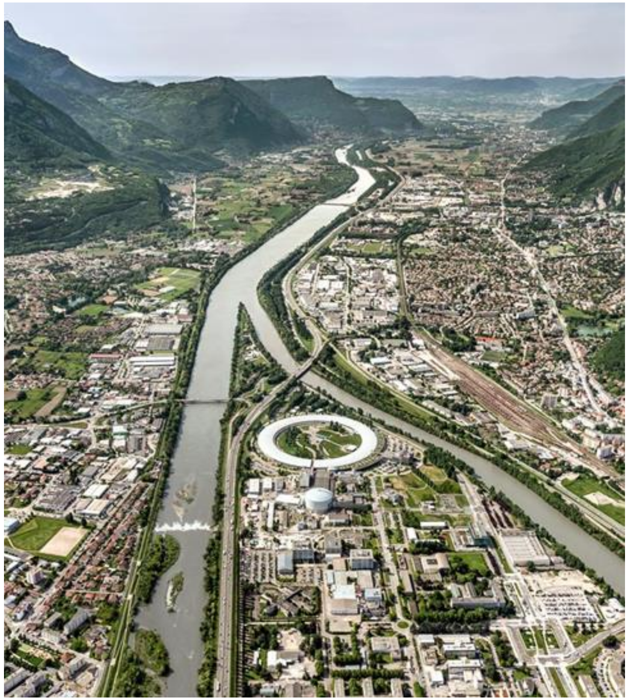

1ST OASYS SCHOOL:

THE SRW PROPAGATORS

R. Celestre

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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.

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.

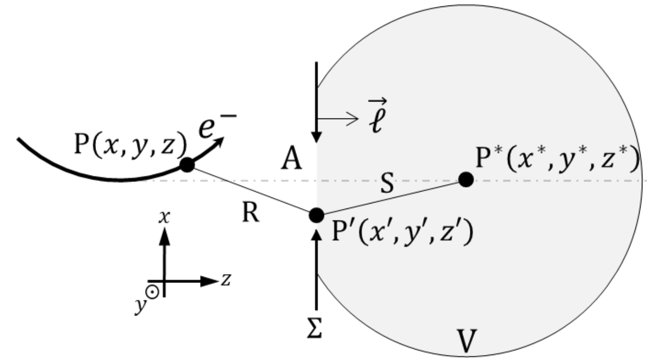
SRW development is partially supported by **US DOE SBIR.**

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:

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

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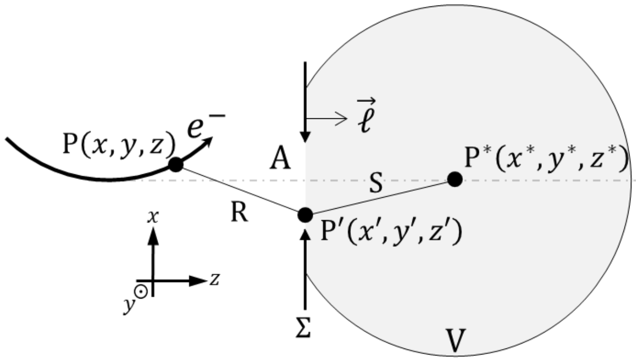

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a) $z^2 \gg (x^* - x')^2 + (y^* - y')^2$;
b) binomial expansion of the square root:

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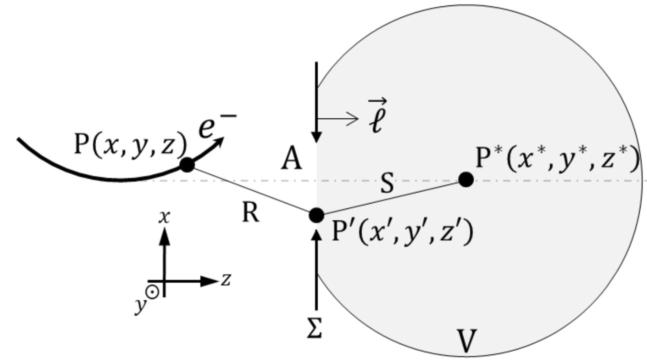

