

# Wavefront propagation for X-ray beamlines with SRW

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# Wavefront propagation for X-ray beamlines with SRW

## Outline:

- Prologue
- Brief introduction to scalar wave optics
- Free-space propagation with SRW
- Thin optical elements
- Thick optical elements
- Where to learn more?

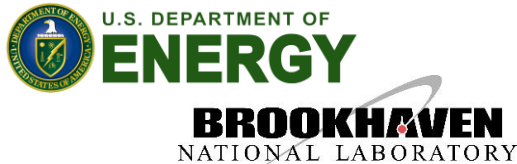
# “Synchrotron Radiation Workshop”

(electrodynamics simulation code for SR emission and propagation)

The project was started in **1997-98** by **Pascal Elleaume** and **Oleg Chubar** after completion of the **Radia** project. **First official version** of SRW was developed at ESRF (written in C++, interfaced to IGOR Pro); Chubar and Elleaume "Accurate and efficient computation of synchrotron radiation in the near field region", Proc. EPAC-98, 1177-1179 (1998).

The **main** open-source **repository** (2012), containing all C/C++ sources, C API, all interfaces and project development files, is on **GitHub**:

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



diamond



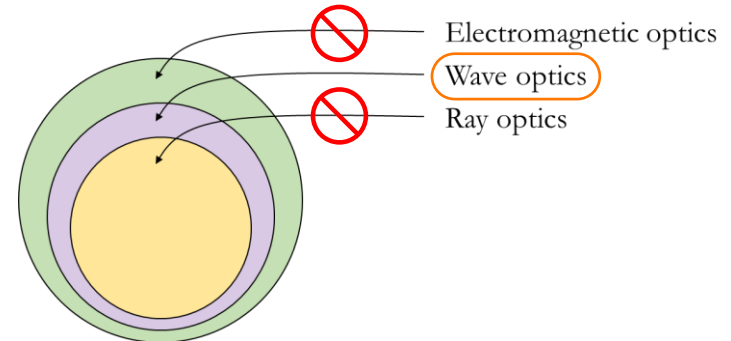
# Prologue

Choosing an **adequate optical theory** for simulations:

“As simple as possible, as accurate as necessary.”

We use **physical optics** when **diffraction effects cannot be neglected**:

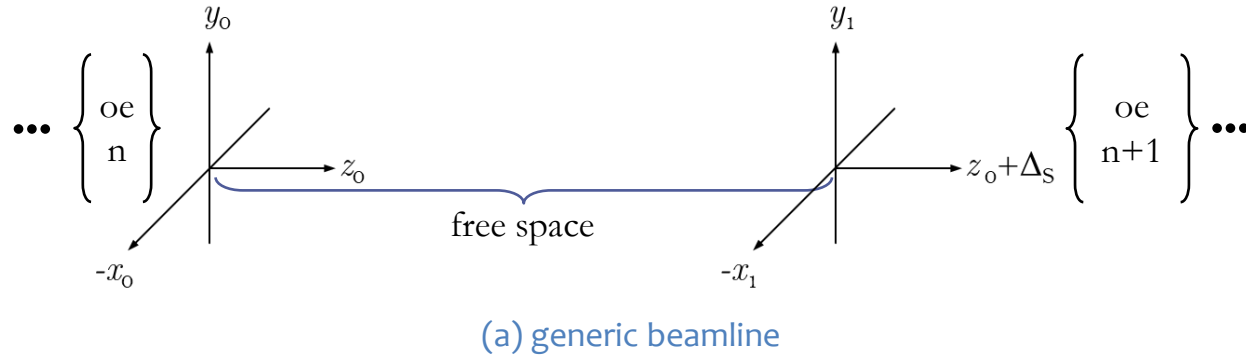
- IR, UV and soft x-ray beamlines in current and low-emittance light sources;
- whenever spatial filtering causes the increase in the coherent fraction (CF):
  - “increasing the propagation distance” – cf. van Cittert-Zenike theorem
  - “closing the aperture to match the coherence length”
  - “slitting down the secondary source”...



(a) hierarchical optical theories

# Prologue

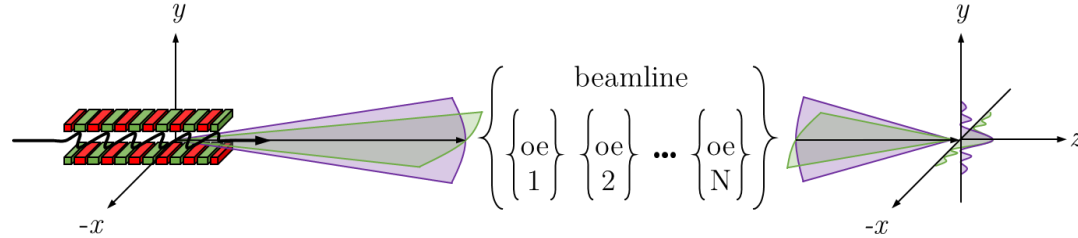
Wave-optical simulations deal with two classes of beamline elements:



- (thin or thick) **optical elements** as transmission elements in **projection approximation**;
- **free spaces** in between optical elements with near- and far-field **diffraction integrals** (e.g. Huygens-Fresnel, Fresnel or Fraunhofer integrals);

