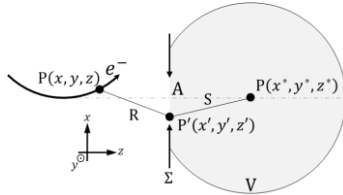


(a) sampling effect (replicas)

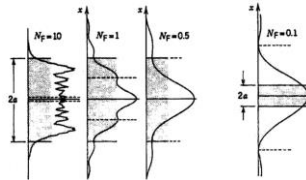
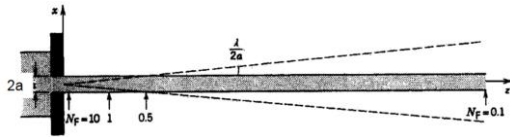


(b) undersampling effect (aliasing)

$$\begin{aligned}
 \nabla \cdot \mathbf{D} &= \cancel{\rho}^0 \\
 \nabla \cdot \mathbf{B} &= 0 \\
 \nabla \times \mathbf{E} &= -\frac{\partial \mathbf{B}}{\partial t} \\
 \nabla \times \mathbf{H} &= \cancel{\mathbf{J}}^0 + \frac{\partial \mathbf{D}}{\partial t}
 \end{aligned}$$



$$\vec{E}_{\omega\perp}(P^*) \approx \frac{-ik}{2\pi} \iint_A \vec{E}_{\omega\perp}(P') \frac{\exp(ikS)}{S} \cos\theta \, ds$$



THE SRW PROPAGATORS

#0 – STANDARD FRESNEL PROPAGATOR

Short description: standard Fresnel propagator calculated by using the convolution theorem (product of spectrums). Uses two FFT.

$$\vec{E}_2(x_2, y_2) \approx \frac{k}{2\pi i L} \iint \vec{E}_1(x_1, y_1) \cdot \overbrace{\exp\{ik\sqrt{L^2 + (x_2 - x_1)^2 + (y_2 - y_1)^2}\}}^K dx_1 dy_1$$

$$\begin{aligned} \Rightarrow g(x, y) * h(x, y) &= \iint_{-\infty}^{\infty} g(\xi, \eta) \cdot h(x - \xi, y - \eta) d\xi d\eta \\ &= \mathcal{F}^{-1}\{\mathcal{F}\{g(x, y)\} \cdot \mathcal{F}\{h(x, y)\}\} \end{aligned}$$

$$\boxed{\vec{E}_2(x_2, y_2) \propto \mathcal{F}^{-1}\{\mathcal{F}\{\vec{E}_1(x_1, y_1)\} \cdot \mathcal{F}\{K\}\}}$$

has analytical Fourier transform

Auto Resize Before Propagation	No
Auto Resize After Propagation	No
Relative precision for propagation with autoresizing (1.0 is nominal)	1.0
Propagator	Standard
Do any resizing on fourier side using fft	No
H range modification factor at resizing	1.0
H resolution modification factor at resizing	1.0
V range modification factor at resizing	1.0
V resolution modification factor at resizing	1.0

#0 – STANDARD FRESNEL PROPAGATOR

Short description: standard Fresnel propagator calculated by using the convolution theorem (product of spectrums). Uses two FFT.

$$\vec{E}_2(x_2, y_2) \approx \frac{k}{2\pi i L} \iint \vec{E}_1(x_1, y_1) \cdot \exp \left\{ i k \sqrt{L^2 + (x_2 - x_1)^2 + (y_2 - y_1)^2} \right\} dx_1 dy_1$$

$$\begin{aligned} \Rightarrow g(x, y) * h(x, y) &= \iint_{-\infty}^{\infty} g(\xi, \eta) \cdot h(x - \xi, y - \eta) d\xi d\eta \\ &= \mathcal{F}^{-1} \{ \mathcal{F}\{g(x, y)\} \cdot \mathcal{F}\{h(x, y)\} \} \end{aligned}$$

$$\vec{E}_2(x_2, y_2) \propto \mathcal{F}^{-1} \left\{ \mathcal{F}\{\vec{E}_1(x_1, y_1)\} \cdot \mathcal{F}\{K\} \right\}$$

has analytical Fourier transform

Auto Resize Before Propagation	No
Auto Resize After Propagation	No
Relative precision for propagation with autoresizing (1.0 is nominal)	1.0
Propagator	Standard
Do any resizing on fourier side using fft	No
H range modification factor at resizing	1.0
H resolution modification factor at resizing	1.0
V range modification factor at resizing	1.0
V resolution modification factor at resizing	1.0