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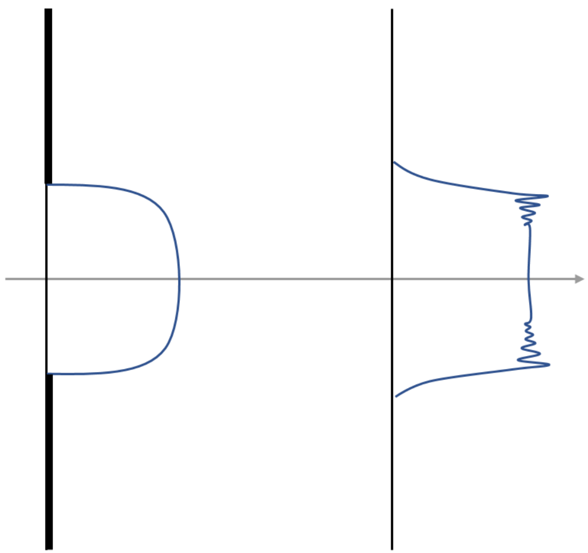
The Fraunhofer approximation:
a) $z \gg \frac{k(x'^2 + y'^2)_{\max}}{2}$.

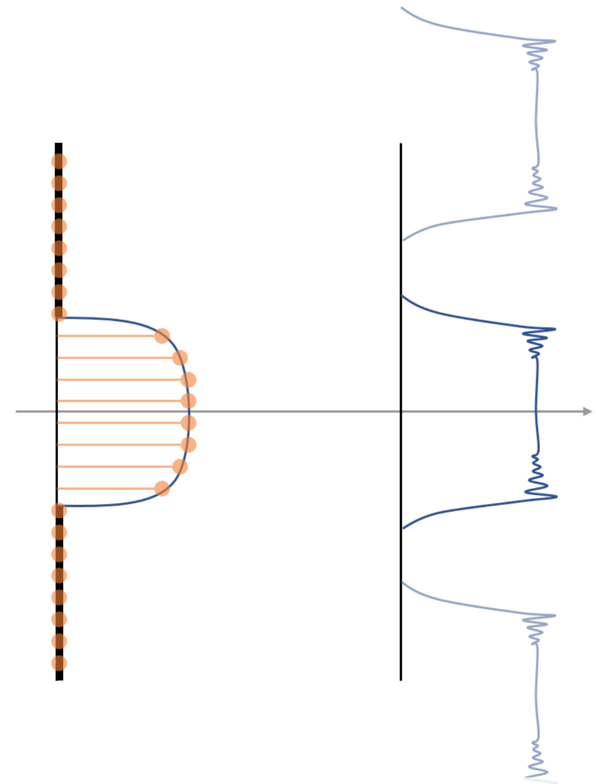
$$U(P^*) = \frac{e^{ikz} e^{i\frac{k}{2z}\left(x^{*2} + y^{*2}\right)}}{i\lambda z} \iint_{-\infty}^{\infty} U(P') \exp\left[-i\frac{2\pi}{\lambda z}(x^*x' + y^*y')\right] \mathrm{d}x'\mathrm{d}y'$$

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



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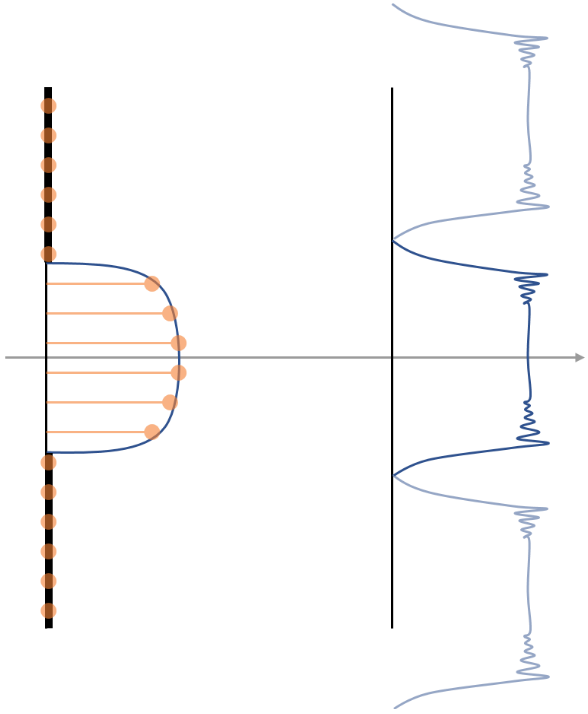

