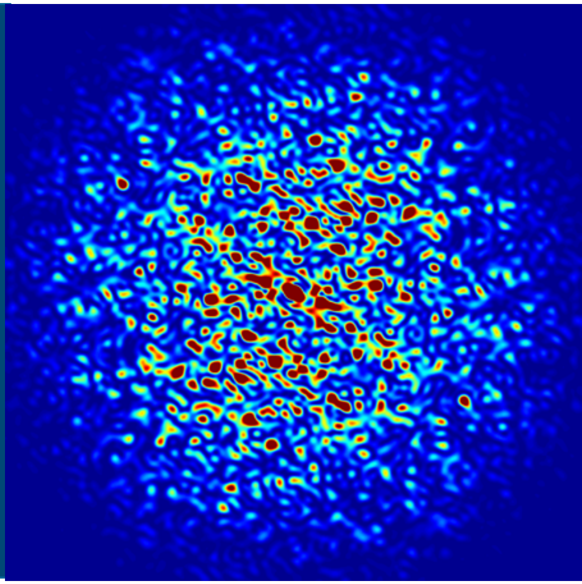
Introduction to SRW



Luca Rebuffi (ANL)

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Outline

- Introduction to Wavefront Propagation
- SRW Propagators

INTRODUCTION TO WAVEFRONT PROPAGATION

Electromagnetic field propagation in free space

From Maxwell equations: wave equation describing spatial and temporal evolution of the electromagnetic fields in free space (D'Alembert equation)

$$\left(\frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \nabla^2\right)\vec{\mathcal{E}} = 0$$

Scalar theory: describe each component of the fields separately

$$\left(\frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \nabla^2\right)U(x,y,z,t) = 0$$

$U(x,y,z,t)$ stands for any of the three component of the vector fields $\vec{\mathcal{E}}$ or magnetic field $\vec{\mathcal{B}}$ or, for light propagating along the *z* direction, any of the two electric field components $\mathcal{E}_\sigma$ and $\mathcal{E}_\pi$.

$U(x,y,z,t)$ can be spectrally decomposed as a superposition of monochromatic fields, using the Fourier Integral:

$$U(x,y,z,t) = \frac{1}{2\pi}\int_0^\infty u_\omega(x,y,z)e^{-i\omega t}d\omega$$

Electromagnetic field propagation in free space

This expression can be used in the D'Alembert equation:

$$\int_0^\infty \left[\left(\nabla^2 + \frac{\omega^2}{c^2}\right) u_\omega(x,y,z)\right] e^{-i\omega t} d\omega = 0$$

The terms in square bracket has to go to 0, so we obtain the separation of the temporal component and a new equation (Helmholtz equation)

$$(\nabla^2 + k^2) u_\omega(x,y,z) = 0$$

$$k = \frac{\omega}{c}$$

⇒ Non-monochromatic light can be solved by calculating separately every monochromatic component

Trivial solutions of the Helmholtz equation are plane waves:

$$u_\omega^{PW}(x,y,z) = e^{i(k_x x + k_y y + k_z z)}$$

$$k = \sqrt{k_x^2 + k_y^2 + k_z^2}$$

Electromagnetic field propagation in free space

$$u_\omega^{PW}(x,y,z) = e^{i(k_x x + k_y y)} e^{iz\sqrt{k^2-k_x^2-k_y^2}} = u_\omega^{PW}(x,y,z=0)e^{iz\sqrt{k^2-k_x^2-k_y^2}}$$

This expression shows that the wavefield of a single monochromatic wave propagated at z is the wavefield calculated at z=0 multiplied by the factor $\boldsymbol{e^{iz\sqrt{k^2-k_x^2-k_y^2}}}$, that can be termed **Free Space Propagator**. Then, for a generic unpropagated field:

$$u_\omega(x,y,z=0) = \frac{1}{2\pi}\iint \breve{u}_\omega(k_x,k_y,z=0)e^{i(k_x x+k_y y)}dk_x dk_y$$

Where $\breve{u}_\omega(k_x,k_y,z=0)$ is the Fourier Transform of $u_\omega(x,y,z=0)$ with respect x and y. From a physical point of view the last expression decompose the unpropagated wavefield into a linear combination of plane waves ($e^{i(k_x x+k_y y)} = u_\omega^{PW}(x,y,z=0)$).