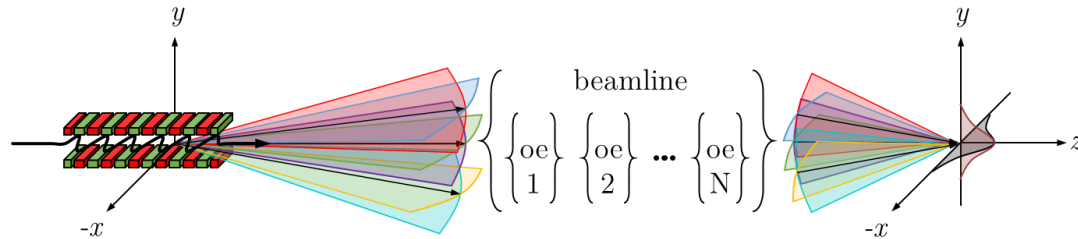
# Prologue

## Fully-coherent simulations (point source):



(a) fully-coherent simulation (filament beam, zero emittance, single electron...)

## Partially-coherent simulations (extended source):



(b) partially-coherent simulation (thick beam, finite emittance, multi-electron...)

# Scalar wave theory – how did we get here?

$$\nabla \times \mathbf{E}(x, y, z, t) = -\frac{\partial \mathbf{B}(x, y, z, t)}{\partial t} \quad \left( \varepsilon_0 \mu_0 \frac{\partial^2}{\partial t^2} - \nabla^2 \right) u(x, y, z, t) = 0$$

$$\left( \varepsilon_0 \mu_0 \frac{\partial^2}{\partial t^2} - \nabla^2 \right) \mathbf{E}(x, y, z, t) = \mathbf{0}$$

$$u = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} U(x, y, z) \exp(-\omega t) dt$$

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

1.) application of  $\nabla \times \bullet$  to both sides of **Faraday's law** in an **uncharged** and **non-conducting medium**. Also remembering that  $\nabla \times (\nabla \times \bullet) = \nabla(\nabla \cdot \bullet) - \nabla^2 \bullet$  results in the **d'Alembert wave equation**.

2.) **each component** of  $\mathbf{E}(x, y, z, t)$  **individually satisfies** the **wave equation**. The complex scalar **solution** of the **wave equation** can be **decomposed** as **superposition** of **monochromatic fields**.

3.) this is the **Helmholtz equation**. Given a volume in space and boundary conditions, the scalar diffraction theory consists in finding solution to the Helmholtz equation.

$$\iiint_V (U \nabla^2 G - G \nabla^2 U) dv = \iint_S \left( U \frac{\partial G}{\partial n} - G \frac{\partial U}{\partial n} \right) ds$$

$$U(x, y, z) = \frac{1}{4\pi} \iint_S \left\{ \frac{\partial U}{\partial n} \left[ \frac{\exp(jk|\vec{r}|)}{|\vec{r}|} \right] - U \frac{\partial}{\partial n} \left[ \frac{\exp(jk|\vec{r}|)}{|\vec{r}|} \right] \right\} ds$$

4.) **Calculation** of  $U(x, y, z)$  at an observation point in space can be done using **Green's theorem**. An **arbitrary** and **careful choice** of the **Green's function**  $G$  results in the **integral theorem of Helmholtz and Kirchhoff**. Yet another careful **choice of Green's function** and **boundary conditions** yield in the **Rayleigh-Sommerfeld** formulation of **diffraction**.

# Scalar wave theory – Rayleigh-Sommerfeld formulation

If  $u_0(x, y)$  vanishes in the shadow of the screen and is undisturbed in  $\Sigma$  (aperture):

$$u_L(x, y) = -\frac{1}{2\pi} \iint_{\Sigma} u_0(\xi, \eta) \left( jk - \frac{1}{|\vec{r}|} \right) \frac{\exp(jk|\vec{r}|)}{|\vec{r}|} \cos(\vec{\ell}, \vec{r}) ds,$$

with  $|\vec{r}| = \sqrt{L^2 + (x - \xi)^2 + (y - \eta)^2}$ ,  $\cos(\vec{\ell}, \vec{r}) = L/|\vec{r}|$  and  $ds = d\xi d\eta$ .

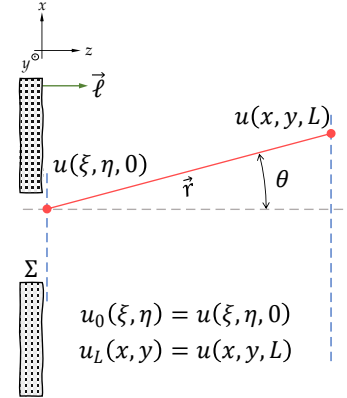
The above equation is a **convolution** between the input field and a kernel:

$$\begin{aligned} u_0(x, y) * h(x, y) &= \iint_{-\infty}^{\infty} u_0(\xi, \eta) \cdot h(x - \xi, y - \eta) d\xi d\eta \\ &= \mathcal{F}^{-1}\{\mathcal{F}\{u_0(x, y)\} \cdot \mathcal{F}\{h(x, y)\}\} \end{aligned}$$

The kernel of the RS diffraction integral is given by:

$$h_{\text{RS}}(x, y) = h_1 + h_2 = \frac{L}{j\lambda} \frac{\exp(jk|\vec{r}|)}{|\vec{r}|^2} + \frac{L}{2\pi} \frac{\exp(jk|\vec{r}|)}{|\vec{r}|^3}$$

For most cases of interest  $|\vec{r}| \gg \lambda$  and hence,  $h$  can be approximated by  $h_1$ .