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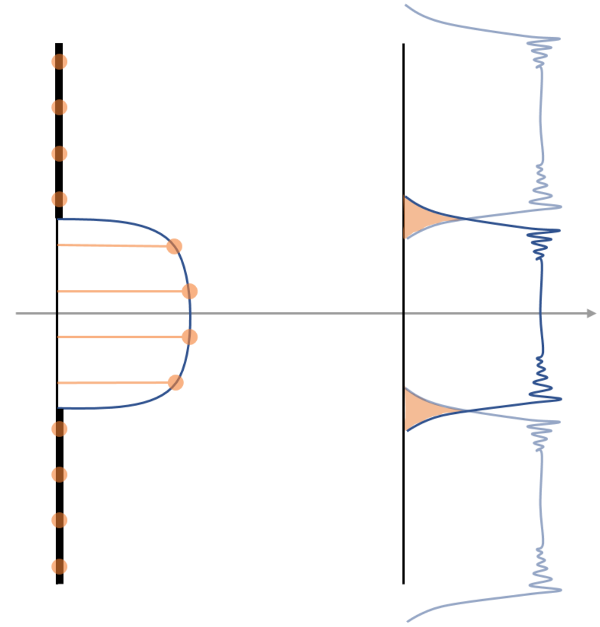

(b) undersampling effect (aliasing)

PHYSICAL OPTICS: THIN TRANSMISSION ELEMENT

$\boldsymbol{T}(x, y, z, \lambda)$ is a complex transmission operator:

$$\boldsymbol{T}(x, y, z, \omega) = \exp\left(\frac{-2\pi i}{\lambda}\int_{C} n\,\mathrm{d}s\right)$$

$$= \exp\left[\frac{-2\pi i}{\lambda}\int_{C} (1 - \delta + i\beta)\mathrm{d}s\right] \Rightarrow \begin{cases} \phi = \dfrac{2\pi}{\lambda}\delta\Delta z & \text{Phase shift} \\ \mathrm{T_{BL}} = \exp\left(-\dfrac{4\pi}{\lambda}\beta\Delta z\right) & \text{Beer-Lambert law} \end{cases}$$

The complex transmission operator can be rewritten as:

$$\boldsymbol{T}(x, y, \omega) = \sqrt{\mathrm{T_{BL}}}\mathrm{e}^{i\phi}\mathrm{e}^{-ik\Delta z}$$

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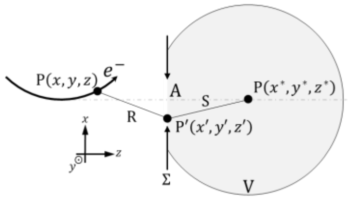
Propagation through a **thin optical element** in the projection approximation is, then, given by:

$$\boxed{U_T(x, y) = \boldsymbol{T}(x, y, \omega) \cdot U(x, y)}$$

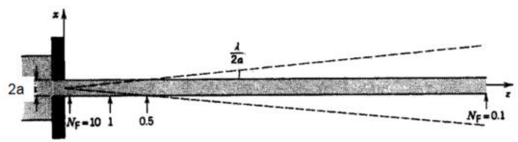
Propagation through **a thick optical element** from transverse plane before the element to a transverse plane just after it:

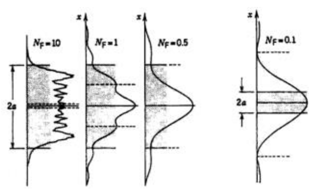
$$\boxed{U_T(x_2, y_2) = \boldsymbol{G}(x_2, y_2, \omega)\exp[ik\Lambda(x_2, y_2, \omega)] \cdot U\left[x_1\left(x_{2,}y_2\right), y_1\left(x_{2,}y_2\right)\right]}$$

$$\nabla \cdot \mathbf{D} = \cancel{\rho}^{\,0}$$
$$\nabla \cdot \mathbf{B} = 0$$
$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t}$$
$$\nabla \times \mathbf{H} = \cancel{\mathbf{J}}_{0} + \frac{\partial \mathbf{D}}{\partial t}$$



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



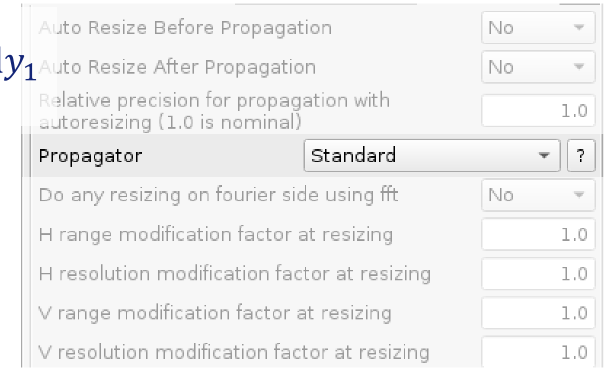


THE SRW PROPAGATORS

#0 – STANDARD FRESNEL PROPAGATOR

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

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



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

$$\boxed{\vec{E}_2(x_2, y_2) \propto \mathcal{F}^{-1}\left\{\mathcal{F}\{\vec{E}_1(x_1, y_1)\} \cdot \underbrace{\mathcal{F}\{\mathrm{K}\}}_{\text{has analytical Fourier transform}}\right\}}$$