Electromagnetic field propagation in free space

By multiplying each of this plane waves for the free space propagator we obtain the propagated wavefield at $z = z^* > 0$:

$$u_\omega(x, y, z = z^*) = \frac{1}{2\pi} \iint \breve{u}_\omega(k_x, k_y, z = 0) e^{i(k_x x + k_y y)} e^{iz^* \sqrt{k^2 - k_x^2 - k_y^2}} dk_x dk_y$$

Rewriting the whole procedure in terms of operators:

$$u_\omega(x, y, z = z^*) = \mathcal{D}_{z^*} u_\omega(x, y, z = 0)$$

$$\mathcal{D}_{z^*} = \mathcal{F}^{-1} e^{iz^* \sqrt{k^2 - k_x^2 - k_y^2}} \mathcal{F}$$ = **Diffraction Operator**

Fresnel Approximation

We assume $u_\omega(x, y, z = 0)$ to be paraxial, implying that all directions of propagations, for each of the non-negligible plane wave components in the angular-spectrum decomposition of the field over $z = 0$, make a small angle with respect to the positive z-axis.

This means that $|k_x|, |k_y| \gg k_z$, and so: $\sqrt{k^2 - k_x^2 - k_y^2} \approx k - \frac{k_x^2 + k_y^2}{2k}$

The Diffraction Operator becomes: $\mathcal{D}_{z^*} \approx \mathcal{D}_{z^*}^F = e^{ikz^*} \mathcal{F}^{-1} e^{-\frac{iz^*\left(k_x^2 + k_y^2\right)}{2k}} \mathcal{F}$

Fresnel Approximation

By using the convolution theorem:

$$f(x,y) \otimes g(x,y) = \iint_{-\infty}^{+\infty} f(x',y')g(x-x',y-y')dx'dy'$$
$$= 2\pi\mathcal{F}^{-1}\{\mathcal{F}\{f(x,y)\}\times\mathcal{F}\{g(x,y)\}\}$$

the following expression can be derived by the previous operator formula:

$$u_\omega(x,y,z=z^*) = u_\omega(x,y,z=0) \otimes P(x,y,z^*)$$

Where

$$P(x,y,z^*) = \frac{1}{2\pi} e^{ikz^*}\mathcal{F}^{-1}\left\{e^{-\frac{iz^*\left(k_x^2+k_y^2\right)}{2k}}\right\} = -\frac{ike^{ikz^*}}{2\pi z^*} e^{\frac{ik\left(x^2+y^2\right)}{2z^*}}$$

$$\Longrightarrow u_\omega\,(x,y,z=z^*) = -\frac{ike^{ikz^*}}{2\pi z^*}\left\{u_\omega(x,y,z=0) \otimes e^{\frac{ik\left(x^2+y^2\right)}{2z^*}}\right\}$$

Fresnel Approximation

It is worth noting that this convolution expression, which expresses the propagated field as the sum of the propagated disturbances, which are due to each of the points on the incident wavefront over the plane $z = 0$. This is the mathematical embodiment of the Huygens-Fresnel principle, which views the propagated disturbance as a sum of the propagated disturbances that emanate from each point on the initial wavefront.