General use:

- propagation over a drift-space with gentle (de)magnification;
- before slits, ideal lenses and smooth phase elements.

Comments:

- preserves number of pixel and ranges;
- given proper sampling, can be used for focusing;
- works for strongly astigmatic systems.

#1 – FRESNEL WITH ANALYTICAL TREATMENT OF THE QUADRATIC PHASE TERMS

Short description: before applying the convolution theorem, the quadratic phase term of the wavefront is removed, to relax sampling requirements. Uses two FFT.

$$\vec{E}_1(x_1, y_1) = \vec{F}_1(x_1, y_1) \exp \left\{ ik \left[\left(\frac{x_1 - x_0}{2R_x} \right)^2 + \left(\frac{y_1 - y_0}{2R_y} \right)^2 \right] \right\}$$

$$\vec{E}_2(x_2, y_2) \approx \frac{k}{2\pi i L} \exp \left\{ ik \left[L + \frac{(x_2 - x_0)^2}{2(R_x + L)} + \frac{(y_2 - y_0)^2}{2(R_y + L)} \right] \right\} \cdot K'$$

$$\cdot \iint \vec{F}_1(x_1, y_1) \cdot \exp \left\{ ik \left[\frac{R_x + L}{2R_x L} \left(x_1 - \frac{R_x x_2 + L x_0}{R_x + L} \right) + \frac{R_y + L}{2R_y L} \left(y_1 - \frac{R_y y_2 + L y_0}{R_y + L} \right) \right] \right\} dx_1 dy_1$$

$$\boxed{\vec{E}_2(x_2, y_2) \propto \mathcal{F}^{-1} \left\{ \mathcal{F} \{ \vec{F}_1(x_1, y_1) \} \cdot \mathcal{F} \{ K' \} \right\}}$$

has analytical Fourier transform

Auto Resize Before Propagation	No
Auto Resize After Propagation	No
Relative precision for propagation with autoresizing (1.0 is nominal)	1.0
Propagator	Quadratic Term
Do any resizing on fourier side using fft	No
H range modification factor at resizing	1.0
Resolution modification factor at resizing	1.0
Resolution modification factor at resizing	1.0
Resolution modification factor at resizing	1.0

#1 – FRESNEL WITH ANALYTICAL TREATMENT OF THE QUADRATIC PHASE TERMS

Short description: before applying the convolution theorem, the quadratic phase term of the wavefront is removed, to relax sampling requirements. Uses two FFT.

$$\vec{E}_1(x_1, y_1) = \vec{F}_1(x_1, y_1) \exp \left\{ ik \left[\left(\frac{x_1 - x_0}{2R_x} \right)^2 + \left(\frac{y_1 - y_0}{2R_y} \right)^2 \right] \right\}$$

$$\vec{E}_2(x_2, y_2) \approx \frac{k}{2\pi i L} \exp \left\{ ik \left[L + \frac{(x_2 - x_0)^2}{2(R_x + L)} + \frac{(y_2 - y_0)^2}{2(R_y + L)} \right] \right\} \cdot K'$$

$$\cdot \iint \vec{F}_1(x_1, y_1) \cdot \exp \left\{ ik \left[\frac{R_x + L}{2R_x L} \left(x_1 - \frac{R_x x_2 + L x_0}{R_x + L} \right) + \frac{R_y + L}{2R_y L} \left(y_1 - \frac{R_y y_2 + L y_0}{R_y + L} \right) \right] \right\} dx_1 dy_1$$

$$\boxed{\vec{E}_2(x_2, y_2) \propto \mathcal{F}^{-1} \left\{ \mathcal{F} \{ \vec{F}_1(x_1, y_1) \} \cdot \mathcal{F} \{ K' \} \right\}}$$