(a) formulation of diffraction by a plane-screen



# Scalar wave theory – Huygens-Fresnel formulation

Applying  $r \gg \lambda$  to the first Rayleigh-Sommerfeld solution:

$$u_L(x, y) = \frac{1}{j\lambda} \iint_{\Sigma} u_0(\xi, \eta) \frac{\exp(jk|\vec{r}|)}{|\vec{r}|} \frac{L}{|\vec{r}|} ds$$

Which is a **convolution** with kernel given by:

$$h_{\text{HF}}(x, y) = \frac{L}{j\lambda} \frac{\exp(jk|\vec{r}|)}{|\vec{r}|^2}$$

The propagated wave can be calculated as:

$$u_L(x, y) = \mathcal{F}^{-1}\{\mathcal{F}\{u_0(x, y)\} \cdot \mathcal{F}\{h_{\text{HF}}(x, y)\}\}$$

The kernel  $\mathcal{F}\{h_{\text{HF}}(x, y)\}$  has no known closed form, so three FFTs are necessary for numerical evaluation. Using the convolution theorem with FFTs is computationally advantageous for numerical problems.

# Scalar wave theory – Huygens-Fresnel formulation

$$u_L(x, y) = \mathcal{F}^{-1}\{\mathcal{F}\{u_0(x, y)\} \cdot \mathcal{F}\{h_{\text{HF}}(x, y)\}\}$$

*“the split propagator/Huygens-Fresnel diffraction integral”*

**Short description:** the **Huygens-Fresnel diffraction integral** is implemented by using the convolution theorem with **3x FFT**.

## **General use:**

- strong (de)magnification systems (e.g. nano KB, FZP...) where the paraxial approximation is less recommended;

## **Comments:**

- preserves number of pixel and ranges of the input plane;
- works for strongly astigmatic systems;
- recently implemented and not extensive used as the other propagators.

# Scalar wave theory – the Fresnel diffraction

“standard”

The **paraxial approximation** of the Huygens-Fresnel integral can be obtained by using the binomial expansion to the square root in  $|\vec{r}|$  provided that  $L^2 \gg (x - \xi)^2$ ,  $L^2 \gg (y - \eta)^2$ :

$$u_L(x, y) = \frac{\exp(jkL)}{j\lambda L} \iint_{\Sigma} u_0(\xi, \eta) \exp\left\{\frac{jk}{2L} [(x - \xi)^2 + (y - \eta)^2]\right\} ds$$

The diffraction integral above is a **convolution** between the input field  $u_0$  and a kernel  $h_F$  :

$$h_F(x, y) = \frac{\exp(jkL)}{j\lambda L} \exp\left[\frac{jk}{2L} (x^2 + y^2)\right],$$

which has analytical Fourier transform  $H_F(f_x, f_y) = \exp(jkL) \exp[-j\pi\lambda L(f_x^2 + f_y^2)]$ . Hence, the calculation of the Fresnel diffraction integral is done using two FFT operations

$$u_L(x, y) = \mathcal{F}^{-1}\{\mathcal{F}\{u_0(x, y)\} \cdot H_F(f_x, f_y)\}$$

# Scalar wave theory – the Fresnel diffraction

*“standard”*

$$u_L(x, y) = \exp(jkL) \cdot \mathcal{F}^{-1}\{\mathcal{F}\{u_0(x, y)\} \cdot \exp[-j\pi\lambda L(f_x^2 + f_y^2)]\}$$

*“Standard Fresnel”*

**Short description:** the **standard Fresnel** diffraction integral is implemented by using the convolution theorem with **2x FFT**.

## **General use:**

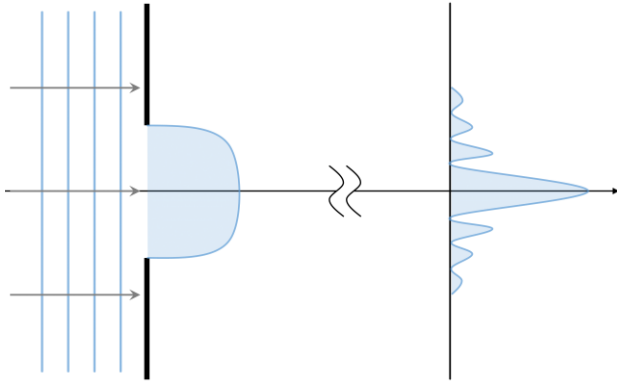
- propagation over free-space with gentle (de)magnification;
- to be used before slits, ideal lenses and smooth phase elements;

