The Wavefront Propagation Tool PHASE

Johannes Bahrdt
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Limits of Ray Tracing Algorithms

Ray tracing codes have been developed over the last 30 years at 1^{st}, 2^{nd}, 3^{rd} generation synchrotron radiation facilities

geometrical optic is justified if radiation
is emittance dominated:

$$\sigma_{electron} = \sqrt{\varepsilon \cdot \beta} >> \sigma_{photon} = \frac{1}{\pi\sqrt{2}}\sqrt{\lambda \cdot L}$$

$$\sigma'_{electron} = \sqrt{\varepsilon / \beta} >> \sigma'_{photon} = \sqrt{\lambda / 2L}$$

this limitation is wavelength dependent
vertical emittance usually 1% of horizontal emittance

⇨ in 3rd generation light sources coherent effects show up
for low energies
in vertical plane

⇨ 4th generation machines have a high degree of transverse coherence
physical optics propagation methods are required

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Brightness definition from electric fields:

$$B_0(\vec{x},\vec{\Phi}) = c\int A(\vec{x},\vec{\xi})\cdot \exp\left[i\frac{2\pi}{\lambda}\vec{\Phi}\cdot\vec{\xi}\right]\cdot d\vec{\xi}$$

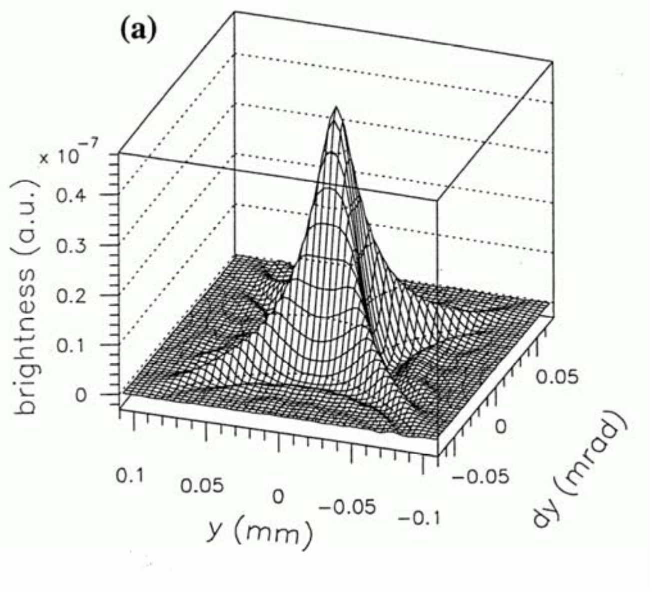
$$A(\vec{x},\vec{\xi}) = \vec{E}_y^*(\vec{x}+\vec{\xi}/2)\cdot\vec{E}_y(\vec{x}-\vec{\xi}/2) + \vec{E}_z^*(\vec{x}+\vec{\xi}/2)\cdot\vec{E}_z(\vec{x}-\vec{\xi}/2)$$

brightness is not positive definite:
derivation of physical properties via integration over space or solid angle

Diffraction at an Aperture:
Convolution with aperture function:

$$G(\vec{x},\vec{\Phi}) = \frac{1}{\lambda^2}\int d\vec{\xi}\cdot S^*(\vec{x}+\vec{\xi}/2)\cdot S(\vec{x}-\vec{\xi}/2)\cdot\exp(i\frac{2\pi}{\lambda}\vec{\Phi}\cdot\vec{x})$$

Convolution with beam emittance is straight forward

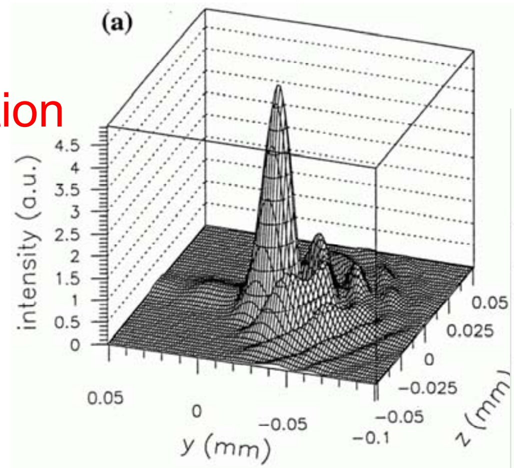


Realistic description of the coordinate and angle correllation of an undulator source in the brightness formalism

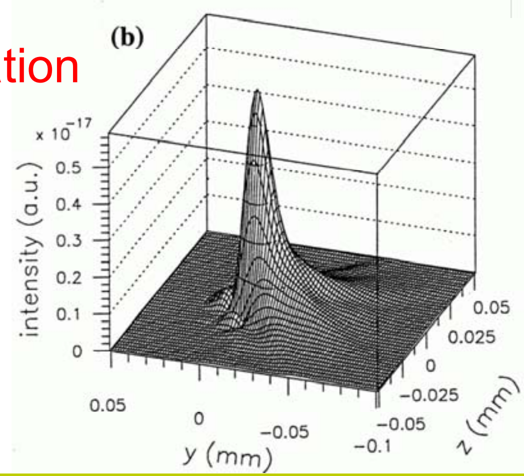
Limits of Brightness Formalism: Mutual Interference

20:1 demagnification of a dipole source
grazing angle 10°

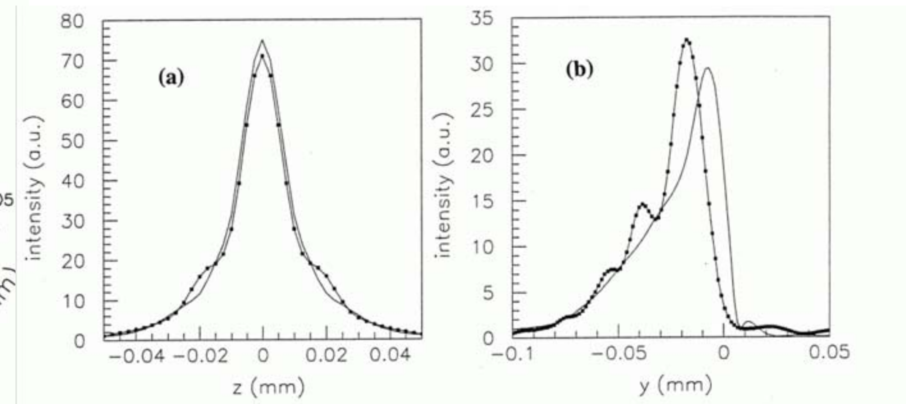
PHASE
transformation



brightness
transformation



comparison with ray tracing result



+ realistic description of source phase space
+ diffraction at apertures
+ simple implementation of beam emittance
- no mutual interference, variation of polarization etc

Features of the Code PHASE

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Geometrical optics

Ray-Tracing including slope errors
Automated beamline optimization

Brightness

Physical optics

free space propagation of electric fields
propagation across optical elements
time / frequency dependent simulations

Wavefront propagation methods of PHASE

stationary phase approximation (SPA)
FFT near field approximation
FFT far field approximation
FFT Fraunhofer approximation

Simulation method of SPA

based on a matrix formalism for nonlinear transformations
of various parameters across the elements
the code is generated with the algebraic code REDUCE

Free Space Propagation

Method A: Integration of the equation of Fresnel and Kirchhoff

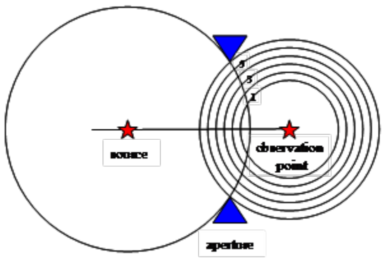
$$\vec{E}(z',y') = \frac{1}{\lambda}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\vec{E}(z,y)\,\frac{e^{i\vec{k}(\vec{r}-\vec{r}\,')}}{|\vec{r}-\vec{r}\,'|}\cos(\beta)\cdot dy\cdot dz$$

Method B: Fourier Optics (FO)

large Fresnel numbers (F>>1)
near field approximation (fixed grid)

small Fresnel numbers (F<<1)
far field and Fraunhofer approximation (non fixed grid)

$$F = \frac{a^2}{\lambda\cdot f}$$



a = radius of aperture
f = focal length = distance to aperture for parallel beams
= distance of mirrors in confocal resonator

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Method B1: Fourier optics, near field approximation

$$\vec{E}_0(\nu_z,\nu_y)=\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\vec{E}(z,y)\cdot e^{-2\pi i(\nu_z z+\nu_y y)}dy\cdot dz$$

