Coherent Ray Tracing of X-Rays with Bmad

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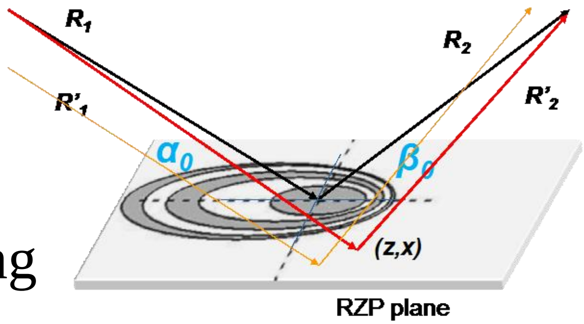
Overview

In Brief: This talk is about how to handle coherence and diffraction effects while doing ray tracing of x-rays and how coherent (and incoherent) ray tracing is being implemented in the Bmad subroutine library.

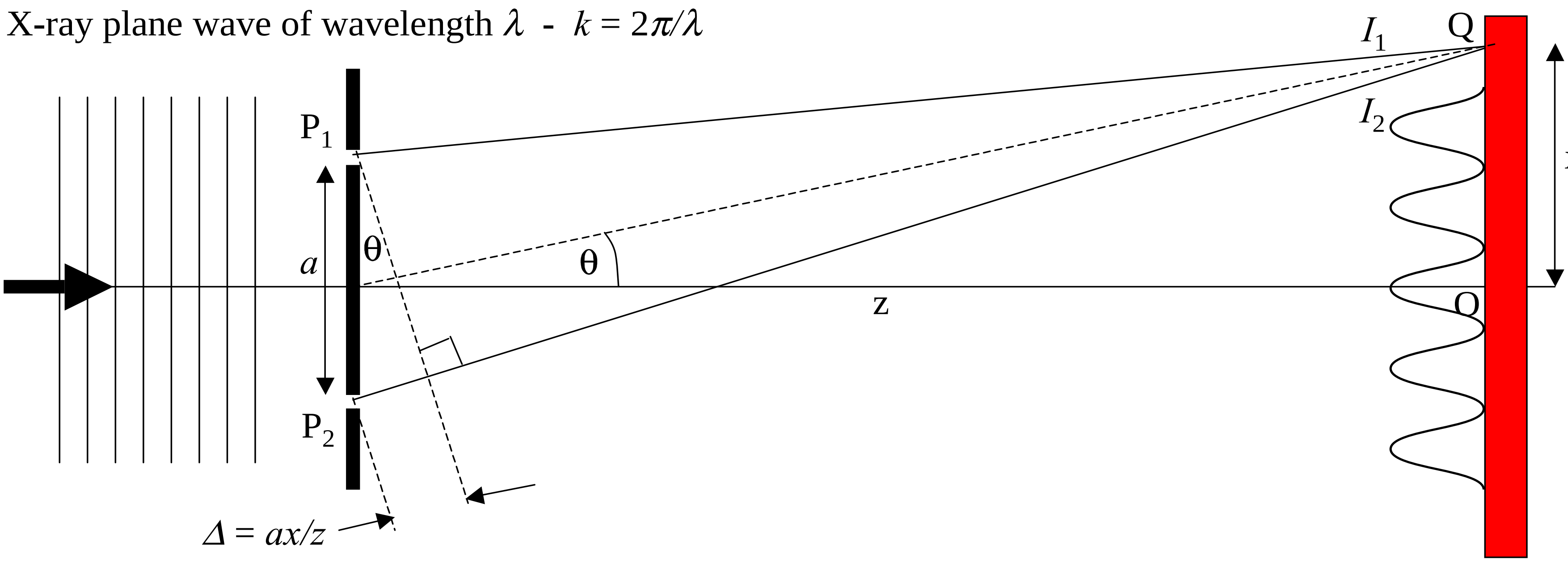
Outline:

- Coherence
  - What is it?
  - How is it useful?
- Simulating X-rays
  - Geometrical (incoherent) ray tracing
  - Wavefront propagation
  - Coherent ray tracing
- State of existing coherent ray tracing codes
- Ray tracing integration with Bmad
- Status, Challenges & Conclusion



Coherence: What is it?

YOUNG'S SLITS EXPERIMENT IN COHERENT ILLUMINATION



ESRF Lecture Series on Coherent X-rays and their Applications, Lecture 2, Malcolm Howells

Coherence means that there is a fixed phase relationship of the EM field between different parts of a beam.

Coherence => Constructive & destructive interference.

Coherence: What is it?