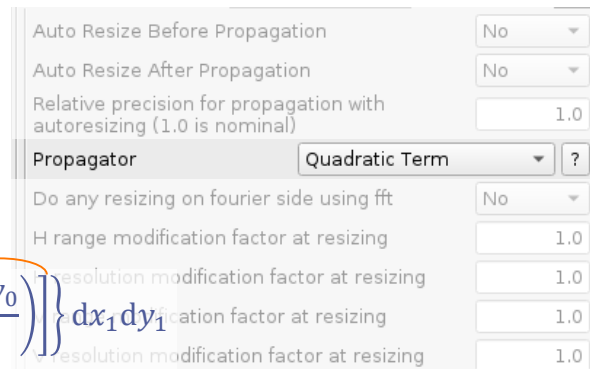
has analytical Fourier transform

General use:

- propagation over a drift-spaces in general;
- before complex optical elements (e.g. curved mirrors).

Comments:

- preserves number of pixel, ranges are recalculated to accommodate the wavefront;
- can be used for or from focusing;
- works for strongly astigmatic systems.



#2 – FRESNEL WITH ANALYTICAL TREATMENT OF THE QUADRATIC PHASE TERMS WITH DIFFERENT PROCESSING NEAR THE WAIST

Short description: before applying the convolution theorem, the quadratic phase term of the wavefront is removed, to relax sampling requirements. Uses two FFT.

$$\vec{E}_1(x_2, y_2) = \vec{F}_1(x_1, y_1) \exp \left\{ ik \left[\left(\frac{x_1 - x_0}{2R_x} \right)^2 + \left(\frac{y_1 - y_0}{2R_y} \right)^2 \right] \right\}$$

$$\vec{E}_2(x_2, y_2) \propto \mathcal{F}^{-1} \left\{ \mathcal{F} \{ \vec{F}_1(x_1, y_1) \} \cdot \mathcal{F} \{ K' \} \right\}$$

has analytical Fourier transform

→ Different calculation of R_x and R_y ; → Different processing near the waist;

Auto Resize Before Propagation	No
Auto Resize After Propagation	No
Relative precision for propagation with autoresizing (1.0 is nominal)	1.0
Propagator	Quadratic Term Special ?
Do any resizing on fourier side using fft	No
H range modification factor at resizing	1.0
H resolution modification factor at resizing	1.0
V range modification factor at resizing	1.0
V resolution modification factor at resizing	1.0

#2 – FRESNEL WITH ANALYTICAL TREATMENT OF THE QUADRATIC PHASE TERMS WITH DIFFERENT PROCESSING NEAR THE WAIST

Short description: before applying the convolution theorem, the quadratic phase term of the wavefront is removed, to relax sampling requirements. Uses two FFT.

$$\vec{E}_1(x_2, y_2) = \vec{F}_1(x_1, y_1) \exp \left\{ ik \left[\left(\frac{x_1 - x_0}{2R_x} \right)^2 + \left(\frac{y_1 - y_0}{2R_y} \right)^2 \right] \right\}$$

$$\vec{E}_2(x_2, y_2) \propto \mathcal{F}^{-1} \left\{ \mathcal{F} \{ \vec{F}_1(x_1, y_1) \} \cdot \mathcal{F} \{ K' \} \right\}$$

has analytical Fourier transform

→ Different calculation of R_x and R_y ; → Different processing near the waist;

General use:

- propagation over a drift-spaces in general;
- specially adequate when (strongly astigmatic) wavefront is being focused or emerging from very small slits;
- strong diffracting elements (gratings).

Comments:

- preserves number of pixel, ranges are recalculated to accommodate the wavefront;
- can be used for or from focusing;
- works for strongly astigmatic systems.