Plane wave expansion of electric fields

$$\vec{E}(\nu_z,\nu_y)=\vec{E}_0(\nu_z,\nu_y)\cdot e^{2\pi i\cdot\Delta x\cdot\sqrt{1/\lambda^2-\nu_z^2-\nu_y^2}}$$

multiplication with a phase factor

$$\vec{E}(z',y')=\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\vec{E}(\nu_z,\nu_y)\cdot e^{2\pi i\cdot(\nu_z z+\nu_y y)}\cdot d\nu_y\cdot d\nu_z$$

back transformation

Grid size in source and image plane is equal
choose grid extension in source plane appropriately
to get equal resolution in source and image plane

Method B2: Fourier optics, far field approximation

$$\vec{E}(z',y',\Delta x)=\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\vec{E}(z,y,0)\cdot t(y'-y,z'-z,x'-x)\cdot dy\cdot dz$$

$$t(y'-y,z'-z,x'-x)=\frac{1}{i\lambda\Delta x}e^{i\frac{kr^2}{2\Delta x}}$$

convolution of source field with point spread function

Rewriting the expressions:

$$\vec{E}(y',z',\Delta x)=\frac{1}{i\lambda\Delta x}e^{i\frac{kr_2^2}{2\Delta x}}FF^{\pm}[\vec{E}(y,z,0)\cdot e^{i\frac{kr_1^2}{2\Delta x}}]$$

where the sign of the FFT depends on the direction of propagation

Both methods, B1 and B2, are mathematically equivalent,
but the noise behaviour is different, depending on the specific application

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Method B3: Fourier optics, Fraunhofer approximation
(very far field approximation)

for large distances the phase factors in method B2 are approximately one.

$$\vec{E}(y',z',\Delta x) = \frac{1}{i\lambda\Delta x} FF^{\pm}[\vec{E}(y,z,0)]$$

the sign of the FFT depends on the direction of propagation

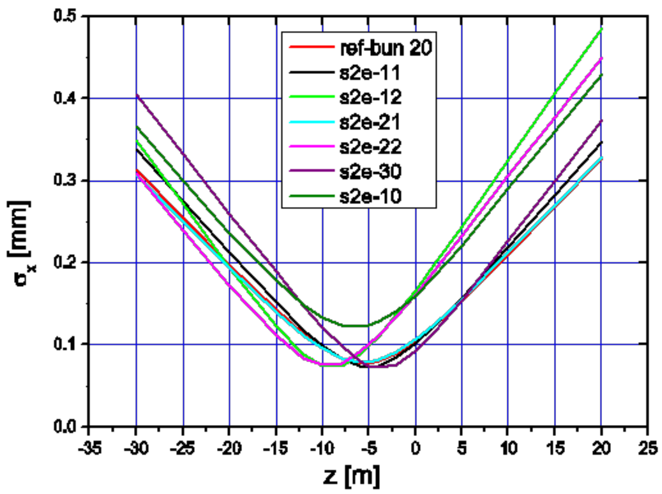
Example: BESSY LE-FEL @114eV

Where is the beam waist?
What is the phase space volume?

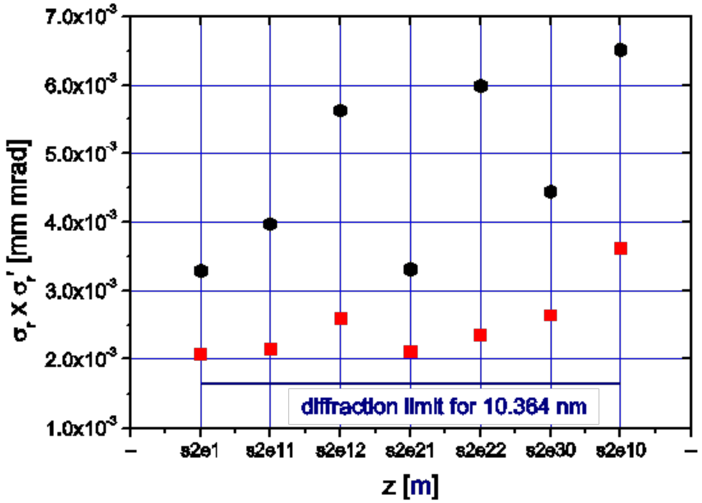
21 slices from time dependent GENESIS simulation
data refer to z=0 (exit of final amplifier)

FFT at each grid point ⟹ frequency spectrum
propagation for frequency of maximum intensity

results from beam propagation



phase space from GENESIS
phase space at the beam waist



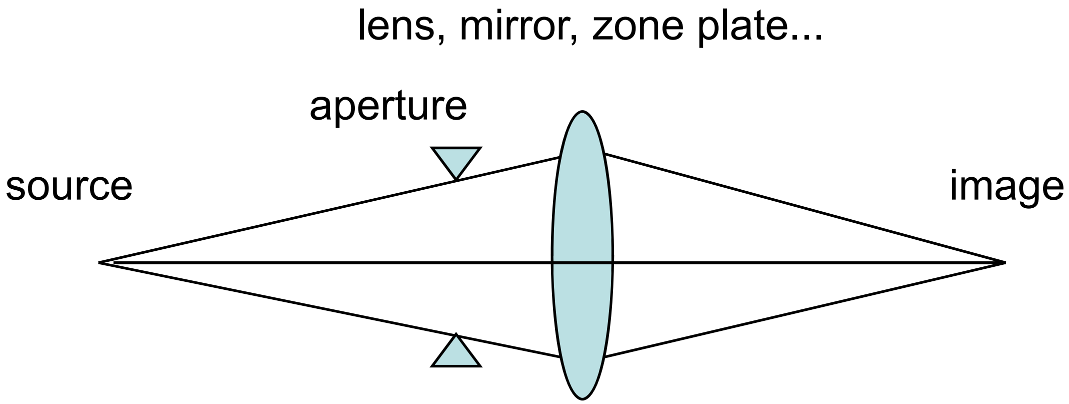
FO-Propagation Across an Optical Element

Normal Iincidence optics:

- free space propagation to the optical element
- multiplication with complex amplitude to account for
  - amplitude variation and
  - phase variation at optical element
- free space propagation

Grazing Incidence optics:

- ray tracing across the optical element instead of multiplication with amplitude / phase factor



Advantages and Limits of Fourier Optics

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Advantages of Fourier optics:

fast: computation time scales with

$$2 \cdot n^2 \cdot \ln(n)$$

as compared to

$$n^4$$

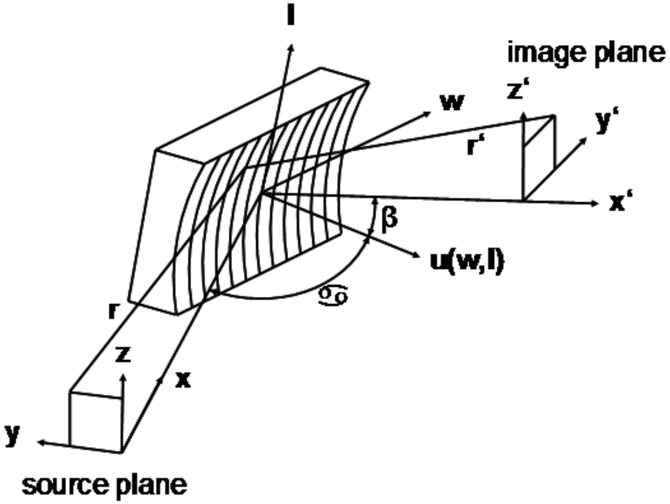
for the stationary phase approximation
(however smaller arrays are needed for SPA)

Limitations of the method:

grid size is not freely choosable
many zeroes have to be computed in case of
strong magnification / demagnification
large arrays are needed
diffraction effects at long mirrors in
grazing incidence geometry are not exactly simulated

Another Method: Stationary Phase Aproximation SPA

Propagation of electric fields along an optical element, starting with Fresnel Kirchhoff:



$$\vec{E}(\vec{a}') = \int h(\vec{a}', \vec{a}) \cdot \vec{E}(\vec{a}) \cdot d\vec{a}$$

with the propagator h

$$h(\vec{a}', \vec{a}) = K \int_{Surface} \frac{\exp(ik(r+r'))}{rr'} \cdot b(w,l) \cdot dw \cdot dl$$

b = complex number describing the optical property of the surface

K = obliquity factor

Matrix Formalism of PHASE

4th order expansion of source coordinates
with respect to image coordinates y‘, z‘, dy‘, dz‘

$$y = \sum_{i+j+k+l \leq 4} a_{ijkl} \cdot y'^{i} \cdot z'^{j} \cdot dy'^{k} \cdot dz'^{l}$$

Similar expansions for phase, determinants...
From expansion above derive expansion of all cross products e.g.:

$$y^2 \cdot z = \sum_{i+j+k+l \leq 4} b_{ijkl} \cdot y'^{i} \cdot z'^{j} \cdot dy'^{k} \cdot dz'^{l}$$

Matrix formalism for transformation of coordinates etc.
(linearization of non linear transformation)