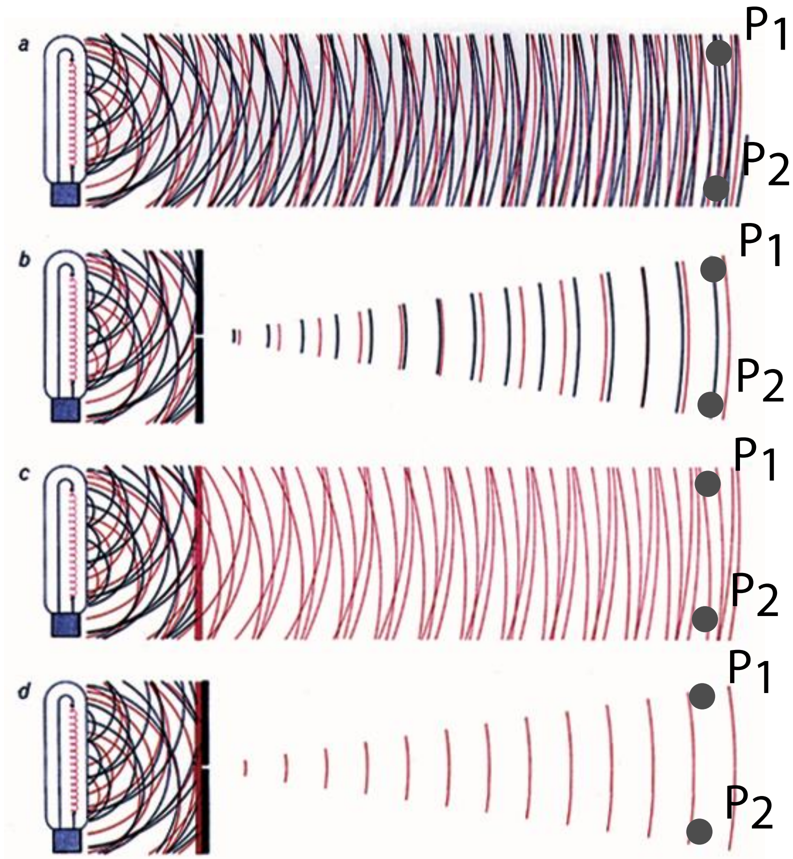
Spatial and Spectral Filtering to Produce Coherent Radiation

Incoherent:

Partially coherent:

Partially coherent:

Coherent:



Courtesy of A. Schawlow, Stanford.

Professor David Attwood
Univ. California, Berkeley

Spatial and Temporal Coherence; Coherent Undulator Radiation, EE290F, 22 Feb 2007

Ch08_F08VG.ai

Radiation may be coherent, incoherent, or somewhere in between

Coherence: How is it Useful?

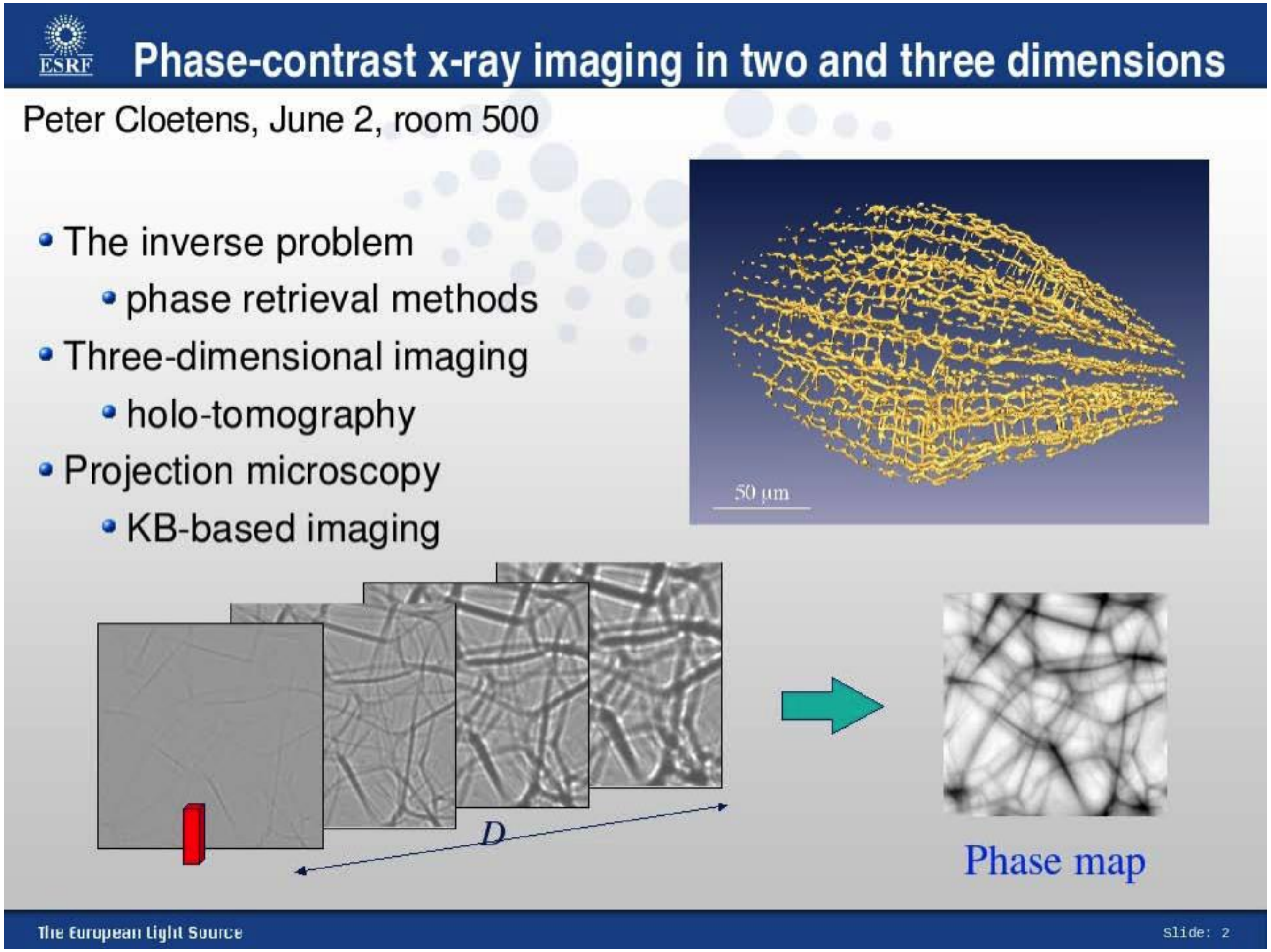
- Measurement of the phase of a scattered beam can be used to help reconstruct the sample under consideration:

> “Coherent x-rays have long been sought as a tool to discover microscopic details of physical and biological assemblies. Such radiation would permit biologists, chemists and physicists to probe with spatial resolutions better than 1,000 Å (perhaps 10 to 100 Å in special circumstances), and with an ability to distinguish concentrations of specific atomic elements.”

Undulators as a Primary Source of Coherent X-rays

D. T. Attwood ; K.-J. Kim ; K. Halbach ; M. R. Howells, 1986

Coherence: How is it useful?

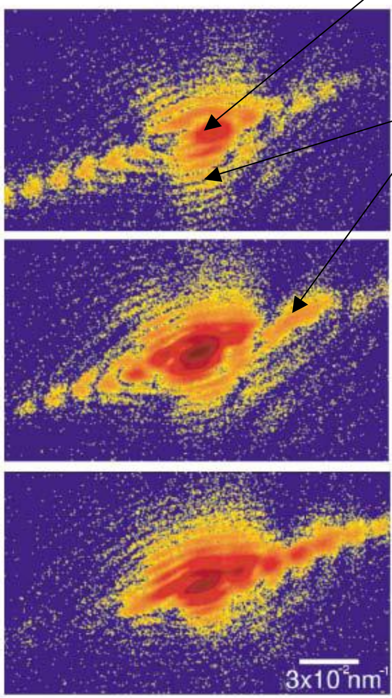


From: Coherent x-rays: overview
ESRF Lecture Series on Coherent X-rays and their Applications, Lecture 1, Malcolm Howells

Coherence: How is it Useful?

APPLICATION TO IMAGING NANOCRYSTALS

Robinson et al PRL, **87**, 195505 (2001), Williams et al PRL, **90**, 175501 (2003)

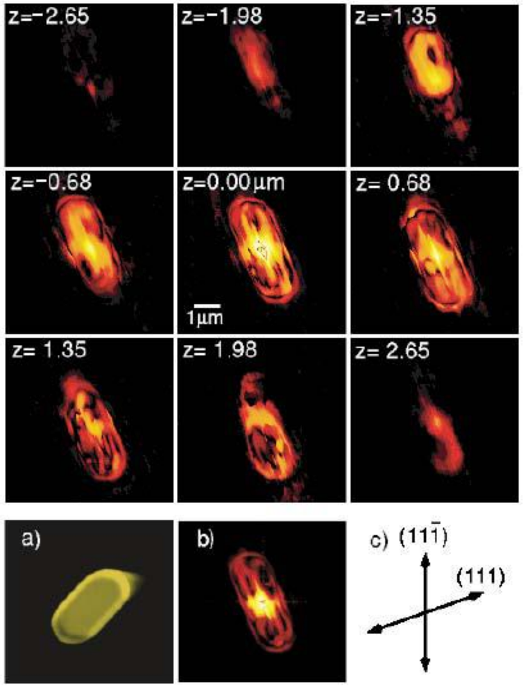


111 Bragg spot of 2 μm Au crystal

Diffraction pattern around the spot (sampled at 30 planes)