## **Comments:**

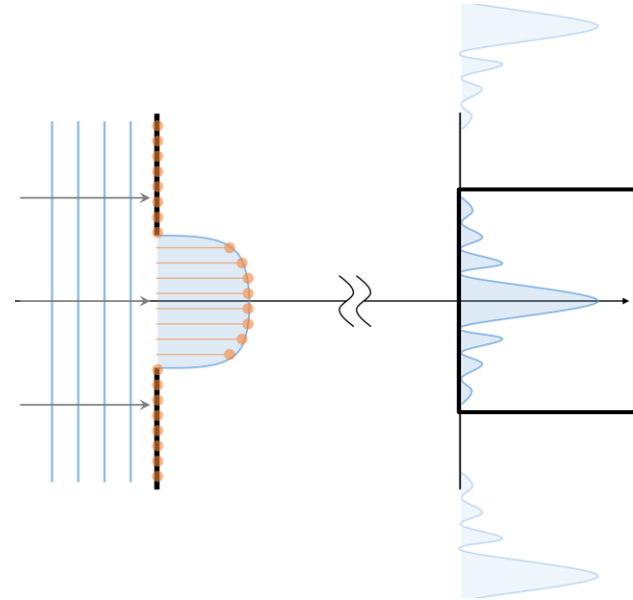
- preserves number of pixel and ranges of the input plane;
- works for strongly astigmatic systems;

# Scalar wave theory – the Fresnel diffraction

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



(a) analytical solution

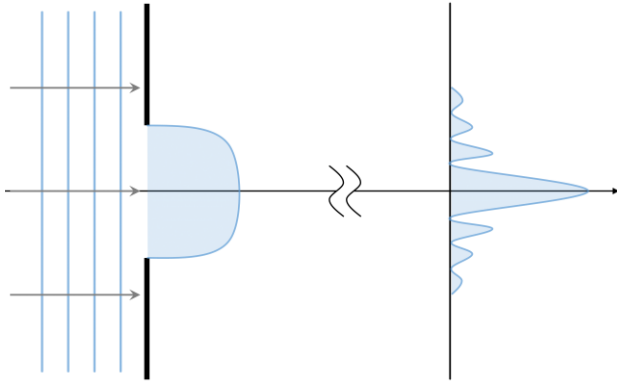


(b) numerical calculation with sampling artifacts (replicas)

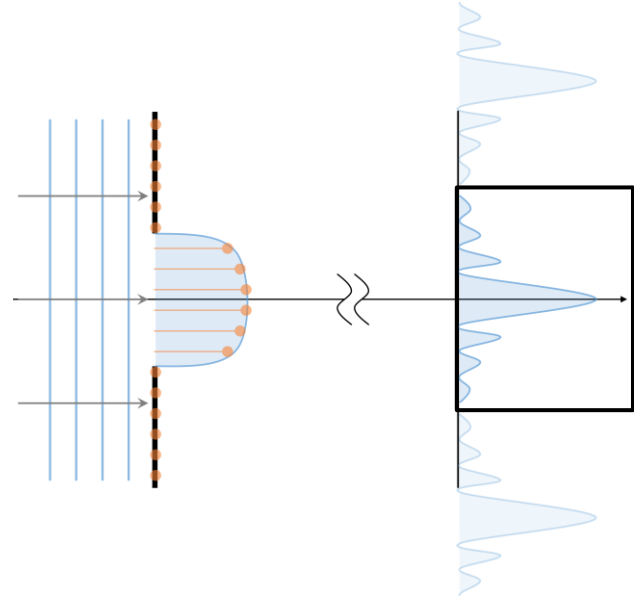
Kelly, J. Opt. Soc. Am. A 31(4), 755 (2014)

# Scalar wave theory – the Fresnel diffraction

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



(a) analytical solution



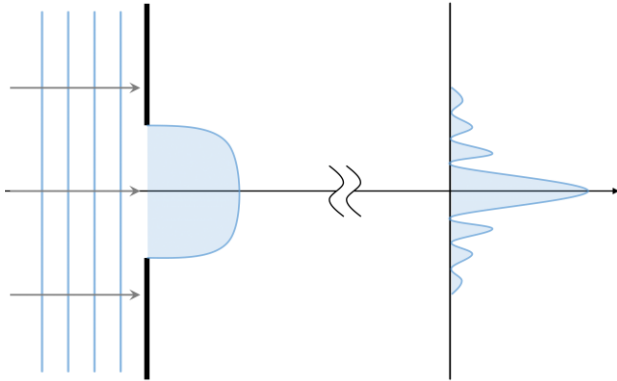
(b) numerical calculation with sampling artifacts (replicas)

Kelly, J. Opt. Soc. Am. A 31(4), 755 (2014)