- coordinate vector with y, z, dy, dz and all cross products: $\overline{Y}$
- representation of optical element with a (70 x 70) matrix: $\overline{\overline{M}}$
- transformation of coordinate vector across one element:

$$\overline{Y}_f = \overline{\overline{M}} \cdot \overline{Y}_i$$

Simplification of Propagator h for one optical element

Second order expansion of the optical path length PL around (w_0, l_0) :

$$h(\vec{a},\vec{a}') \propto \frac{1}{r_{w_0,l_0} \cdot r'_{w_0,l_0}} \exp[ik(r_{w_0,l_0} + r'_{w_0,l_0})] \cdot$$

$$\int \exp[ik(\frac{\partial^2 PL}{\partial \Delta w^2} \cdot \frac{\Delta w^2}{2} + \frac{\partial^2 PL}{\partial \Delta l^2} \cdot \frac{\Delta l^2}{2} +$$

$$\frac{\partial^2 PL}{\partial \Delta w \cdot \partial \Delta l} \Delta w \cdot \Delta l)] \cdot d\Delta w \cdot d\Delta l$$

perform analytical integration to infinity

$$\vec{E}(\vec{a}') \propto$$

$$\int \vec{E}(\vec{a}) \cdot \exp[ik(r_{w_0,l_0} + r'_{w_0,l_0})]/(r_{w_0,l_0} \cdot r'_{w_0,l_0}) \cdot$$

$$\left| \frac{\partial^2 PL}{\partial \Delta w^2} \cdot \frac{\partial^2 PL}{\partial \Delta l^2} - \left(\frac{\partial^2 PL}{\partial \Delta w \cdot \partial \Delta l} \right)^2 \right|^{-1/2} \cdot d\vec{a}$$

→ **SPA reduces the dimensions of integration from 6 to 4!**

Propagator h for several optical elements I

Heuristic Approach: valid for one optical element

$$\left| \frac{\partial^2 PL}{\partial \Delta w^2} \cdot \frac{\partial^2 PL}{\partial \Delta l^2} - \left(\frac{\partial^2 PL}{\partial \Delta w \cdot \partial \Delta l} \right)^2 \right| \cong \frac{\cos(\alpha) \cdot \cos(\beta)}{r^2 r'^2} \cdot \left| \frac{\partial(y,z)}{\partial(dy',dz')} \right|$$

General approach needed for a combnation of N optical elements

Path length PL for N optical elements:

$$PL = \sum_{\substack{p,q=1\ldots N \\ r_p=\{0,2\} \\ s_q=\{0,2\} \\ r_p+s_q=2 \\ k+l+m+n\leq 4}} PLC(k,l,m,n,r_p,s_q) \cdot y_i^k \cdot z_i^l \cdot dy_i^m \cdot dz_i^n \cdot \Delta w_p^{\ r_p} \cdot \Delta l_q^{\ s_q}$$

The propagator has the form:

$$\tilde{h}(w_{10}, l_{10}, \ldots w_{N0}, l_{N0}) \propto \frac{1}{\prod_{i=1}^{N+1} r_0^i} \cdot \exp[ik(r_0^1 + \ldots + r_0^{N+1})] \cdot$$

$$\int \cdots \int \exp[ik(\sum_{p,q=1}^{N} \sum_{r_p+s_q=2}^{2} \frac{\partial^{r_p+s_q} PL}{\partial \Delta w_p^{r_p} \cdot \partial \Delta l_q^{s_q}} \cdot \frac{\Delta w_p^{r_p} \cdot \Delta l_q^{s_q}}{r_p! \cdot s_q!})] \cdot d\Delta w_1 \cdot d\Delta l_1 \cdots d\Delta l_N$$

PL = quadratic form

Propagator h for several optical elements II

The quadratic form can be represented by

$$PL = \overrightarrow{X}^T \cdot \overline{\overline{G}} \cdot \overrightarrow{X}$$

$$\overrightarrow{X} = (x_1, \cdots x_{2N}) = (\Delta w_1, \Delta l_1 \cdots \Delta l_N)$$

The matrix $\overline{\overline{G}}$ can be converted to a diagonal form using an orthogonal transformation $\overline{\overline{K}}$ (principle axis theorem)

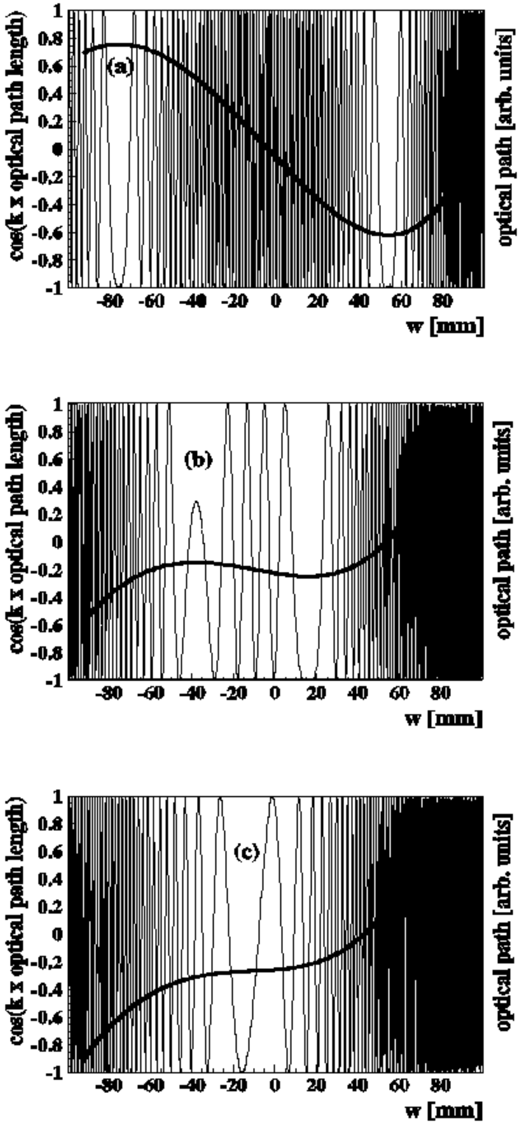
$$\begin{pmatrix} \lambda_1 & 0 & 0 \\ 0 & \ldots & 0 \\ 0 & 0 & \lambda_N \end{pmatrix} = \overline{\overline{K}}^T \cdot \overline{\overline{G}} \cdot \overline{\overline{K}}$$

A seperation of integrals and an analytic integration simplifies the expression of the propagator:

$$\tilde{h}(w_{10}, l_{10}, \ldots w_{N0}, l_{N0}) \propto$$

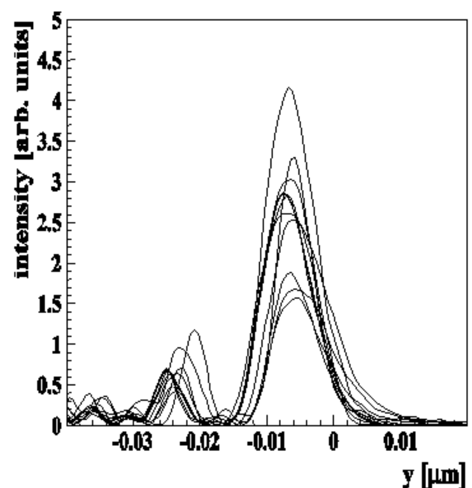
$$= \frac{1}{\prod_{i=1}^{N+1} r_i} \cdot \frac{\partial(\Delta w_1 \cdots \Delta l_N)}{\partial(\upsilon_1 \cdots \upsilon_{2N})} \cdot \left(\frac{2\pi}{k}\right)^N \cdot \frac{1}{\sqrt{|\lambda_1 \cdots \lambda_{2N}|}} \cdot e^{im\pi/2} \cdot e^{-iN\pi/2}$$

Singularities



The anayltic integration requires a sufficient separation of principle rays (top).