Views of the reconstructed image at nine depth values

SEM of nanocrystal



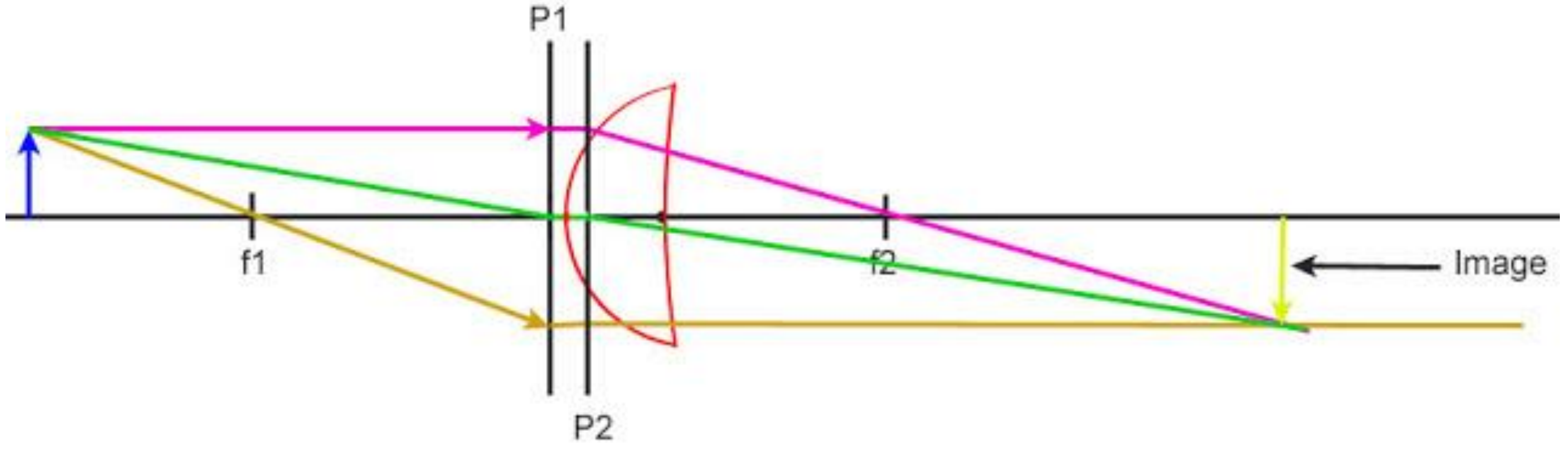
rays and their Applications, Lecture 7, Malcolm Howells

From: ESRF Lecture Series on Coherent X-rays and their Applications, Lecture 7, Malcolm Howells

Geometrical (Incoherent) Ray Tracing

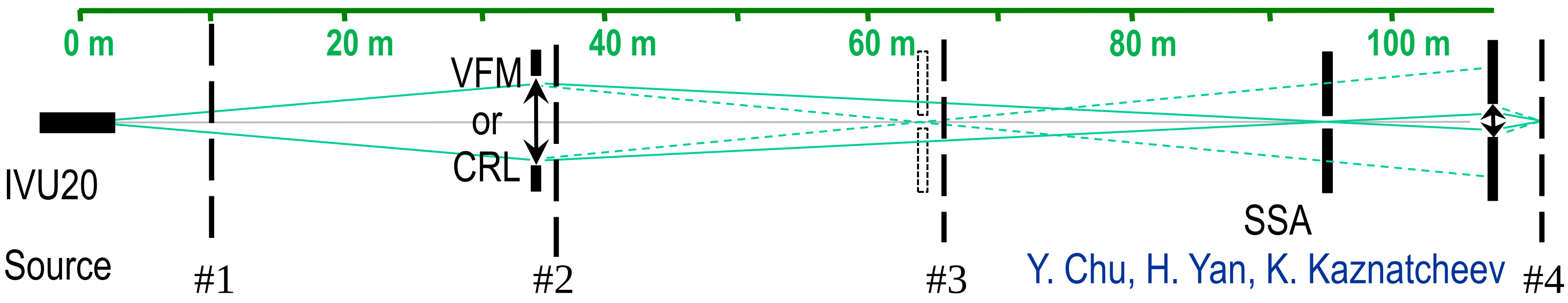
- Photons are "ballistic" (move in straight lines)
- Photons have intensity
- Photon intensity adds at the detector

  ➔No coherence properties



Wavefront Propagation

Wavefront propagation a way to handle coherence.