By calculating the convolution in its integral form, we obtain a version of the formula more convenient for numerical calculations, and to make a smooth transition to the Fraunhofer approximation:

$$u_\omega(x, y, z = z^*) = -\frac{ike^{ikz^*}}{2\pi z^*} \iint_{-\infty}^{+\infty} u_\omega(x', y', z = 0) e^{\frac{ik}{2z^*}\left[(x-x')^2 + (y-y')^2\right]} dx'dy' =$$

$$= -\frac{ike^{ikz^*}}{2\pi z^*} e^{\frac{ik}{2z^*}(x^2+y^2)} \iint_{-\infty}^{+\infty} u_\omega(x', y', z = 0) e^{\frac{ik}{2z^*}(x'^2+y'^2)} e^{-\frac{ik}{z^*}(xx'+yy')^2} dx'dy'$$

Fresnel Approximation

This expression is also rewritten in terms of a kernel function K(x, y):

$$K(x, y, z, k) = -\frac{ik}{2\pi z} e^{\frac{ik}{2z}(x^2+y^2)}$$

$$\Longrightarrow u_\omega\ (x, y, z = z^*) = e^{ikz^*} \iint_{-\infty}^{+\infty} u_\omega(x', y', z = 0) K(x - x', y - y', z^*, k) dx'dy'$$

Fraunhofer Approximation

Propagated wavefield at distances that are very large compared to the characteristic length scale of the unpropagated wavefield, are said to be in the "far-field".

Assume the unpropagated disturbance, in the plane $z = 0$, to be non-negligible only over a region of diameter b. We can introduce the dimensionless Fresnel number, N_F, as:

$$N_F = \frac{b^2}{\lambda z^*} = \frac{kb^2}{2\pi z^*}$$