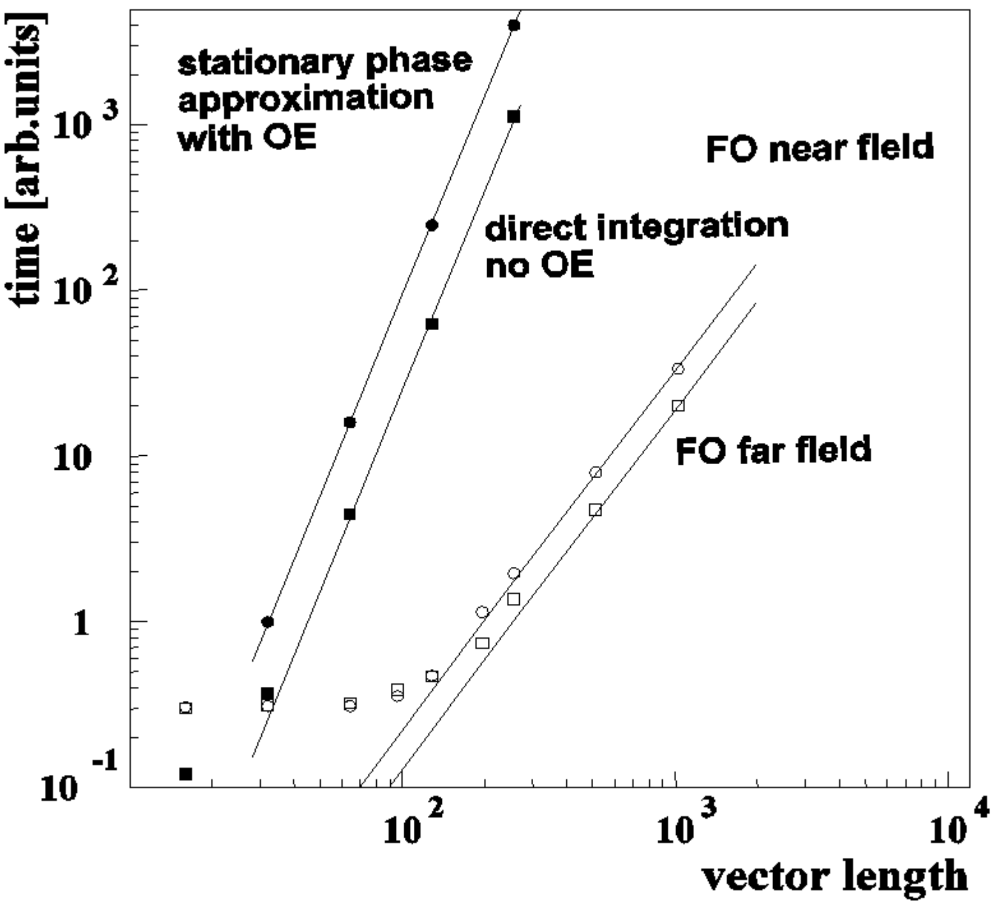
For one or two optical elements the source and image plane have to be chosen appropriately to guarantee a separation of principle rays.



Thick line: principle rays are well separated.
Thin lines: principles rays are close and the results are noisy.

For three or more optical elements the principle rays are well seperated and no singularities show up.

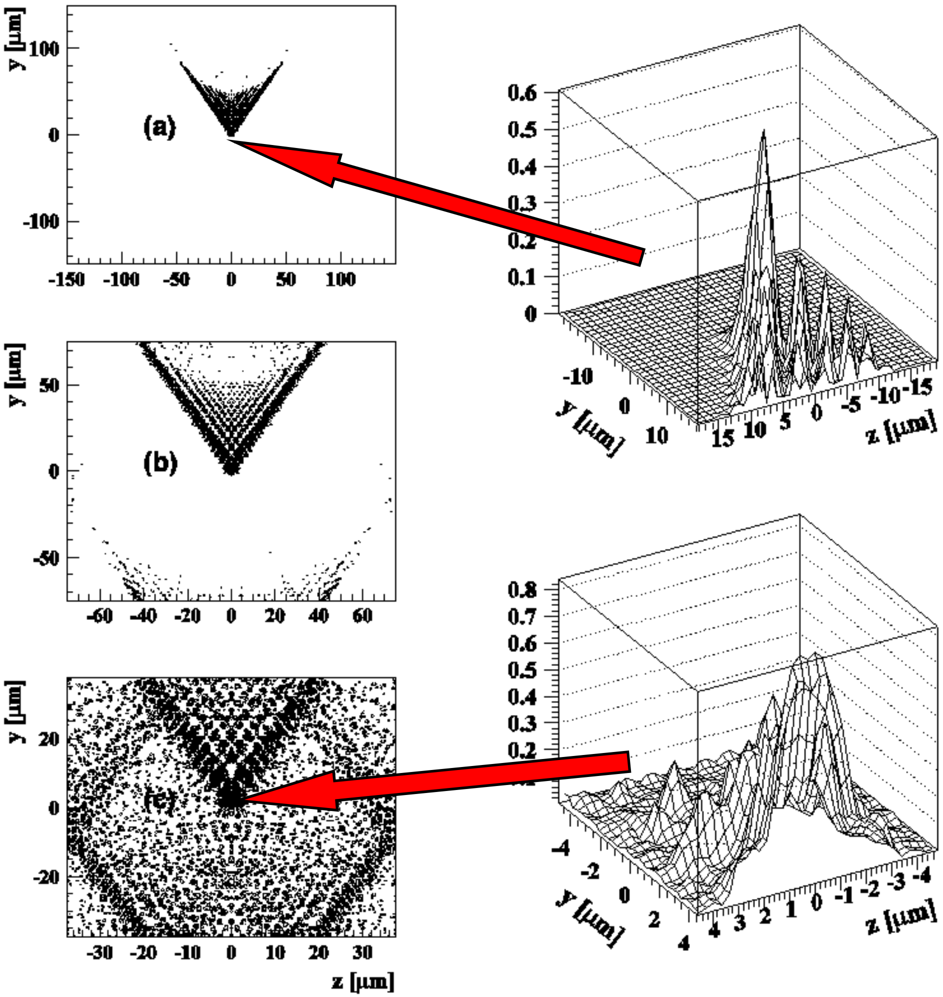
Comparison of Different Propagation Shemes



For a given vectror length Fourier optics (FO) is much faster as compared to the stationary phase approximation (SPA)

However:
the SPA requires much smaller vectors than FO to propagate the same information

Strong Demagnification in Fourier Optics



20:1 demagnification of a Gaussian source. The noise in the image plane increases if the image size is reduced.

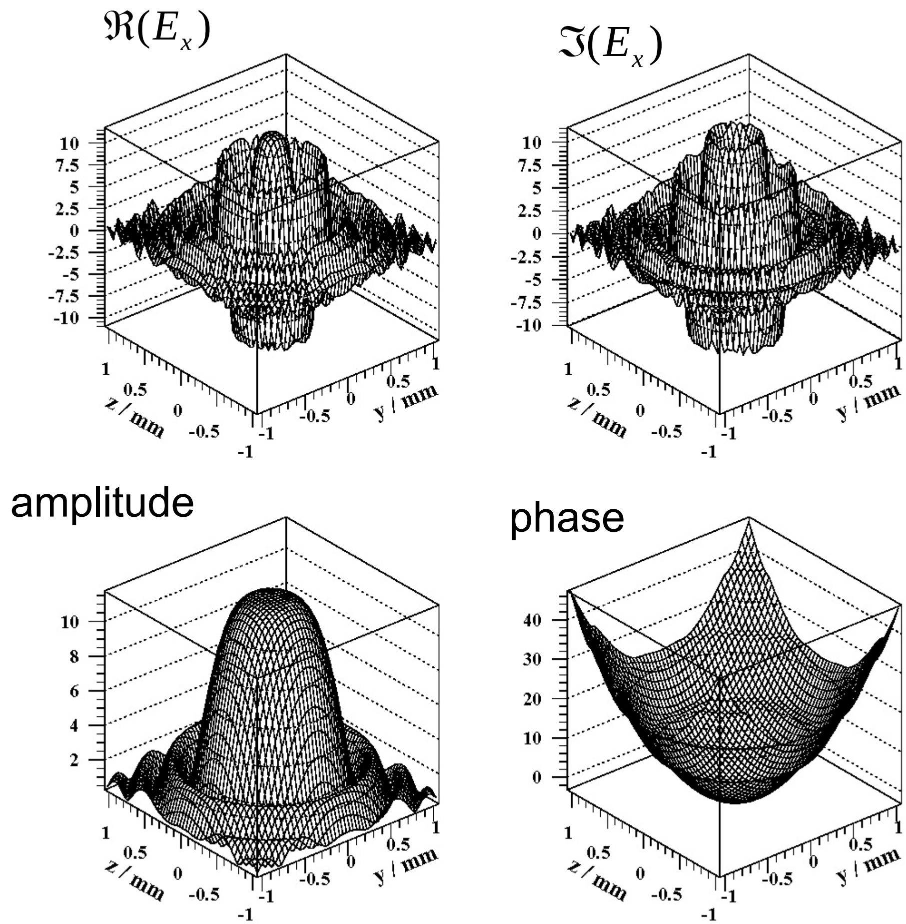
Though the information is concentrated only in a small area large arrays have to be propagated.

Within the SPA only the relevant part in the image plane has to be evaluated.