Idea:
1. Divide beamline into planes.
2. Calculate Field on the 1st plane using synchrotron radiation formulas and the particle beam parameters (emittance, etc.).
3. Propagate field from plane to plane using Huygens-Fresnel principle (equivalent to Kirchoff's integral):

$$E(\mathbf{r}_{plane2}) = \frac{k}{4\pi i} \int_{Plane1} d\mathbf{r}' \, E(\mathbf{r}') \frac{\exp(ik|\mathbf{r} - \mathbf{r}'|)}{|\mathbf{r} - \mathbf{r}'|}$$

- ✓ Partial coherence is handled by propagating multiple wavefronts.
- ✓ Alternative: instead of E(**r**), propagate the coherence function S($\mathbf{r}_1$, $\mathbf{r}_2$)

Wavefront Propagation Programs

- SRW [Oleg Chubar, BNL]
- PHASE [J. Bahrdt, BESSY]
- Commersial packages ...

ZEMAX	[Radiant Zemax]
GLAD	[Applied Optics Research]
VirtualLab	[LightTrans]
OSLO	[Sinclair Optics]
Microwave Studio	[CST]

"Commercial codes are expensive, and yet don't have all functions required for SR / X-ray Optics simulations"

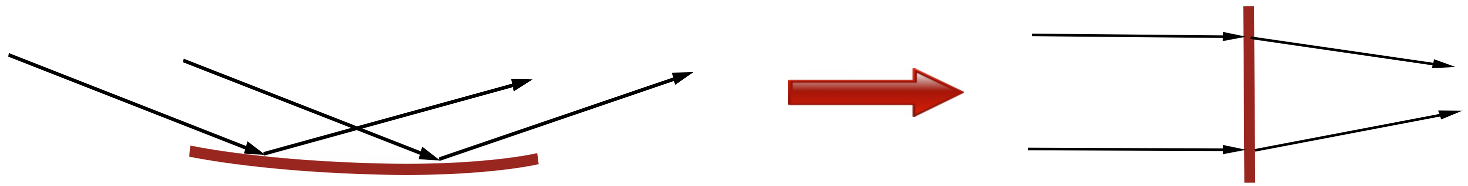
Problems With Wavefront Propagation

Wavefront propagation involves an integration which can be complicated when the beamline elements are not planer.

SRW makes the following approximations:

- Normal incidence geometries only.
- Thin optics approximation.

Example: Focusing mirror handled as a thin normal incidence element with a positional dependent phase shift.



SRW has problems handling “complicated” geometries.

Coherent Ray Tracing

Idea: Use rays for Monte Carlo integration of Kirchoff's integral

- Photons characterized by an electric field and energy:

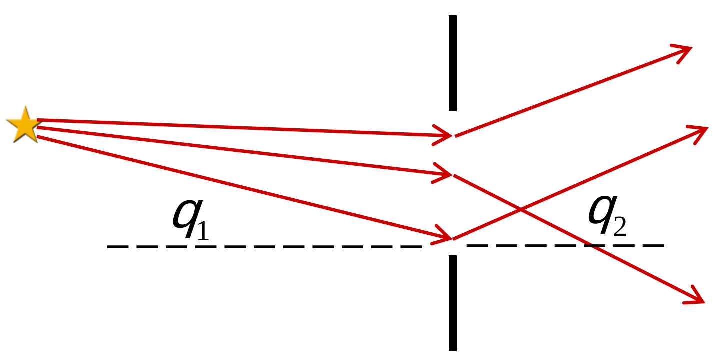
  (E_x, φ_x, E_y, φ_y, Energy)

- To simulate partial coherence, divide photons into sets ("wavefronts").
  All photons in a given set are 100% coherent and photons in different sets are incoherent.

- Where there are no apertures, use ballistic propagation.
  [This is justified by using the stationary phase approximation with Kirchhoff's integral]

- At an aperture, photons are given a random direction and the photon field is scaled:

$$\mathbf{E}_{x,y} \to \mathbf{E}_{x,y} \cdot \frac{k}{4pi}(\cos q_1 + \cos q_2)$$



Coherent Ray Tracing

Advantages of coherent ray tracing:

- Very easy to parallelize
- Can handle complex geometries
  (arbitrary shaped surfaces, surface roughness, etc.)
- Can handle near field problems easily.

Disadvantages of coherent ray tracing:

- Computation time may become excessive

"Monte Carlo modeling is popular because it is simple and easily adapted to odd geometries and boundary conditions”

- D. G. Fischer et al.

Coherent Ray Tracing is Not New...