The "far-field" condition is reached when the propagation distance z^* is large enough that: $N_F \ll 1$

In this condition: $e^{\frac{ik}{2z^*}(x'^2+y'^2)} \approx 1 \Longrightarrow$

$$u_\omega(x,y,z=z^*) = -\frac{ike^{ikz^*}}{2\pi z^*} e^{\frac{ik}{2z^*}(x^2+y^2)} \iint_{-\infty}^{+\infty} u_\omega(x',y',z=0) e^{-\frac{ik}{z^*}(xx'+yy')^2} dx'dy'$$

Wavefront and Propagator discretization

A complex wavefield $u_\omega(x,y,z)$ can be represented in a computer by giving its values on a grid that must be finite and discrete. This numeric wavefield is defined in a finite domain that must be large enough to contain all points where the wavefront disturbance is significantly different from zero. The grid must also be dense enough to follow with enough detail all the variations of U. Both the conditions can be subjected to big limitations.
The propagated wavefield can be calculated approximately by discretizing the integrals into sums:

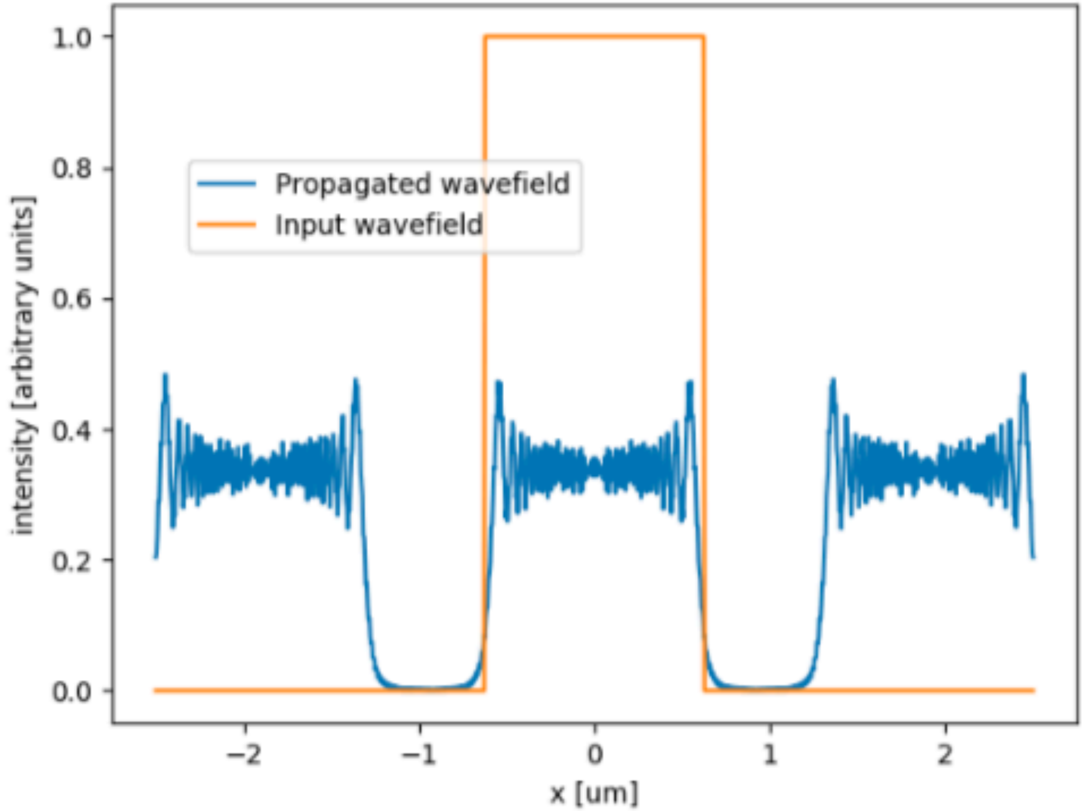
$$u_\omega(x,y,z=z^*) = -\frac{ike^{ikz^*}}{2\pi z^*}\sum_{i=0}^{N_x-1}\sum_{j=0}^{N_y-1} u_\omega\left(x_i',y_j',z=0\right)e^{\frac{ik}{2z^*}\left[\left(x-x_i'\right)^2+\left(y-y_j'\right)^2\right]}\left(x_{i+1}'-x_i'\right)\left(y_{j+1}'-y_j'\right)$$