Representation of the Source (One Slice)

Real and imaginary parts
of electric field from:
- **Integration of Jackson equation**
  (spontaneous emission)
- **FEL code (GENESIS…)**
  (stimulated emission)

Amplitude and phase
representation permits faster
integration algorithm



Polarization Analysis of Results: Stokes Vectors

Results: Electric fields

$$E_z = A_z \exp\left[i(\vec{k}\cdot\vec{r} - \omega t)\right]$$
$$E_y = A_y \exp\left[i(\vec{k}\cdot\vec{r} - \omega t) + \delta\right]$$

Projection vectors

$$\vec{S}_h = [(1,0)]$$
$$\vec{S}_v = [(0,1)]$$
$$\vec{S}_{45} = [(1,1)]/\sqrt{2}$$
$$\vec{S}_{135} = [(1,-1)]/\sqrt{2}$$
$$\vec{S}_r = [(1,i)]/\sqrt{2}$$
$$\vec{S}_l = [(1,-i)]/\sqrt{2}$$

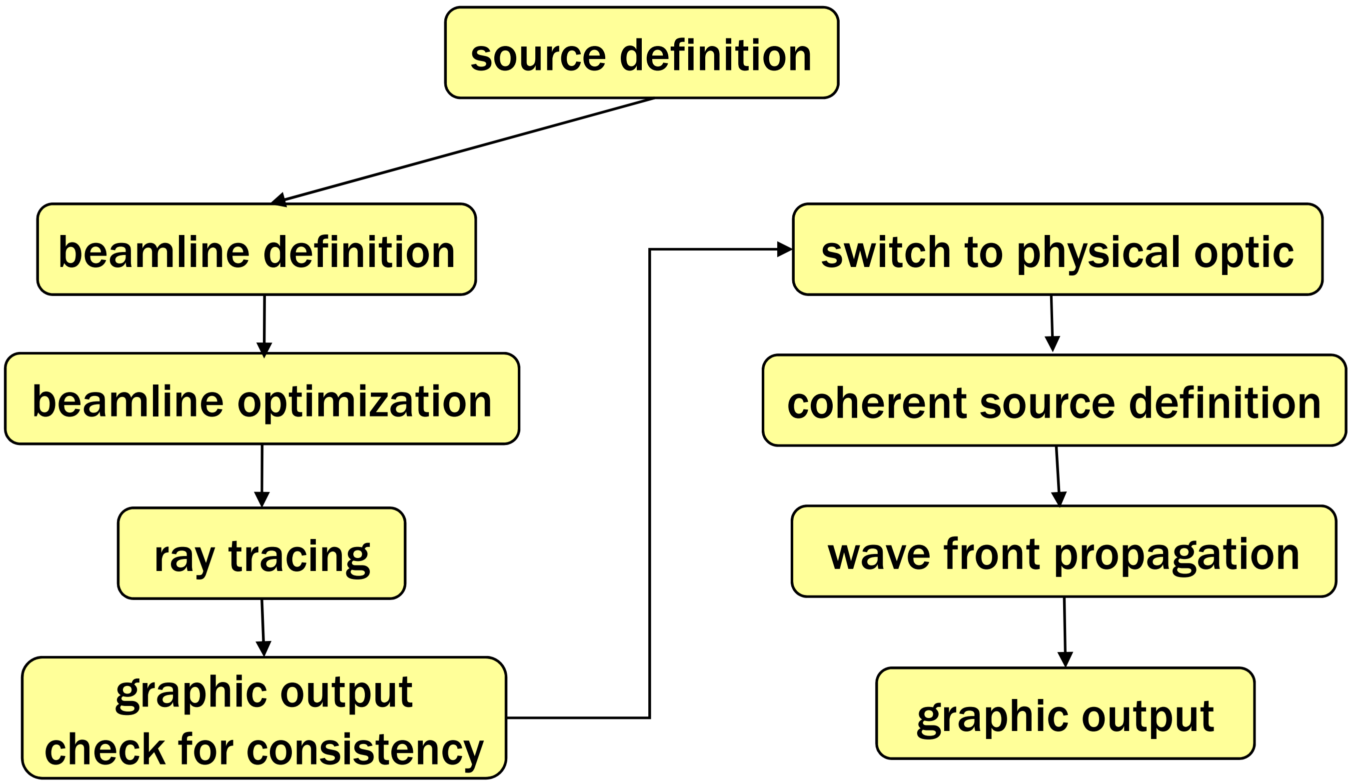
Polarization filter
e.g. circular right handed

$$I_r = \left|\vec{E}\cdot\vec{S}_r^{\,*}\right|^2 = \frac{1}{2}\left|E_z - iE_y\right|^2$$

Stokes parameters

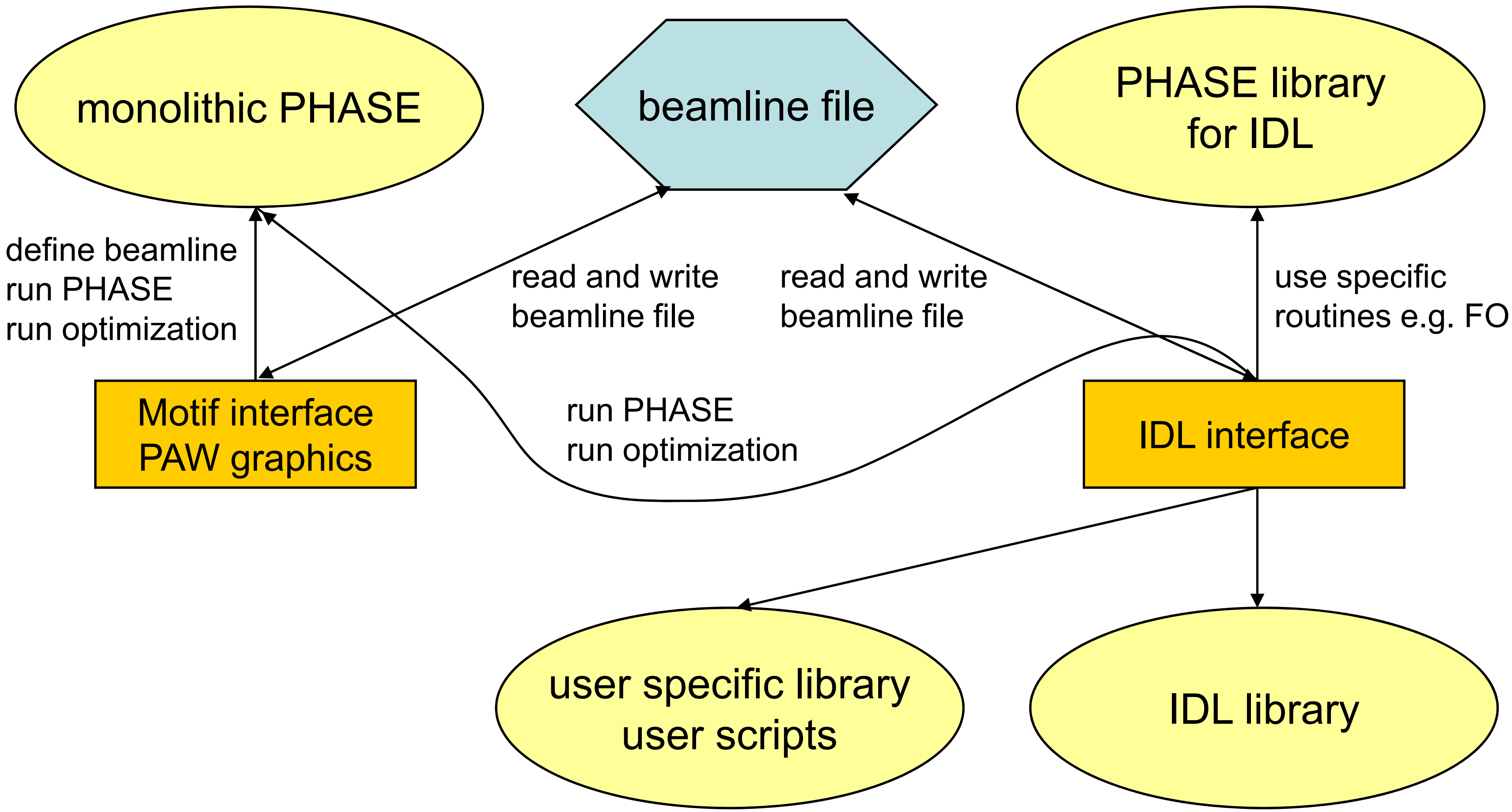
$$S_0 = |A_z|^2 + |A_y|^2 = I_h + I_v$$
$$S_1 = |A_z|^2 - |A_y|^2 = I_h - I_v$$
$$S_2 = 2\cdot|A_z||A_y|\cos(\delta) = I_{45} - I_{135}$$
$$S_3 = 2\cdot|A_z||A_y|\sin(\delta) = I_r - I_l$$