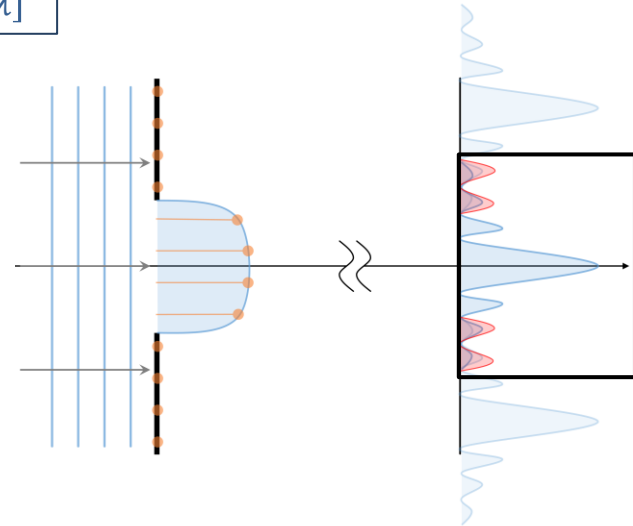
# Scalar wave theory – the Fresnel diffraction

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

$$N = \lceil p \cdot \Delta\Omega^2 \cdot R / \lambda \rceil$$



(a) analytical solution



(b) numerical calculation with sampling artifacts (replicas)

Kelly, J. Opt. Soc. Am. A 31(4), 755 (2014)

# Scalar wave theory – the Fresnel diffraction

“quadratic term”

Assuming the input field has a **quadratic phase term** defined by the wavefront curvature  $(R_x, R_y)$  centred at  $(x_0, y_0)$ :

$$u_0(x, y) = g_0(x, y) \cdot \exp \left\{ \frac{jk}{2} \left[ \frac{(x - x_0)^2}{R_x} + \frac{(y - y_0)^2}{R_y} \right] \right\},$$

The Fresnel diffraction integral can be re-written as:

$$u_L(x, y) = \exp \left\{ \frac{ik}{2} \left[ \frac{(x - x_0)^2}{(R_x + L)} + \frac{(y - y_0)^2}{(R_y + L)} \right] \right\} \cdot \frac{\exp(jkL)}{j\lambda L} \cdot \iint_{\Sigma} g_0(\xi, \eta) \exp \left\{ \frac{ik}{2L} \left[ \frac{R_x + L}{R_x} \left( \frac{R_x x + Lx_0}{R_x + L} - \xi \right)^2 + \frac{R_y + L}{R_y} \left( \frac{R_y y + Ly_0}{R_y + L} - \eta \right)^2 \right] \right\} ds$$

Which is a **convolution** integral with the reduced coordinates:

$$(\hat{x}, \hat{y}) = \left( \frac{R_x x + Lx_0}{R_x + L}, \frac{R_y y + Ly_0}{R_y + L} \right)$$



# Scalar wave theory – the Fresnel diffraction

*“quadratic term”*

The kernel of the transformation as a function of the reduced coordinates is given by:

$$h_{\text{QPT}}(x, y) = \frac{\exp(jkL)}{j\lambda L} \exp \left[ \frac{ik}{2L} \left( \frac{R_x + L}{R_x} \hat{x}^2 + \frac{R_y + L}{R_y} \hat{y}^2 \right) \right],$$

with analytical Fourier transform  $H_{\text{QPT}}(f_x, f_y)$ :

$$H_{\text{QPT}}(f_x, f_y) = \exp(jkL) \cdot \sqrt{\frac{R_x R_y}{(R_x + L)(R_y + L)}} \cdot \exp \left[ -j\pi L \lambda \left( \frac{R_x}{R_x + L} f_x^2 + \frac{R_y}{R_y + L} f_y^2 \right) \right]$$

The calculation of the **Fresnel transform** with the **analytical treatment of the quadratic phase term**:

$$u_L(x, y) = \exp \left\{ \frac{ik}{2} \left[ \frac{(x - x_0)^2}{(R_x + L)} + \frac{(y - y_0)^2}{(R_y + L)} \right] \right\} \cdot \mathcal{F}^{-1} \{ \mathcal{F} \{ g_0(x, y) \} \cdot H_{\text{QPT}}(f_x, f_y) \}$$

# Scalar wave theory – the Fresnel diffraction

*“quadratic term”*

$$u_L(x, y) = \exp \left\{ \frac{ik}{2} \left[ \frac{(x - x_0)^2}{(R + L)} + \frac{(y - y_0)^2}{(R + L)} \right] \right\} \cdot \mathcal{F}^{-1} \{ \mathcal{F} \{ g_0(x, y) \} \cdot H_{\text{QPT}}(f_x, f_y) \}$$

*“Fresnel with analytical treatment of the quadratic (leading) phase terms”*

**Short description:** the **quadratic phase term** of the input wave is removed, relaxing sampling requirements. This implementation of the Fresnel diffraction integral uses the convolution theorem with **2x FFT**.

## General use:

- most prolific SRW propagator – being used with a wide range of free-space propagation;
- to be used before complex optical elements (e.g. transmission elements, curved mirrors... );
- can be used for propagation from and to image planes;

## Comments:

- preserves number of pixel but the ranges are re-scaled as  $\Delta x_L = \Delta x_0(R + L)/R$  and  $\Delta y_L = \Delta y_0(R + L)/R$ ;
- works for strongly astigmatic systems;
- has singularities when  $R \approx -L$ .