To calculate the disturbance in a grid in the detector plane, the numbers of operation would be $\left(N_x N_y\right)^2$

Wavefront and Propagator discretization

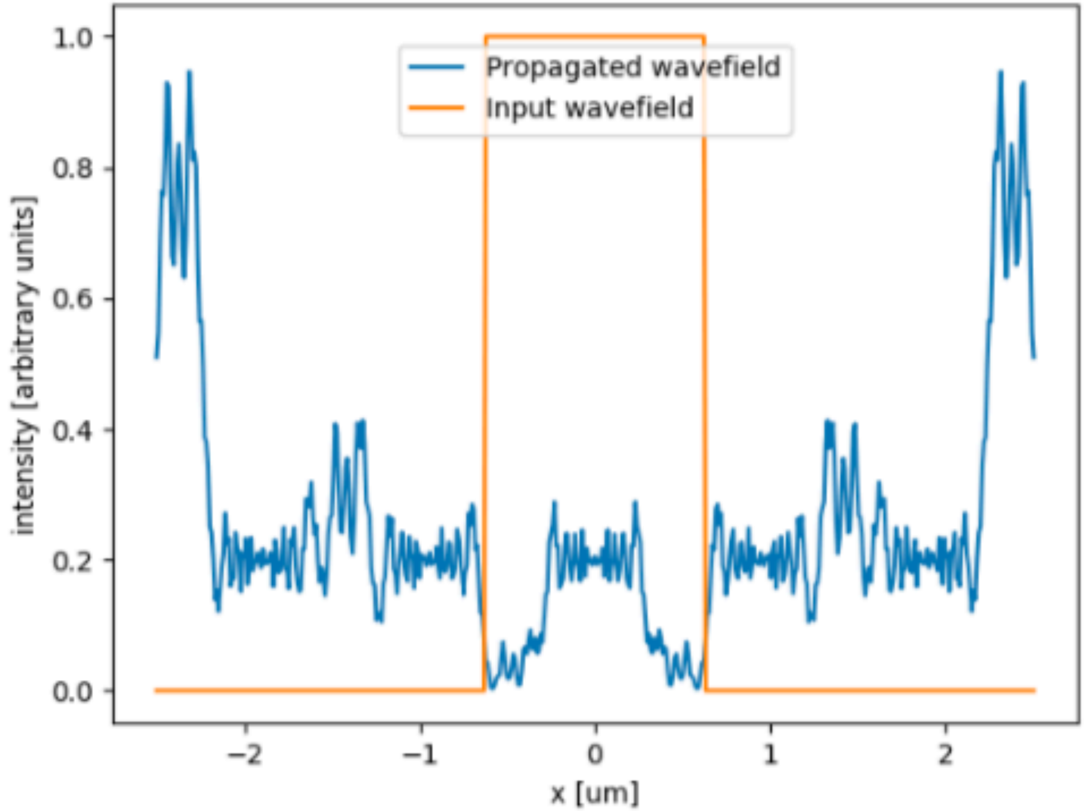
Effect of the discretization: Replicas

Replicas can be avoided by increasing the sampling or by isolating the main feature at the image plane, if the replica are well separated.



Effect of under-sampling: Aliasing

Under-sampling produces an overlapping of the replicas, thus completely distorting the expected result. This effect is called *aliasing.*



SRW PROPAGATORS

Analytical treatment of the quadratic radiation phase terms

Assume that the electric field before the propagation has quadratic terms in its phase, defined by the radii of the wavefront curvature in the horizontal and vertical planes R_x, R_y and the transverse ordinates of the center point $(x_0\,,y_0)$

$$u_\omega(x,y,z=0) = F(x,y,z=0)e^{\frac{ik}{2}\left[\frac{(x-x_0)^2}{R_x}+\frac{(y-y_0)^2}{R_y}\right]}$$

The propagated wavefield becomes:

$$u_\omega(x,y,z=z^*) = -\frac{ike^{ikz^*}}{2\pi z^*}\iint_{-\infty}^{+\infty} F(x',y',z=0)e^{\frac{ik}{2}\left[\frac{(x'-x_0)^2}{R_x}+\frac{(y'-y_0)^2}{R_y}+\frac{(x-x')^2+(y-y')^2}{z^*}\right]}dx'dy' =$$

$$= F(x,y,z=z^*)e^{\frac{ik}{2}\left[\frac{(x-x_0)^2}{R_x+z^*}+\frac{(y-y_0)^2}{R_y+z^*}\right]}$$

Chubar, O. and Celestre, R., Opt. Express 27, 28750-28759 (2019)

Analytical treatment of the quadratic radiation phase terms

Where:

$$F(x,y,z=z^*) = -\frac{ike^{ikz^*}}{2\pi z^*}\iint_{-\infty}^{+\infty} F(x',y',z=0)e^{\frac{ik}{2z^*}\left[\frac{R_x+z^*}{R_x}\left(\frac{R_x x+z^* x_0}{R_x+z^*}-x'\right)^2+\frac{R_y+z^*}{R_y}\left(\frac{R_y y+z^* y_0}{R_y+z^*}-y'\right)^2\right]}dx'dy'$$

Like the expression of $u_\omega(x,y,z=z^*)$, this is a convolution-type integral, though it applies to the function $F(x',y',z=0)$ that can be considered as the initial electric field after the "subtraction" of its quadratic phase terms. $F(x,y,z=z^*)$ can be considered as a propagated electric field with its (evolved) quadratic terms subtracted.