Working with PHASE



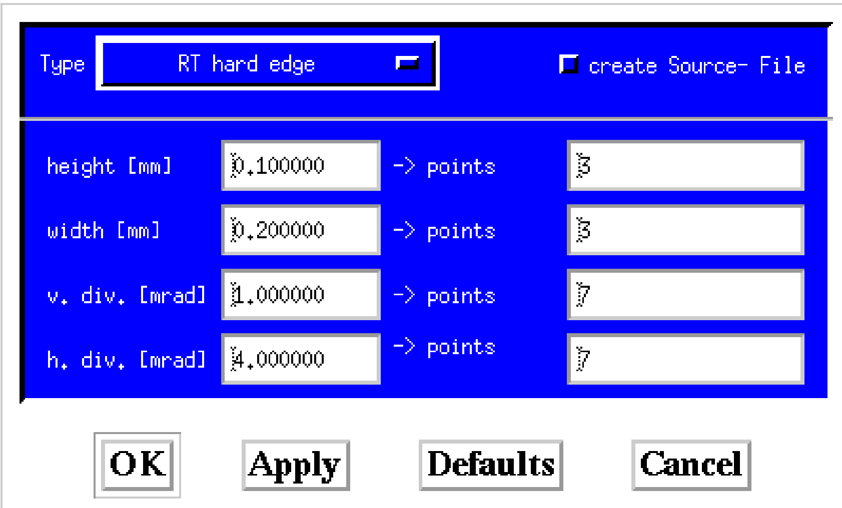
Structure of PHASE

User Interfaces : Motif, IDL
Graphics : PAW (CERN library), IDL
Platform : LINUX



PHASE: Motif Based User Interface I

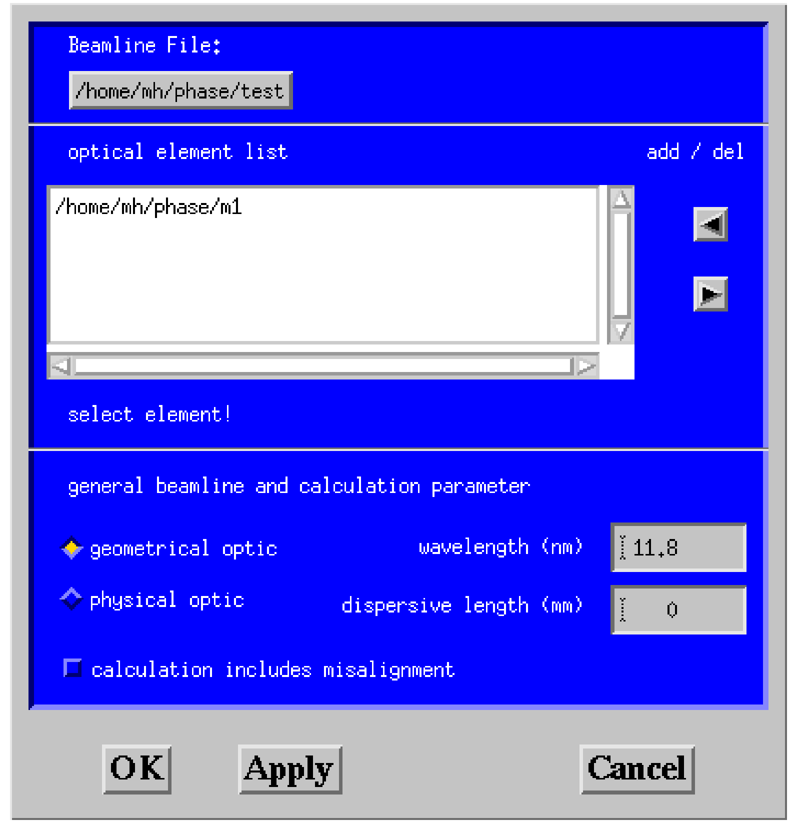
Definition of source



Sources:

- Gaussian source
- hard edge
- undulator source
- source from file

Beamline layout



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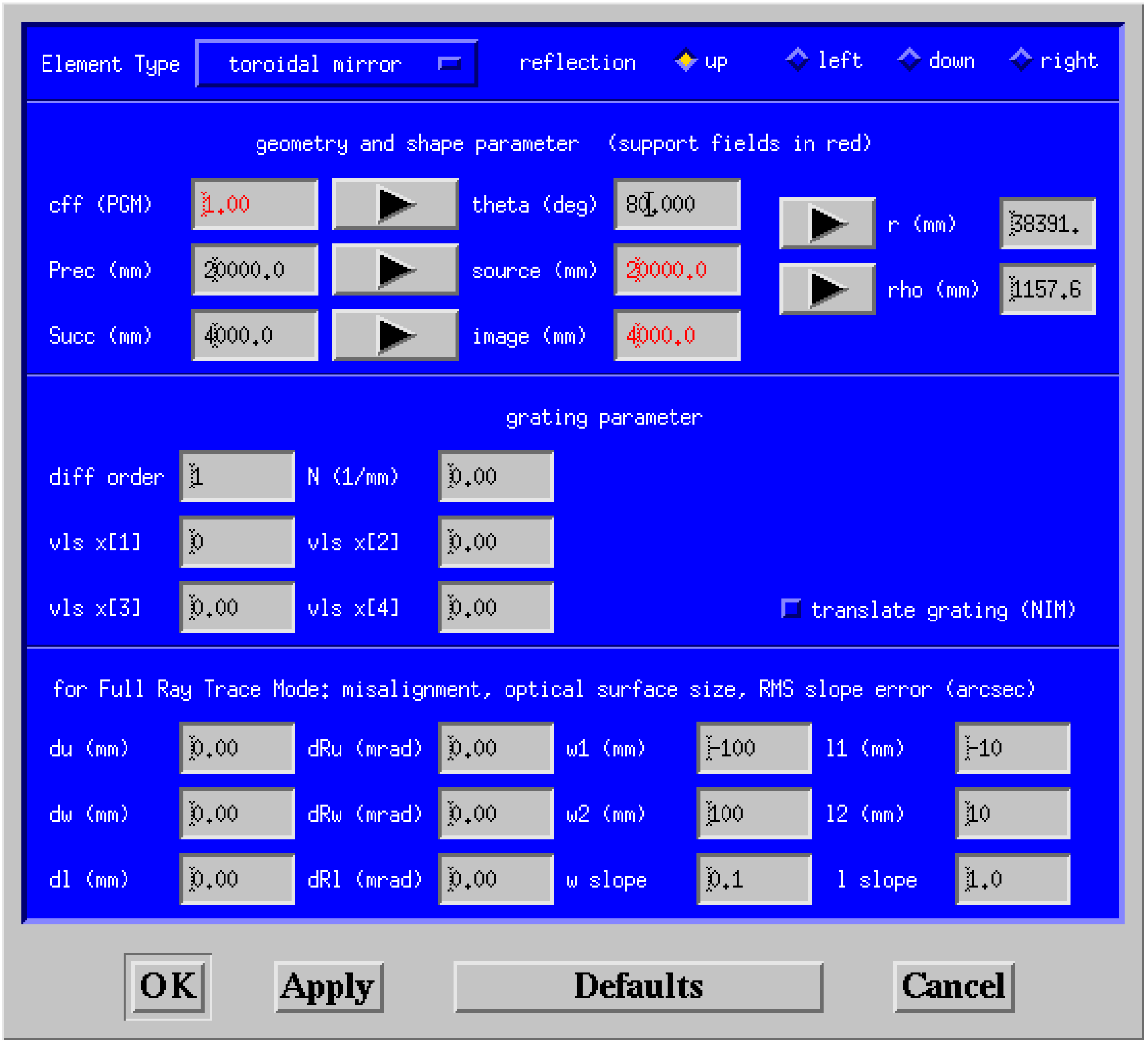
Definition of optical elements



Optical elements
- mirrors
- gratings (VLS)

Surface profile
- limited to 5th order might be enhanced in the future

Slope errors
- Gaussian distribution (ray tracing mode only)