Chubar and Celestre, *Opt. Express* 27(20), 28750 (2019)

# Scalar wave theory – the Fresnel diffraction

“quadratic term –  
special”

$$u_L(x, y) = \exp \left\{ \frac{ik}{2} \left[ \frac{(x - x_0)^2}{(R_x + L)} + \frac{(y - y_0)^2}{(R_y + L)} \right] \right\} \cdot \mathcal{F}^{-1} \{ \mathcal{F} \{ g_0(x, y) \} \cdot H_{\text{QPT}}(f_x, f_y) \}$$

*“Fresnel with analytical treatment of the quadratic (leading) phase terms, yet with different processing near a waist”*

**Short description:** the **quadratic phase term** of the input wave is removed, relaxing sampling requirements. This implementation of the Fresnel diffraction integral uses the convolution theorem with **2x FFT** but **with a different estimation of  $R_x$  and  $R_y$  near the beam waist**.

## General use:

- to be used before complex optical elements (e.g. transmission elements, curved mirrors... );
- can be used for propagation from and to image planes (e.g. very small slits);
- strong diffracting elements

## Comments:

- preserves number of pixel but the ranges are re-scaled;
- works for strongly astigmatic systems;
- has singularities when  $R_x \approx -L$  and  $R_y \approx -L$ .

Chubar and Celestre, Opt. Express 27(20), 28750 (2019)

# Scalar wave theory – the Fraunhofer diffraction

*“from waist”*

Expanding the quadratic terms in the exponential function and collecting terms in the standard Fresnel propagator:

$$u_L(x, y) = \frac{\exp(jkL)}{j\lambda L} \exp\left[\frac{jk}{2L}(x^2 + y^2)\right] \iint_{\Sigma} u_0(\xi, \eta) \cdot \exp\left[\frac{jk}{2L}(\xi^2 + \eta^2)\right] \cdot \exp\left\{-\frac{jk}{L}(x\xi + y\eta)\right\} ds$$

For sufficiently large propagation distances, i.e.  $a^2/\lambda L \ll 1$ , we arrive at the **Fraunhofer** regime:

$$u_L(x, y) = \frac{\exp(jkL)}{j\lambda L} \exp\left[\frac{jk}{2L}(x^2 + y^2)\right] \iint_{\Sigma} u_0(\xi, \eta) \cdot \exp\left\{-\frac{jk}{L}(x\xi + y\eta)\right\} ds$$

which, apart from the multiplicative factors, is the Fourier transform of the input field  $u_0(x, y)$  evaluated at frequencies  $f_x = x/\lambda L$  and  $f_y = y/\lambda L$ :

$$u_L(x, y) \propto \mathcal{F}\{u_0(x, y)\}$$

# Scalar wave theory – the Fraunhofer diffraction

*“from waist”*

$$u_L(x, y) \propto \mathcal{F}\{u_0(x, y)\}$$

*“For propagation from a waist over a ~large distance”*

**Short description:** propagator based on the far-field approximation (Fraunhofer) using 1x FFT.

## General use:

- propagation of a wavefront emerging from a focal plane in both vertical and horizontal directions – *from a waist to a ~large distance*;
- output plane several times larger than the input plane (e.g. scattering experiments);

## Comments:

- preserves number of pixel but the ranges are re-scaled;
- fails for astigmatic systems.

# Scalar wave theory – the optical Fourier transform

*“to waist”*

We consider now a converging wavefront  $u_0(x, y) = g_0(x, y) \cdot \exp[-jk(x^2 + y^2)/2q]$ , where  $q$  is the distance between wave and focusing plane. We then plug it into the Fresnel integral:

$$u_L(x, y) = \frac{\exp(jkL)}{j\lambda L} \exp\left[\frac{jk}{2L}(x^2 + y^2)\right] \cdot \iint_{\Sigma} g_0(\xi, \eta) \cdot \exp\left[-\frac{jk}{2q}(\xi^2 + \eta^2)\right] \cdot \exp\left[\frac{jk}{2L}(\xi^2 + \eta^2)\right] \cdot \exp\left\{-\frac{jk}{L}(x\xi + y\eta)\right\} ds$$

If the wavefront  $u_0(x, y)$  is propagated to the image plane, that is, if  $L = q$ , the above equation becomes:

$$u_L(x, y) = \frac{\exp(jkL)}{j\lambda L} \exp\left[\frac{jk}{2L}(x^2 + y^2)\right] \cdot \iint_{\Sigma} g_0(\xi, \eta) \cdot \exp\left\{-\frac{jk}{L}(x\xi + y\eta)\right\} ds$$

Which is a Fourier transform of the field  $g_0(x, y)$ :

$$u_L(x, y) \propto \mathcal{F}\{g_0(x, y)\}$$

Goodman, *Introduction to Fourier Optics*, (2017)