Fischer et al. Vol. 25, No. 10/October 2008/J. Opt. Soc. Am. A 2571

Monte Carlo modeling of spatial coherence: free-space diffraction

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We present a Monte Carlo method for propagating partially coherent fields through complex deterministic optical systems. A Gaussian copula is used to synthesize a random source with an arbitrary spatial coherence

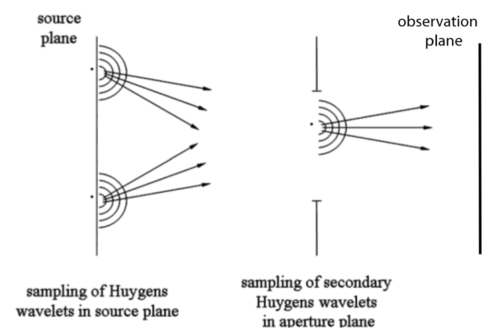


Fig. 3. Illustration of Monte Carlo approximation of the Huygens wavefront.

The following programs have coherent ray tracing:

RAY	[F. Schäfers, BESSY]
McXtrace	[E. Knudsen, Univ. Copenhagen]
(Shadow)	[M. S. del Rio, ESRF]

State of Ray Tracing Codes

The coherent ray tracing discussed by Fisher et al:

- Is 2-dimensional
- Does not not go beyond "proof of principle" examples.

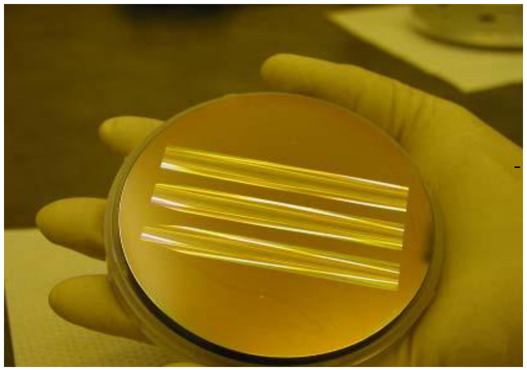
McXtrace:

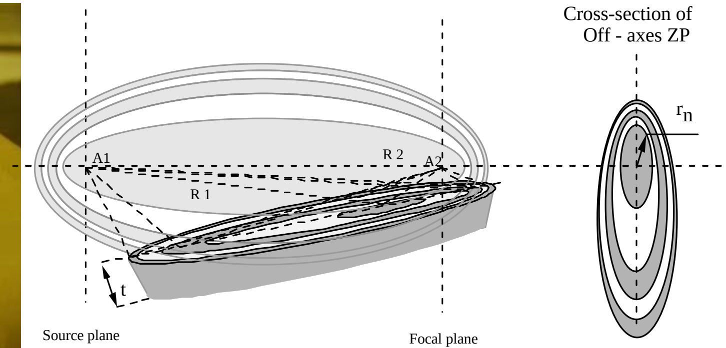
- Coherent ray tracing looks like an "afterthought" and not well developed.

Ray Program

2\. Special optics: Zoneplates (transmission, reflection)

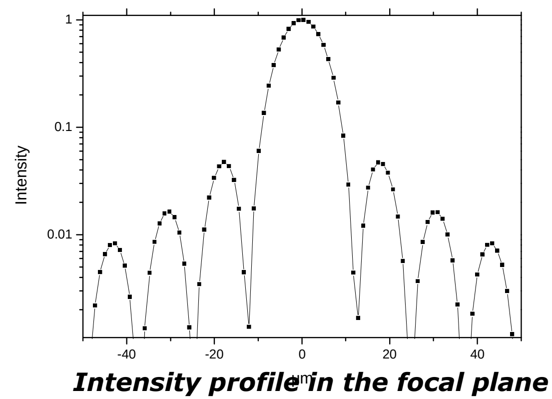
HELMHOLTZ ZENTRUM BERLIN für Materialien und Energie





Ellip[illegible]cal Re[illegible]ec[illegible]n (Bragg-Fresnel) z[illegible]ne plate f[illegible]r [illegible]cussing [illegible]

Gold reflection off-axis zone plates on a Si substrate: 715 eV, 785 eV, 861 eV.
Focal distance: 902 cm. Outer zone: 1 μm.
Aperture: 80 mm x 10 mm