Misalignment
- 3 translations
- 3 rotations

Apertures
- ray tracing mode only in physical optics different algorithm

Beamline Optimization in Geometrical Optics Mode

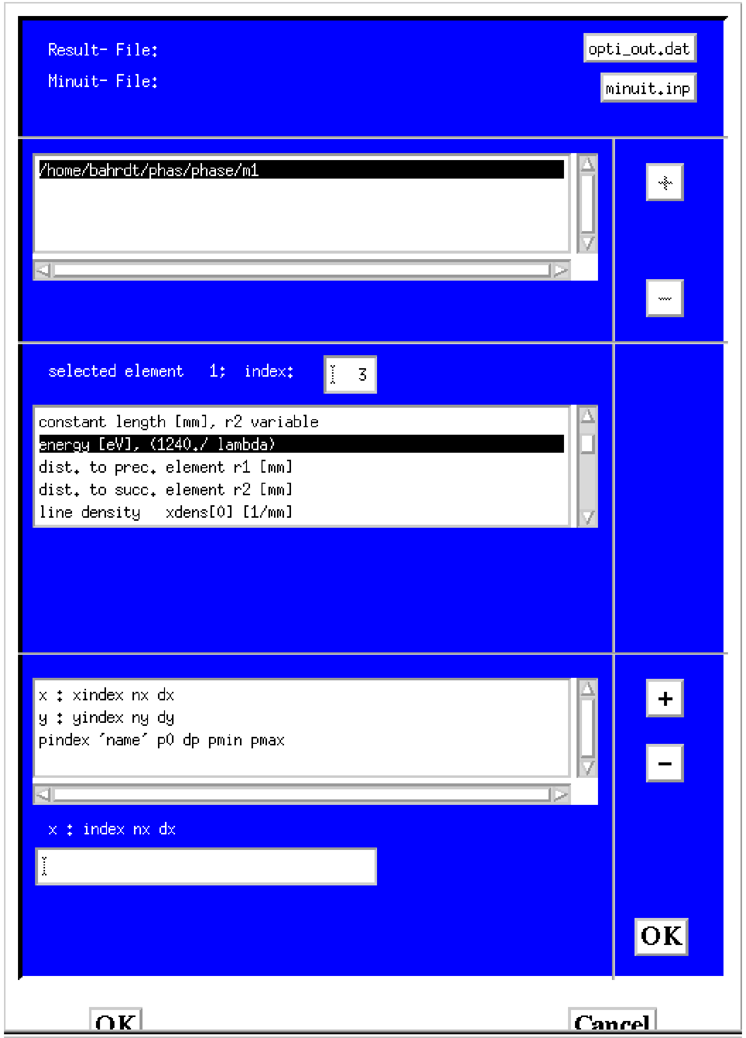


Figure of merit:

- ❑ horizontal focus
- ❑ vertical focus
- ❑ hor. & vert. focus
- ❑ resolving power
- ❑ special cost function

Variables for optimization:

- ❑ distances
- ❑ deflection angles
- ❑ grating line density parameters
- ❑ radii R & rho
- ❑ expansion parameters of surface
- ❑ …

Optimization:

- ❑ multi parameter fit with MINUIT / CERN library
- ❑ systematic variation of 2 specific parameters

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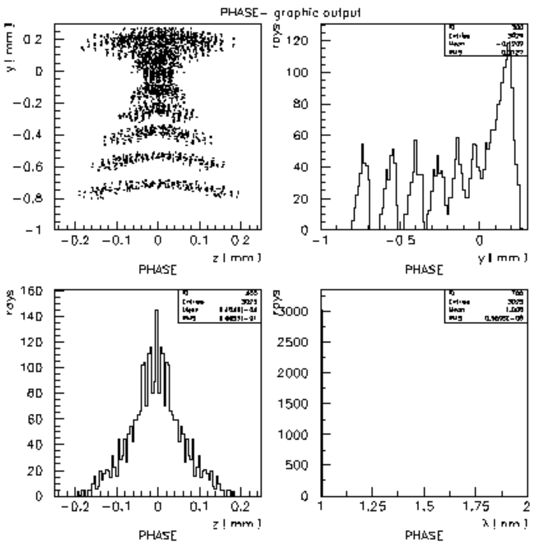
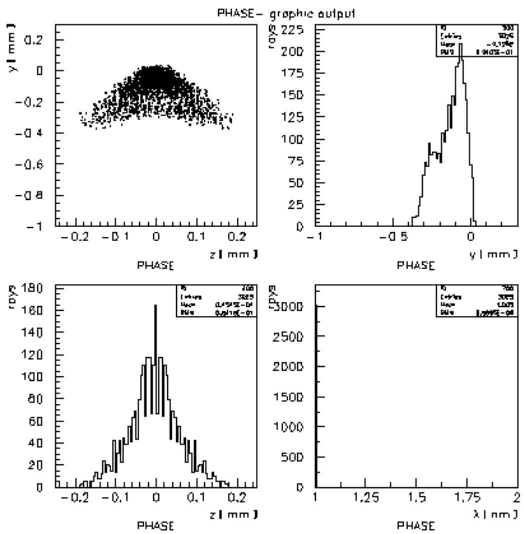
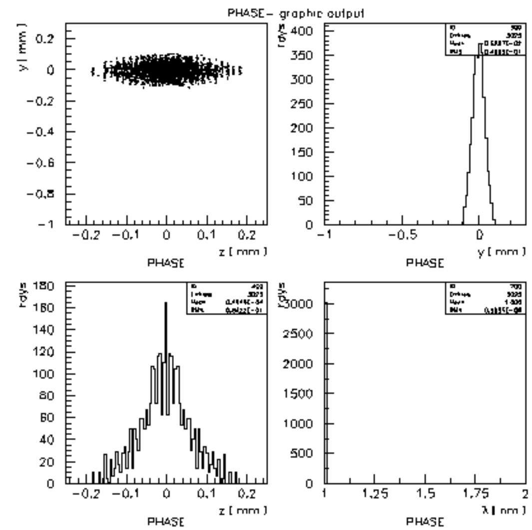
Line density n of the grating:

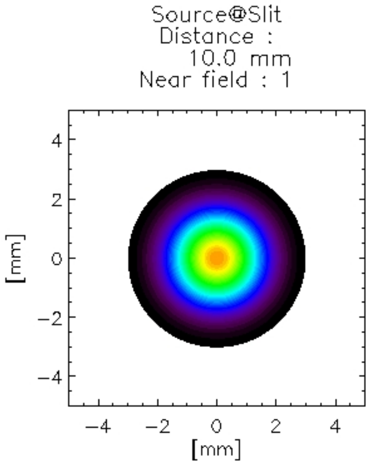
$$n = N_0 + 2 N_1 w + 3 N_2 w^2 + 4 N_3 w^3 + 5 N_4 w^4$$

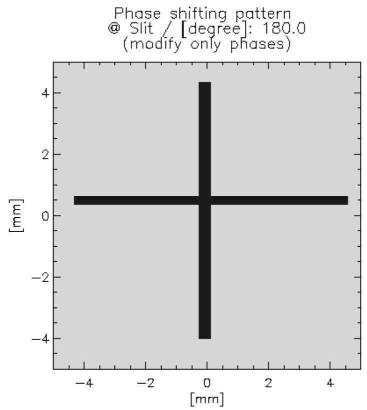


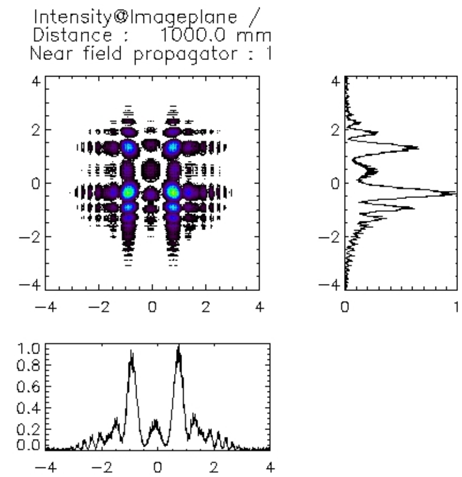


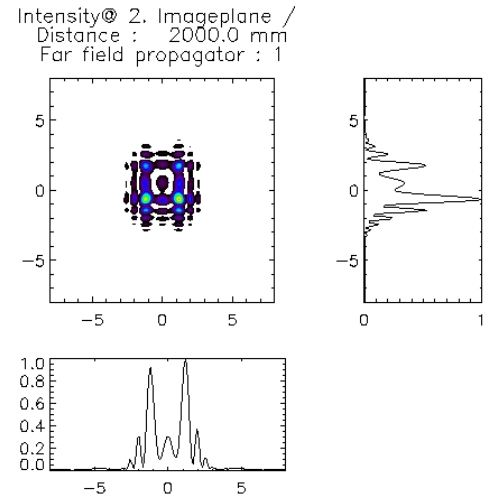


N_0 =1200	N_0 =1200	N_0 =1200
N_1 =0	N_1 =0.244	N_1 =0.244
N_2 =0	N_2 =0	N_2 =0.00178









1 **2** **3** **4**

A short example:

1. beam=phaSrcWFGauss(nz,-size/2, size/2 , ny ,-size/2, size/2, waist, 0, lambda,1,1,0) beam is an array of complex numbers
2. bild = read_bmp('b5_cross.bmp') bild is the phase pattern
   idx = where(bild GT 0.5)
   ezre = beam.zre * cos(phi *!DPI/180D) – beam.zim * sin(phi *!DPI/180D)
   beam.zre(idx) = ezre(idx)
3. phaPropFFTnear, beam, dist1 propagation
4. phaPropFFTfar, beam, dist

Interface Between IDL and Monolithic PHASE

Create new or read old beamline

beamline = phaNewBeamline(blfname) or phaReadBLFile(blfname)

Create source and set apertures

beamline.src.so4 = phaSrcWFGauss(ianzz, zmin, zmax, ianzy, ymin, ymax, w0 , zfoc, xlam, ez0, ey0, dphi_zy)
phaSetApertures, beamline, ….