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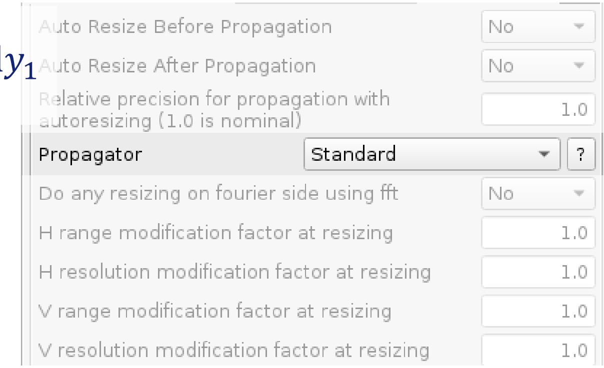

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General use:

- 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.

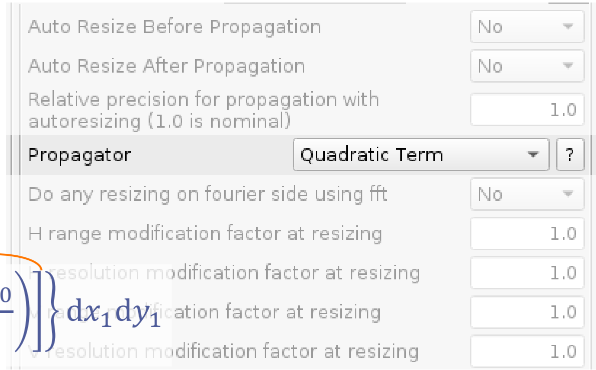
#1 – FRESNEL WITH ANALYTICAL TREATMENT OF THE QUADRATIC PHASE TERMS

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

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

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

$$\cdot\iint \vec{F}_1(x_1,y_1)\cdot\overbrace{\exp\left\{ik\left[\frac{R_x+L}{2R_xL}\left(x_1-\frac{R_xx_2+Lx_0}{R_x+L}\right)+\frac{R_y+L}{2R_yL}\left(y_1-\frac{R_yy_2+Ly_0}{R_y+L}\right)\right]\right\}}^{\mathrm{K}'}\mathrm{d}x_1\mathrm{d}y_1$$



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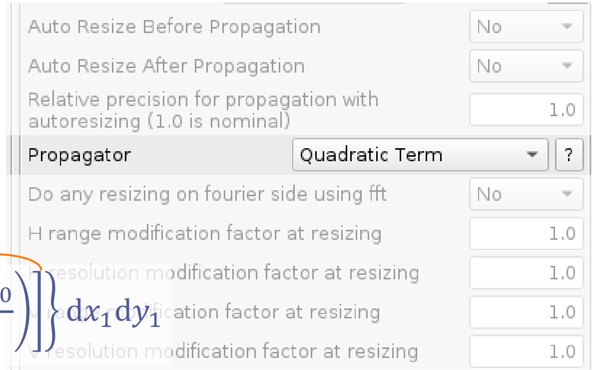

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General use:

- 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.

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

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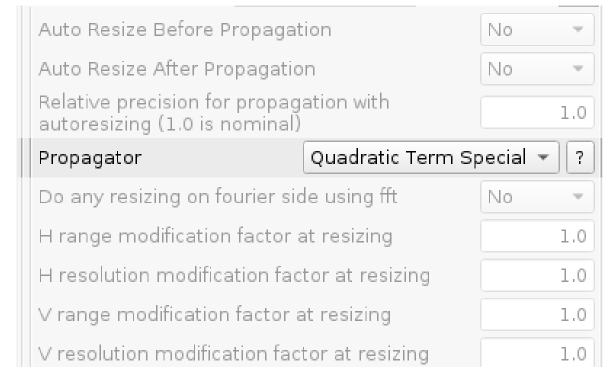

→ Different calculation of R_x and R_y; → Different processing near the waist;

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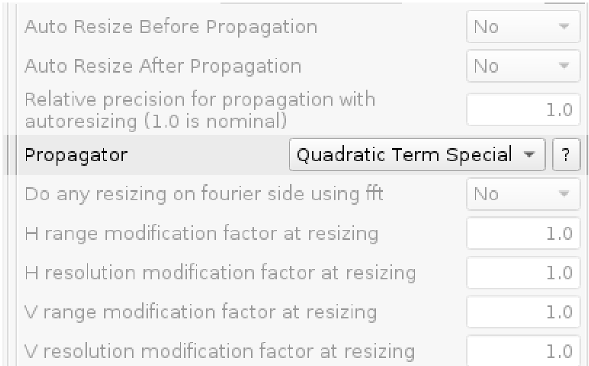


→ Different calculation of R_x and R_y; → Different processing near the waist;

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).