# Scalar wave theory – the optical Fourier transform

*“to waist”*

$$u_L(x, y) \propto \mathcal{F}\{g_0(x, y)\}$$

*“For propagation over some distance to a waist”*

**Short description:** propagator based on the **Fourier transforming property** of a lens using 1x FFT.

## **General use:**

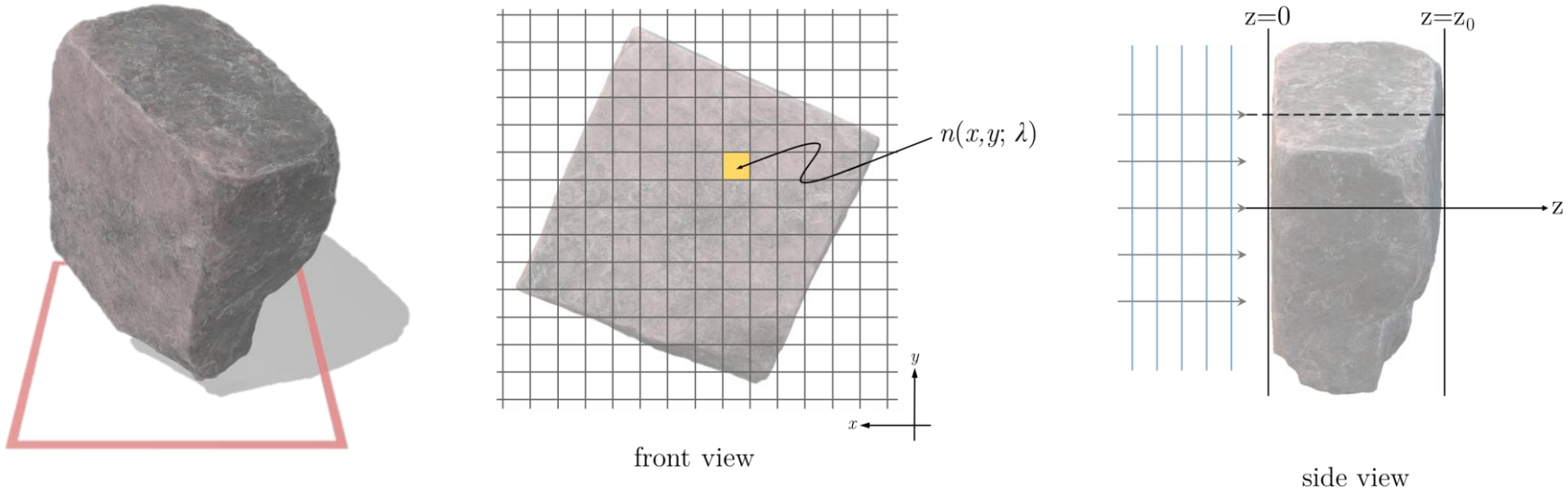
- propagation of a wavefront to a waist (image plane);
- output plane several times smaller than the input plane;

## **Comments:**

- preserves number of pixel but the ranges are re-scaled;
- fails for astigmatic systems.

# Thin optical elements

Consider the following 3D scattering element:



(a) representation of a weak 3D scattering volume



# Thin optical elements

If the scatterer is **sufficiently weak** as to **minimally disturb the path** that the wave-field would have taken in its absence:

$$u_{\text{thin}}(x, y) \approx \exp \left\{ -\frac{jk}{2} \int_{z=0}^{z=z_0} [1 - n^2(x, y)] dz \right\} u_0(x, y)$$

Since  $n = 1 - \delta + j \cdot \beta$  and because  $1 - \delta \approx 1$  we can approximate:  $1 - n^2 \approx 2(\delta + j \cdot \beta)$ :

$$u_{\text{thin}}(x, y) \approx \exp \{ -jk[\delta(x, y) + j \cdot \beta(x, y)]\Delta_z(x, y) \} u_0(x, y)$$

The complex transmission operator in projection approximation can be written as:

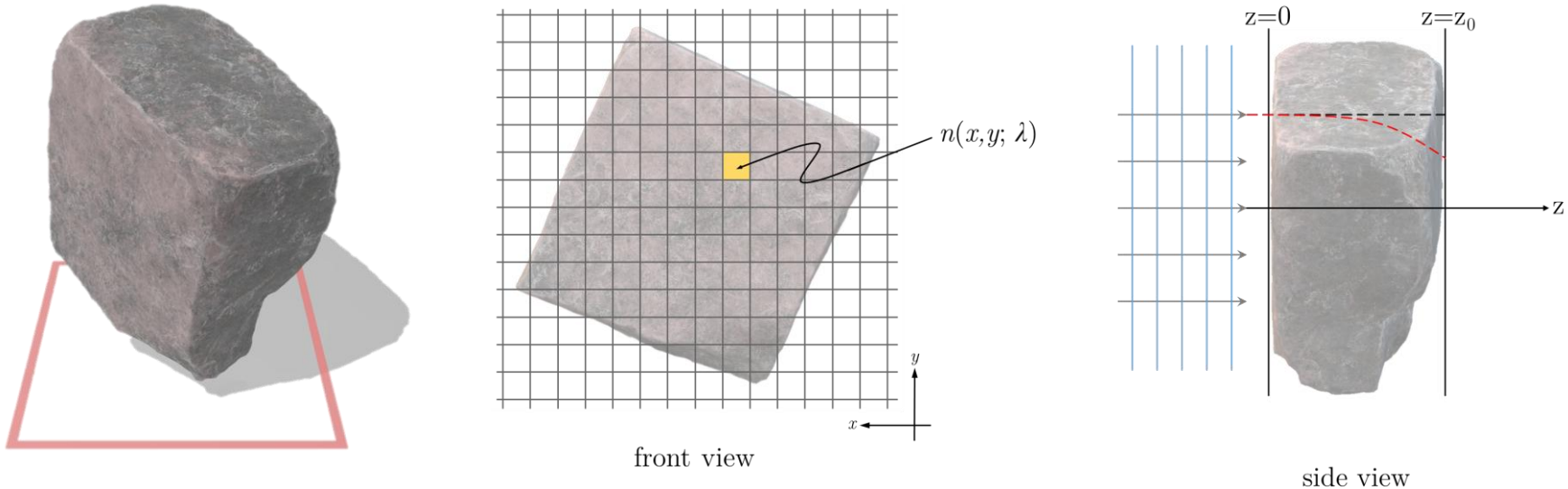
$$T[\Delta_z(x, y)] = \exp \{ -jk[\delta(x, y) + j \cdot \beta(x, y)]\Delta_z(x, y) \} = \sqrt{T_{\text{BL}}(\Delta_z)} \cdot \exp[j\phi(\Delta_z)]$$