Intensity profile in the focal plane calculated with 100 000 000 rays

F. Schaefers
RAY @ BESSY

INT-Seminar 29 Jun 2012 23

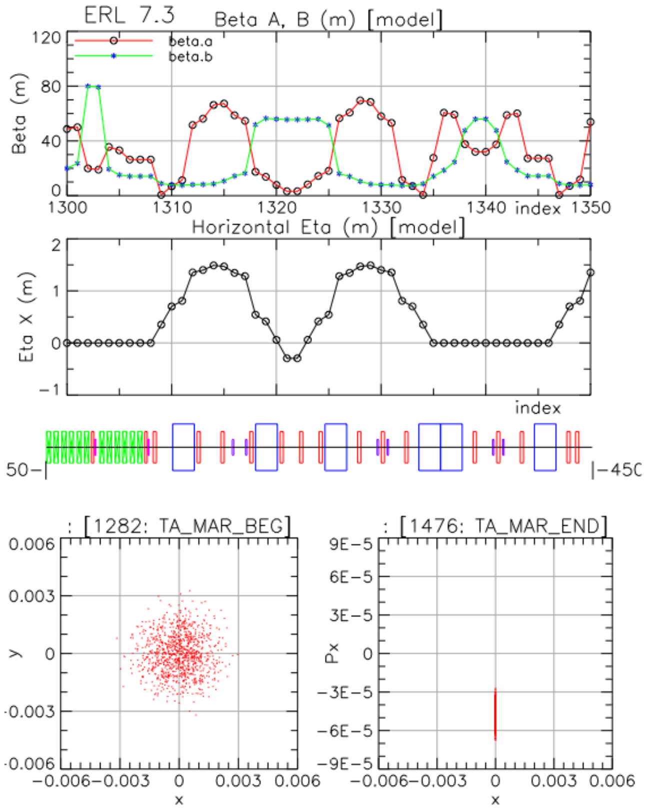
- Coherent ray tracing in Ray started sometime before 2009.

Bmad

Coherent ray tracing is being implemented as part of the Bmad simulation library.

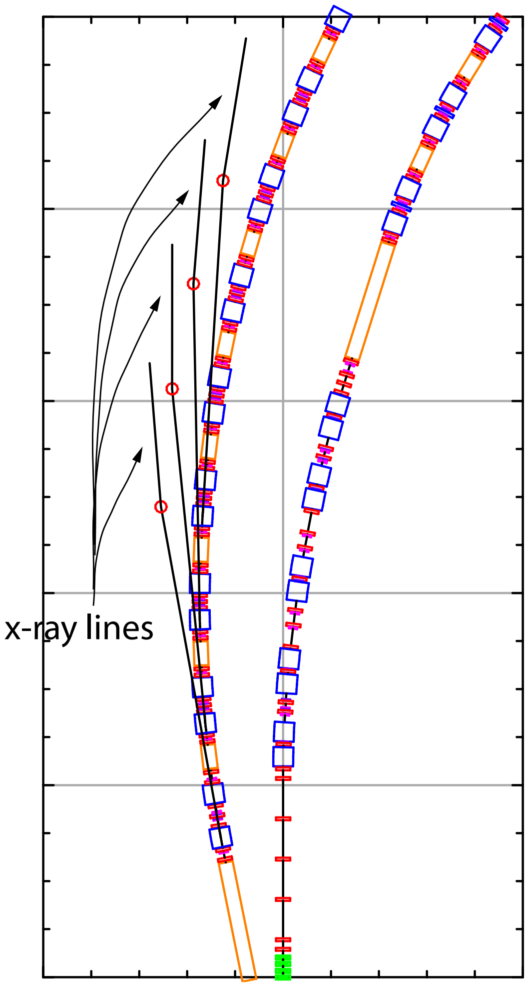
Bmad overview:

- In development since the 1990’s.
- Started as a subroutine library for simulating relativistic charged particles.
- Used as the simulation engine in a number of programs at Cornell.
- Used to measure and correct the orbit and optics in the Cesr storage ring.
- Used for simulations of the Cornell ERL, International Linear Collider, etc.