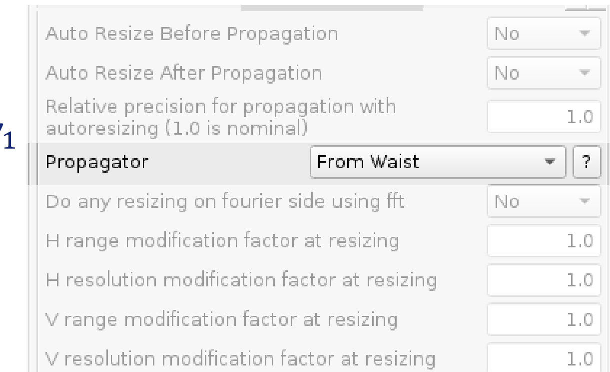
Comments:

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

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

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

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



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

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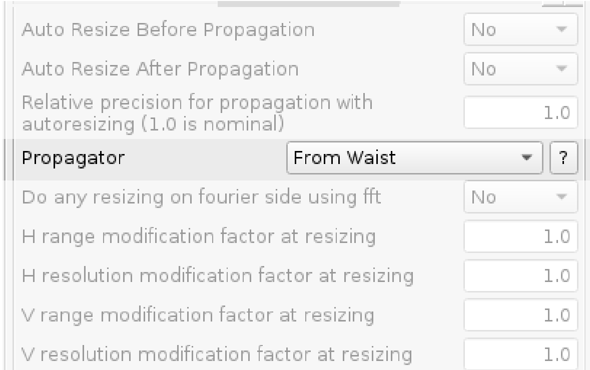

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General use:

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

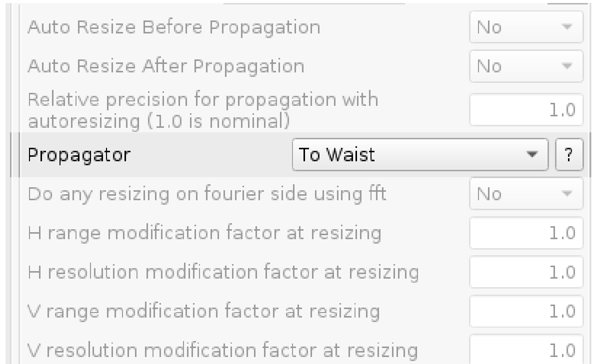
Comments:

- 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.

$$\vec{E}_2(x_2,y_2) \approx \frac{k}{2\pi iL} e^{ikL} e^{i\frac{k}{2L}(x_2^2+y_2^2)} \iint \vec{E}_1(x_1,y_1)\cdot \exp\left[-\frac{ik}{L}(x_2x_1+y_2y_1)\right] \mathrm{d}x_1\mathrm{d}y_1$$



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

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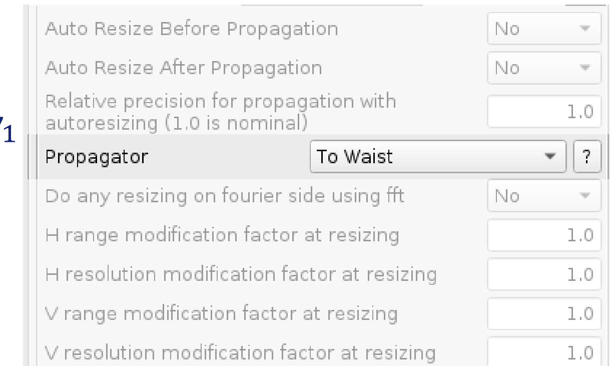

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$$\boxed{\vec{E}_2(x_2, y_2) \propto \mathcal{F}\{\vec{E}_1(x_1, y_1)\}}$$

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. BALTSER: *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 nonparixial scalar diffraction integrals for focused fields*. J. Opt. Soc. Am. A, Vol. 31, No. 8, 1832-1841, 2014.

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