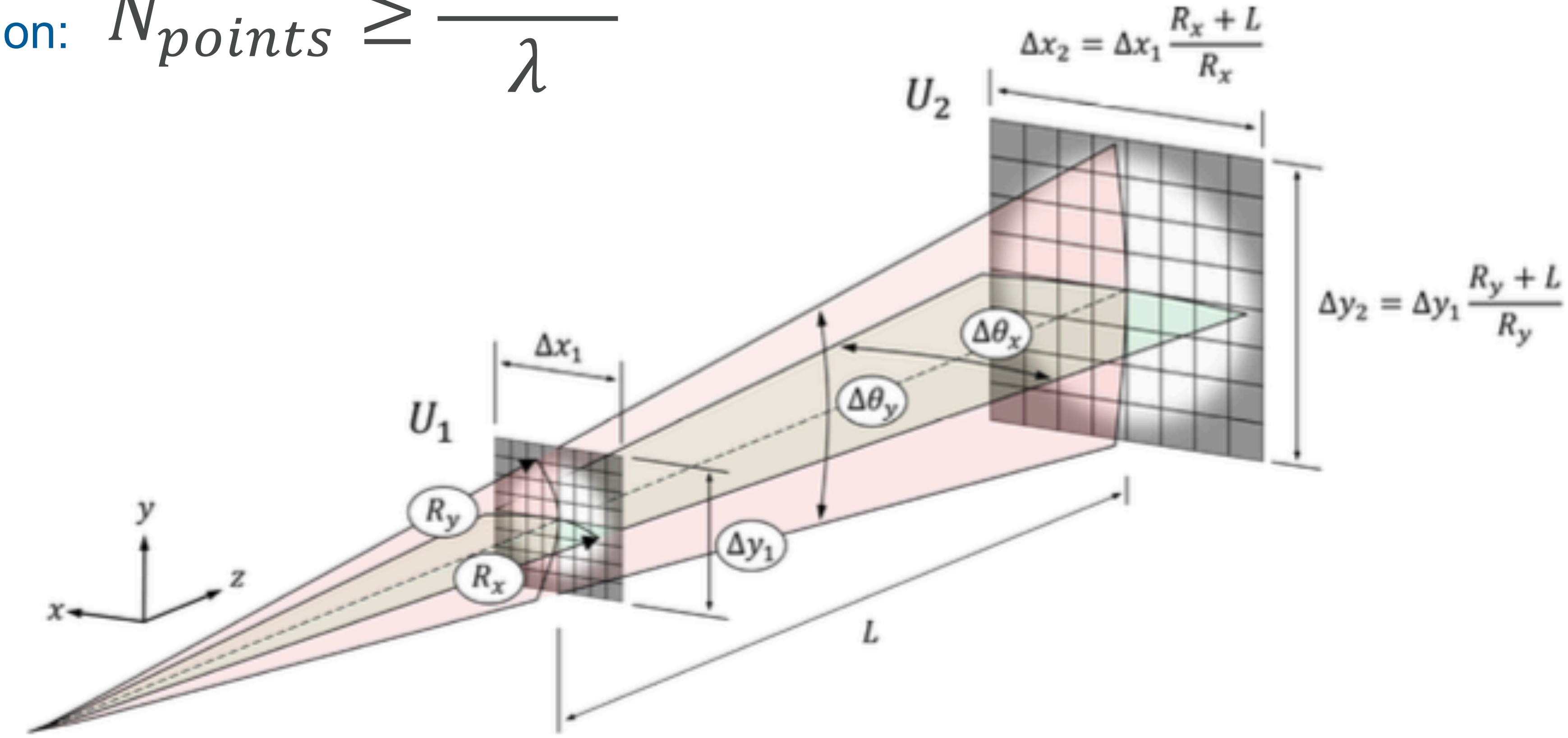
The kernel of the integral is:

$$K(x,y,z,k) = -\frac{ik}{2\pi z}e^{\frac{ik}{2z}\left[\frac{R_x+z}{R_x}x^2+\frac{R_y+z}{R_y}y^2\right]}$$

Chubar, O. and Celestre, R., Opt. Express 27, 28750-28759 (2019)

Number of Points in the Propagation Plane

For each transversal direction: $N_{points} \geq \dfrac{\Delta\theta^2 R}{\lambda}$



Chubar, O. and Celestre, R. Opt. Express 27, 28750-28759 (2019)

Effects of Optics Elements

SRW uses a matrix expression of the propagator acting on all the transverse components of the Electric Field. For a "thin" optical element we can write the kernel function by using a complex transmission matrix function:

$$\boldsymbol{K}(x_j, y_j, x_{j-1}, y_{j-1}, k) \approx \boldsymbol{T}(x_j, y_j, k)\delta(x_{j-1} - x_j)\delta(y_{j-1} - y_j)$$