Bmad & Ray Tracing

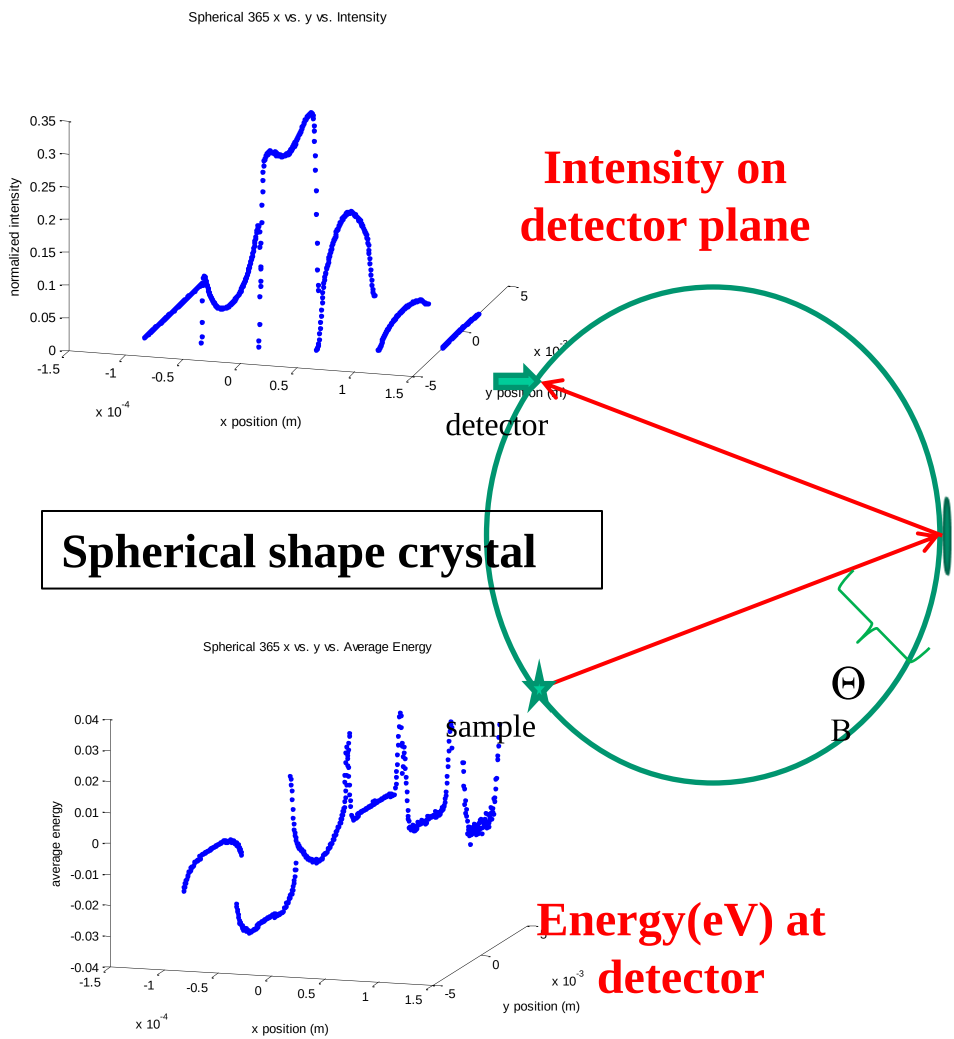
- Elements implemented in Bmad for X-ray tracing:
  - Crystal (dynamical diffraction, Bragg & Laue)
  - Mirror
  - Multilayer Mirror
  - Focusing Capillary
  - Diffraction plate (example: slit or zone plate)
- Elements with surfaces may be curved.
- Can simulate multiple x-ray lines branching from a storage ring or linac.
- Can simulate bend and wiggler radiation.
- All elements can be individually adjusted in space. Both position and orientation.
- Can link a group of elements in space (EG elements mounted on a support table)
- Can simulate “control room knobs”.



Ray Tracing Status

- Geometric ray tracing (no coherence): "Operational" and simulations with Ken Finkelstein and Peter Ko ongoing.

- Coherent ray tracing:
  Bmad simulation shows good agreement with that of Brian Heltsley of the CESR X-ray beam size monitor (XBSM).

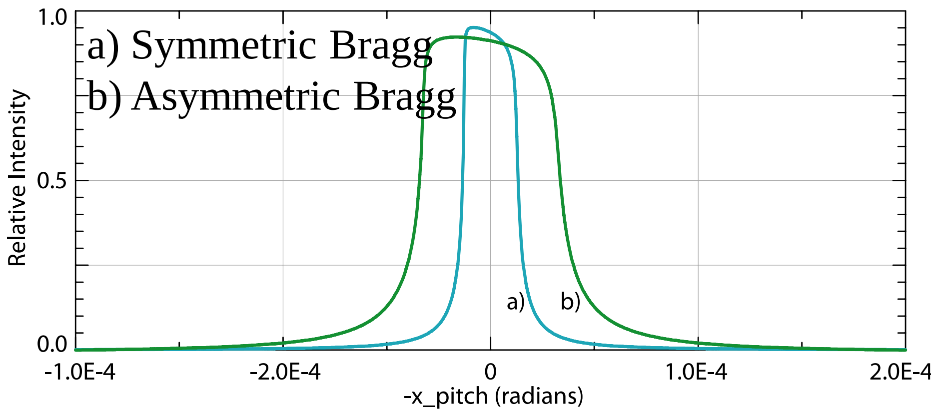


Challenges

Ray tracing in Bmad is still in its infancy and development work is ongoing:

Partial List:

- Generating partially coherent distribution of photons appropriate for undulators or other insertion devices.
- Smarter tracking of photons to cut down on the time spent tracking photons that do not reach the detector.



Conclusion

Bmad:

- Modular code means that Bmad can be adapted to many different problems.
- Aim is to be able to do a “complete” simulation from electron generation at the cathode through x-ray generation in undulators through tracking x-rays to the sample and detector.

Lots to do but beginning to be able to simulate real world X-ray problems.

Spare Slides