Auto Resize Before Propagation	No
Auto Resize After Propagation	No
Relative precision for propagation with autoresizing (1.0 is nominal)	1.0
Propagator	Quadratic Term Special ?
Do any resizing on fourier side using fft	No
H range modification factor at resizing	1.0
H resolution modification factor at resizing	1.0
V range modification factor at resizing	1.0
V resolution modification factor at resizing	1.0

#3 – PROPAGATION FROM A WAIST OVER A ~LARGE DISTANCE

Short description: Propagator based on the far field approximation (Fraunhofer). Uses 1 FFT.

$$\vec{E}_2(x_2, y_2) \approx \frac{k}{2\pi i L} e^{ikL} e^{i\frac{k}{2L}(x_2^2 + y_2^2)} \iint \vec{E}_1(x_1, y_1) \cdot \exp\left[-\frac{ik}{L}(x_2 x_1 + y_2 y_1)\right] d\xi d\eta$$

$$\Rightarrow \mathcal{F}\{g(x, y)\}(f_x, f_y) = \iint_{-\infty}^{\infty} g(\xi, \eta) \cdot \exp[-i2\pi(f_x \xi + f_y \eta)] d\xi d\eta$$

$$\boxed{\vec{E}_2(x_2, y_2) \propto \mathcal{F}\{\vec{E}_1(x_1, y_1)\}}$$

Auto Resize Before Propagation	No
Auto Resize After Propagation	No
Relative precision for propagation with autoresizing (1.0 is nominal)	1.0
Propagator	From Waist ?
Do any resizing on fourier side using fft	No
H range modification factor at resizing	1.0
H resolution modification factor at resizing	1.0
V range modification factor at resizing	1.0
V resolution modification factor at resizing	1.0

#3 – PROPAGATION FROM A WAIST OVER A ~LARGE DISTANCE

Short description: Propagator based on the far field approximation (Fraunhofer). Uses 1 FFT.

$$\vec{E}_2(x_2, y_2) \approx \frac{k}{2\pi i L} e^{ikL} e^{i\frac{k}{2L}(x_2^2 + y_2^2)} \iint \vec{E}_1(x_1, y_1) \cdot \exp\left[-\frac{ik}{L}(x_2 x_1 + y_2 y_1)\right] d\xi d\eta$$

$$\Rightarrow \mathcal{F}\{g(x, y)\}(f_x, f_y) = \iint_{-\infty}^{\infty} g(\xi, \eta) \cdot \exp[-i2\pi(f_x \xi + f_y \eta)] d\xi d\eta$$

$$\boxed{\vec{E}_2(x_2, y_2) \propto \mathcal{F}\{\vec{E}_1(x_1, y_1)\}}$$

Auto Resize Before Propagation	No
Auto Resize After Propagation	No
Relative precision for propagation with autoresizing (1.0 is nominal)	1.0
Propagator	From Waist
Do any resizing on fourier side using fft	No
H range modification factor at resizing	1.0
H resolution modification factor at resizing	1.0
V range modification factor at resizing	1.0
V resolution modification factor at resizing	1.0

General use:

- propagation of a wavefront emerging from a focal position in both vertical and horizontal directions;
- output plane several times larger than the input plane.

Comments:

- preserves number of pixel, ranges are recalculated to accommodate the wavefront;
- should be used when the output plane is larger than the input plane;
- fails for strongly astigmatic systems.

#4 – PROPAGATION TO A WAIST

Short description: Propagator based on the far field approximation (Fraunhofer). Uses 1 FFT.