Finally:

$$u_{\text{thin}}(x, y) = T[\Delta_z(x, y)] \cdot u_0(x, y)$$

# Thick optical elements

We consider now the following 3D scattering element:



(a) representation of thick scattering volume

# Thick optical elements

A **thick** optical **element** can be **sliced** into a number  $N$  of parallel slabs **until the projection approximation holds** between two adjacent slices **separated by vacuum**.

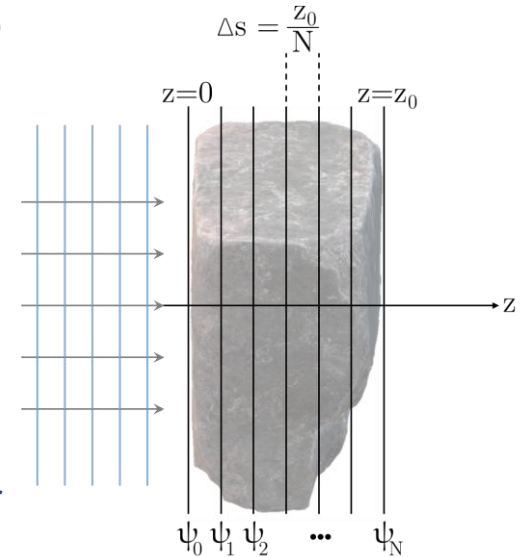
The wave propagation through this thick element is given by:

$$u_{MS}(x, y) = \prod_{i=1}^N \mathcal{D}(\Delta s) \cdot [T_i(\Delta z) \cdot u_0(x, y)]$$

Where  $\mathcal{D}(\Delta s)$  is an operator form of a free-space propagator over  $\Delta s$ .

See also:

- Li, Wojcik and Jacobsen, *Opt. Express* 25(3), 1831 (2017)
- Munro, *J. Opt. Soc. Am. A* 36(7), 1197 (2019)



side view

(a) representation of a thick scattering volume as a series of thin elements (multi-slicing)

Paganin, *Coherent X-Ray Optics*, (2006)

# Thick optical elements

Alternatively, a **thick** optical **element** (e.g. grazing incidence mirrors) can be represented by:

$$u_{\text{thick}}(x, y, x^-, y^-) \approx \mathbf{G}(x, y) \cdot \exp[jk \cdot \Lambda(x, y)] \delta_D[x^- - u(x, y)] \delta_D[y^- - v(x, y)] \cdot u_0(x^-, y^-)$$

where the superscripts ‘-’ indicate ‘before interaction’ and:

- $\mathbf{G}(x, y)$  is a matrix function defining local transformations of the electric field components;
- $\Lambda(x, y)$  is a scalar function defining the corresponding optical path difference;
- $\delta_D[x^- - u(x, y)]$  and  $\delta_D[y^- - v(x, y)]$  are scalar functions defining the transformation of the coordinates for points in the transverse planes before and after the optical element.

Algorithms for their numerical calculation can be found by using the **stationary phase method** and/or by **applying** (locally) the laws of **geometrical optics** and **boundary conditions** for the electric field components

See also:

- Zachariasen, *Theory of X-Ray Diffraction in Crystals* (1945)
- Sutter, Chubar and Suvorov, *Proc. SPIE* 9202(3), 1831 (2014)
- Sutter et al, *Proc. SPIE* 11493(0V), 1831 (2020)

Canestrari, Chubar and Reininger, *J Synchrotron Rad* 21(5), 1110–1121 (2014)

# Where to learn more?

## SRW:

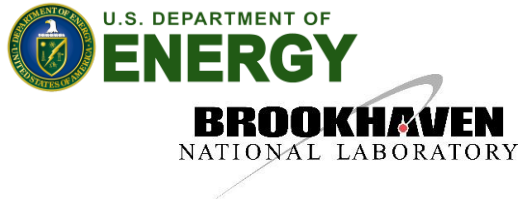
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# Acknowledgment

The author is grateful to **Oleg Chubar**, Brookhaven National Lab, for all the fruitful discussions regarding accurate optical simulations, physical optics and SRW. The author is also thankful to everyone who contributed to the SRW project in any capacity.



**Thank you!**