Where x_j, y_j are transverse coordinate in a plane after the optical element and x_{j-1}, y_{j-1} in a plane before. For an optical element with some extent along optical axis, like a grazing incidence mirror, the kernel function can be written as:

$$\boldsymbol{K}(x_j, y_j, x_{j-1}, y_{j-1}, k) \approx \boldsymbol{G}(x_j, y_j, k)e^{ik\Lambda(x_j, y_j, k)}\delta\left(x_{j-1} - \tilde{x}_{j-1}(x_j, y_j)\right)\delta\left(y_{j-1} - \tilde{y}_{j-1}(x_j, y_j)\right)$$

Where $\boldsymbol{G}(x_j, y_j, k)$ is a matrix function defining local transformations of the wavefield (e.g. reflection from a mirror surface), $\tilde{x}_{j-1}(x_j, y_j)$ and $\tilde{y}_{j-1}(x_j, y_j)$ are functions defining the transformation of coordinates for points in the transverse plane before and after the optical element, $\Lambda(x_j, y_j, k)$ is a function defining the corresponding optical path difference.

Chubar, O., Berman, L., Chu, Y. S., Fluerasu, A., Hubert, S., Idir, M., Kaznatcheev, K., Shapiro, D. Shen, Q. and Baltser, J., Proc. SPIE, 8141:814107 (2011)

SRW Standard Propagator

Is the Fresnel Propagator:

$$u_\omega(x,y,z=z^*) = -\frac{ike^{ikz^*}}{2\pi z^*}\iint_{-\infty}^{+\infty} u_\omega(x',y',z=0)e^{\frac{ik}{2z^*}\left[(x-x')^2+(y-y')^2\right]}dx'dy' =$$

- propagation over a drift space with gentle (de)magnification
- before slits, ideal lenses and smooth phase elements
- preserves number of pixel and ranges
- given proper sampling, can be used for focusing
- works for strongly astigmatic systems

Quadratic Term/Quadratic Term Special Propagator

Is the Fresnel propagator with analytical treatment of the quadratic phase terms

$$u_\omega(x,y,z=z^*) = -\frac{ike^{ikz^*}}{2\pi z^*}\iint_{-\infty}^{+\infty} F(x',y',z=0)e^{\frac{ik}{2}\left[\frac{(x'-x_0)^2}{R_x}+\frac{(y'-y_0)^2}{R_y}+\frac{(x-x')^2+(y-y')^2}{z^*}\right]}dx'dy'$$

Quadratic Term	Quadratic Term Special
- propagation over a drift space in general - before complex optical elements (e.g. curved mirrors). - preserves number of pixel, ranges are recalculated to accommodate the wavefront - can be used for or from focusing - works for strongly astigmatic systems.	- different calculation of Rx and Ry and processing near the waist - 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) - preserves number of pixel, ranges are recalculated to accommodate the wavefront - can be used for or from focusing - works for strongly astigmatic systems.

From Waist/To Waist Propagator

Is the Fraunhofer Propagator:

$$u_\omega(x,y,z=z^*) = -\frac{ike^{ikz^*}}{2\pi z^*} e^{\frac{ik}{2z^*}(x^2+y^2)} \iint_{-\infty}^{+\infty} u_\omega(x',y',z=0) e^{-\frac{ik}{z^*}(xx'+yy')^2} dx'dy'$$

From Waist	To Waist
- propagation of a wavefront emerging from a focal position in both vertical and horizontal directions - output plane (several times) larger than the input plane - preserves number of pixel, ranges are recalculated to accommodate the wavefront - fails for strongly astigmatic systems.	- propagation of a wavefront being focused on both directions - output plane (several times) smaller than the input plane - preserves number of pixel, ranges are recalculated to accommodate the wavefront - fails for strongly astigmatic systems.

References

Official Repository
Official SRW User Interface

https://github.com/ochubar/SRW

https://www.sirepo.com/srw

SRW Publications

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Thank you!