$$\vec{E}_2(x_2, y_2) \approx \frac{k}{2\pi i L} e^{ikL} e^{i\frac{k}{2L}(x_2^2 + y_2^2)} \iint \vec{E}_1(x_1, y_1) \cdot \exp\left[-\frac{ik}{L}(x_2 x_1 + y_2 y_1)\right] d\xi d\eta$$

$$\Rightarrow \mathcal{F}\{g(x, y)\}(f_x, f_y) = \iint_{-\infty}^{\infty} g(\xi, \eta) \cdot \exp[-i2\pi(f_x \xi + f_y \eta)] d\xi d\eta$$

$$\boxed{\vec{E}_2(x_2, y_2) \propto \mathcal{F}\{\vec{E}_1(x_1, y_1)\}}$$

Auto Resize Before Propagation	No
Auto Resize After Propagation	No
Relative precision for propagation with autoresizing (1.0 is nominal)	1.0
Propagator	To Waist ?
Do any resizing on fourier side using fft	No
H range modification factor at resizing	1.0
H resolution modification factor at resizing	1.0
V range modification factor at resizing	1.0
V resolution modification factor at resizing	1.0

#4 – PROPAGATION TO A WAIST

Short description: Propagator based on the far field approximation (Fraunhofer). Uses 1 FFT.

$$\vec{E}_2(x_2, y_2) \approx \frac{k}{2\pi i L} e^{ikL} e^{i\frac{k}{2L}(x_2^2 + y_2^2)} \iint \vec{E}_1(x_1, y_1) \cdot \exp\left[-\frac{ik}{L}(x_2 x_1 + y_2 y_1)\right] d\xi d\eta$$

$$\Rightarrow \mathcal{F}\{g(x, y)\}(f_x, f_y) = \iint_{-\infty}^{\infty} g(\xi, \eta) \cdot \exp[-i2\pi(f_x \xi + f_y \eta)] d\xi d\eta$$

$$\boxed{\vec{E}_2(x_2, y_2) \propto \mathcal{F}\{\vec{E}_1(x_1, y_1)\}}$$

Auto Resize Before Propagation	No
Auto Resize After Propagation	No
Relative precision for propagation with autoresizing (1.0 is nominal)	1.0
Propagator	To Waist ?
Do any resizing on fourier side using fft	No
H range modification factor at resizing	1.0
H resolution modification factor at resizing	1.0
V range modification factor at resizing	1.0
V resolution modification factor at resizing	1.0

General use:

- propagation of a wavefront being focused on both directions.
- output plane several times smaller than the input plane.

Comments:

- preserves number of pixel, ranges are recalculated to accommodate the wavefront;
- should be used when the output plane is smaller than the input plane;
- fails for strongly astigmatic systems.

References (SRW):

- CHUBAR, O. and P. ELLEAUME: *Accurate and efficient computation of synchrotron radiation in the near field region*. Proceedings of the 6th European Particle Accelerator Conference - EPAC-98, pages 1177-1179;
- CHUBAR, O.: *Wavefront calculations*. Proc. SPIE, 4143:48-59, 2001;
- CHUBAR, O., L. BERMAN, Y. S. CHU, A. FLUERASU, S. HULBERT, M. IDIR, K. KAZNATCHEEV, D. SHAPIRO, Q. SHEN and J. BALTZER: *Development of partially-coherent wavefront propagation simulation methods for 3rd and 4th generation synchrotron radiation sources*. Proc. SPIE, 8141:8141-8141-10, 2011;
- CHUBAR, O.: *Recent updates in the "Synchrotron Radiation Workshop" code, on-going developments, simulation activities, and plans for the future*. Proc. SPIE, 9209:9209-9209-10, 2014.

References (wavefront propagation):

- GOODMAN, J. W.: *Foundations of Scalar Diffraction Theory and Fresnel and Fraunhofer Diffraction*. In *Introduction to Fourier Optics*, pages 43-47; 48-120. McGraw-Hill, Fourth edition, 2017.
- KELLY, P. D.: *Numerical calculation of the Fresnel transform*. J. Opt. Soc. Am. A, Vol. 31, No. 4, 755-764, 2014.
- HILLENBRAND, M., P. D. KELLY and S. SINZINGER: *Numerical solution of nonparaxial scalar diffraction integrals for focused fields*. J. Opt. Soc. Am. A, Vol. 31, No. 8, 1832-1841, 2014.

Acknowledgment:



The speaker thanks Oleg Chubar for fruitful discussions on wave propagation and physical optics.