Create or modify optical element

OptElement = phaNewOptElement('Spieglein an der Wand')
phaDefineOpticalElement , OptElement, ….
phaAddOptElement, beamline, OptElement

Set or modify integration parameters

phaSetIntegrationParameter, beamline , ……
phaSetControlFlags, beamline , ……

Write beamline file and run PHASE

beamline = phaWriteBLFile(blfname)
phaBatchMode, BLfile, ResultFile, cmode

Get results

phaLoadEMField, beamline, MainFileName

Time / Frequency Dependent Simulations

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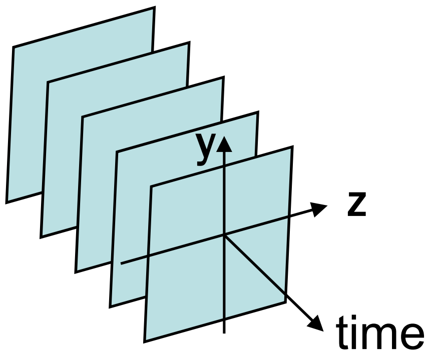
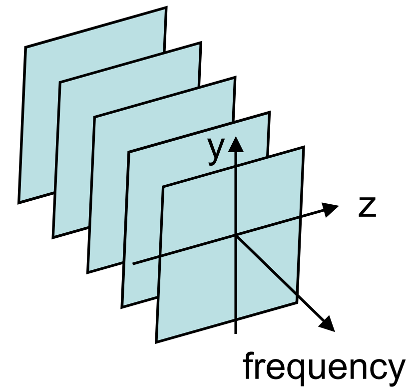
Time domain



FFT for each grid point

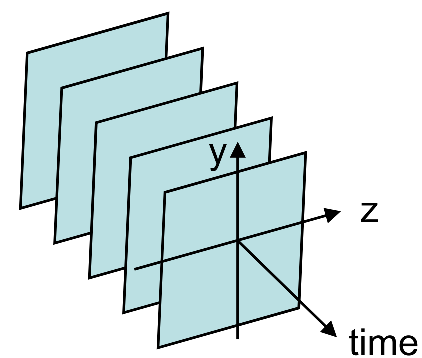
Frequency domain



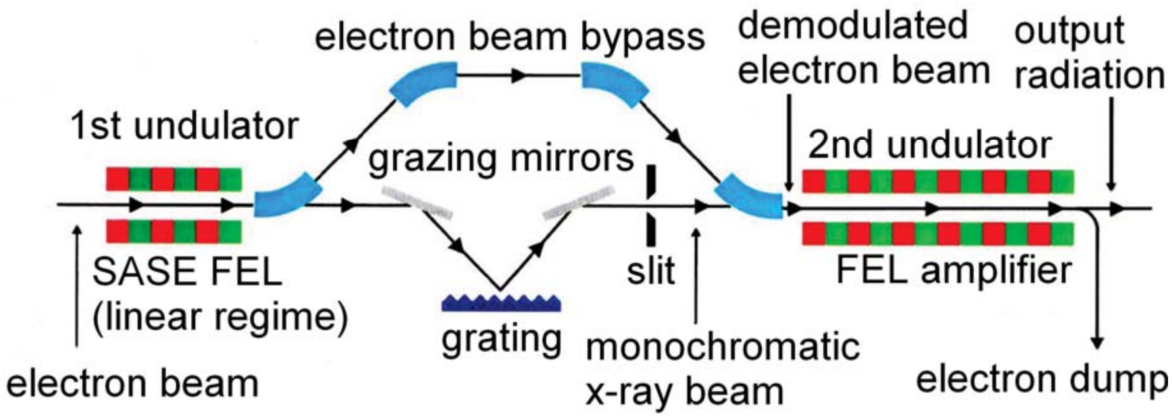
Generation of transverse field distributions with GENESIS, number of slices depends on fine structure in time space: HGHG ⟷ SASE

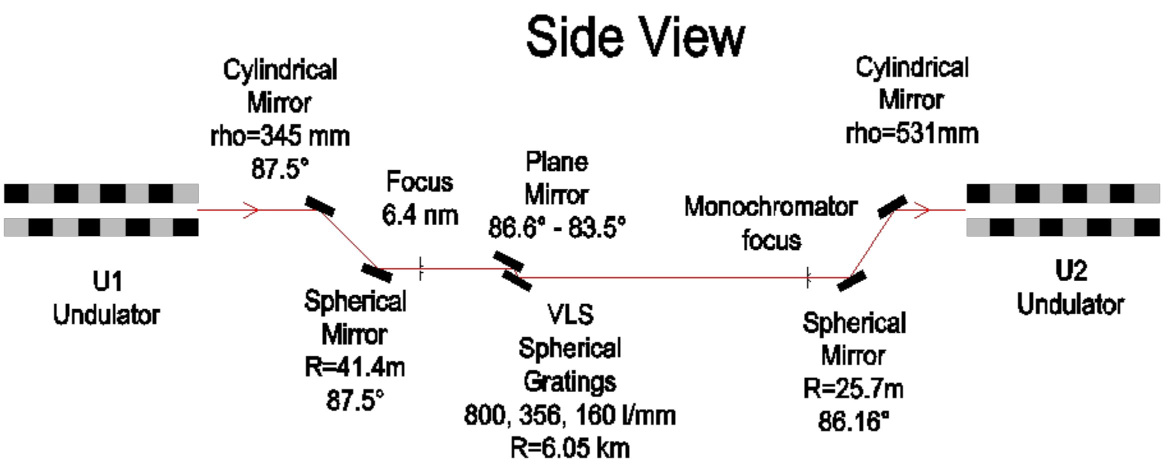
PHASE propagation for each frequency

FFT^{-1} for each grid point



Example: Self Seeding Option at FLASH I





Example: Self Seeding Option at FLASH II

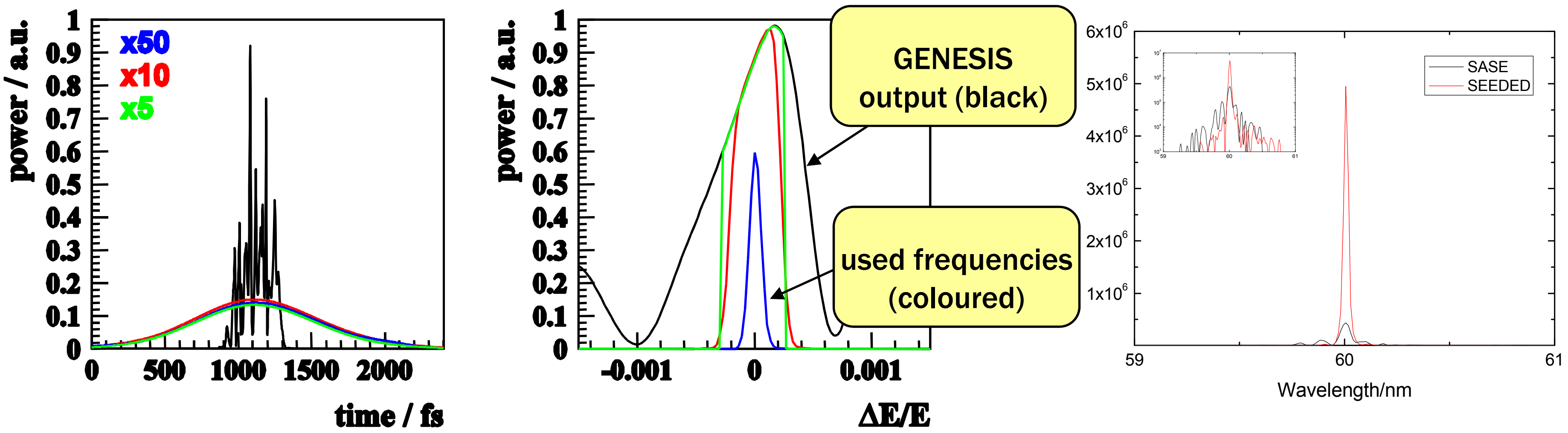
Characteristics of the FEL pulse

behind the 1st undulator & monochromator

behind the 2nd undulator

time domain

frequency domain



Black: directly behind the first undulator
Coloured: behind the monochromator for exit slits of
40µm (blue)
200µm (red)
400µm (green)

unseeded FEL (black)
seeded FEL (red)
one order of magnitude enhancement due to seeding

Summary

- Ray tracing capabilities (limited set of optical elements)
- Automated beamline optimization
- Wavefront propagation with various propagators such as
  Stationary phase approximation propagation
  Fourier optic
- Time and frequency dependent simulations
  using realistic pulse features from time dependent
  FEL codes

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