Which Path to Coherence in McXtrace ?
An exploratory approach to Partial Coherence

Andrea Prodi

McXtrace Team, Niels Bohr Institutet,
Københavns Universitet

European X-FEL GmbH
Hamburg
Septempber 2^{nd} 2010

Outline

Correlation Functions

Given an x-ray field $V(\mathbf{r}, t)$, the 2^{nd}-order statistical properties are described by:

- Cross-correlation Function:

$$\Gamma(\mathbf{r}_1, \mathbf{r}_2; \tau) = \langle V^*(\mathbf{r}_1, t) V(\mathbf{r}_2, t + \tau) \rangle_t$$

Correlation Functions

Given an x-ray field $V(\mathbf{r}, t)$, the 2^{nd}-order statistical properties are described by:

- Cross-correlation Function:

$$\Gamma(\mathbf{r}_1, \mathbf{r}_2; \tau) = \langle V^*(\mathbf{r}_1, t) V(\mathbf{r}_2, t + \tau) \rangle_t$$

- Cross-spectral density:

$$W(\mathbf{r}_1, \mathbf{r}_2; \nu) = \int_{-\infty}^{\infty} \Gamma(\mathbf{r}_1, \mathbf{r}_2; \tau)\, e^{2\pi i \nu \tau}\, d\tau$$

Correlation Functions

Given an x-ray field $V(\mathbf{r}, t)$, the 2^{nd}-order statistical properties are described by:

- Cross-correlation Function:

$$\Gamma(\mathbf{r}_1, \mathbf{r}_2; \tau) = \langle V^*(\mathbf{r}_1, t) V(\mathbf{r}_2, t + \tau) \rangle_t$$

- Cross-spectral density:

$$W(\mathbf{r}_1, \mathbf{r}_2; \nu) = \int_{-\infty}^{\infty} \Gamma(\mathbf{r}_1, \mathbf{r}_2; \tau)\, e^{2\pi i \nu \tau}\, d\tau$$

- All measurable quantities can be related to correlation functions of the field.

Propagation of Coherence

The propagation of cross-spectral density from an arbitrary closed surface can be achieved by:

$$W(\mathbf{r}_1,\mathbf{r}_2;\nu)=\frac{1}{(2\pi)^2}\iint_S W^{(0)}(\mathbf{r}_1,\mathbf{r}_2;\nu)\frac{\partial}{\partial n_1'}G^*(\mathbf{r}_1,\mathbf{r}_1')\frac{\partial}{\partial n_2'}G(\mathbf{r}_2,\mathbf{r}_2')\,d^2\mathbf{r}_1' d^2\mathbf{r}_2'$$

- G is the Green's function

Propagation of Coherence

The propagation of cross-spectral density from an arbitrary closed surface can be achieved by:

$$W(\mathbf{r}_1,\mathbf{r}_2;\nu)=\frac{1}{(2\pi)^2}\iint_S W^{(0)}(\mathbf{r}_1,\mathbf{r}_2;\nu)\frac{\partial}{\partial n_1'}G^*(\mathbf{r}_1,\mathbf{r}_1')\frac{\partial}{\partial n_2'}G(\mathbf{r}_2,\mathbf{r}_2')\,d^2\mathbf{r}_1'd^2\mathbf{r}_2'$$

- G is the Green's function
- COMPUTATIONALLY INTENSIVE !

The Gaussian Schell-model

The Gaussian Schell-model (GSM) is
a partially coherent planar source defined by[7] :

$$W^{(0)}(\mathbf{r}_1, \mathbf{r}_2) = A_0 \; e^{-\frac{(\mathbf{r}_1^2+\mathbf{r}_2^2)}{4\sigma_I^2} - \frac{(\mathbf{r}_2-\mathbf{r}_1)^2}{(2\sigma_\mu^2)}}$$

where σ_I refers to spectral density,
σ_μ to spectral degree of coherence
and $\mathbf{r}_1, \mathbf{r}_2$ lie on the plane of the source.

Open Questions

- Realistic model of a partially coherent x-ray source
- Calculation of correlation functions at different distances from the source
- Time structure ?

Recent ideas in the literature (for *spatial* coherence)

- Coherent Mode Decomposition + Geometrical Optics [7]
- Eikonal approximation + Geometrical Optics [4,5]
- Green Function + Monte Carlo sampling [2,3]

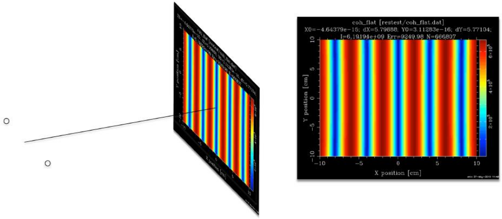
Ray-tracing: state variables and approximations

Geometrical optics justified if radiation is emittance dominated.

In McXtrace, a photon (ray) is described by:

$(\mathbf{r}, \mathbf{k}, P, \phi)$

- k-domain propagation
- ϕ can be used for coherent summation



two point sources out of phase

Stochastic Source + Monte Carlo Sampling of the Green's Function

1. A GSM Stochastic Source with arbitrary spatial coherence is synthesized by means of the "Gaussian copula" statistical tool.

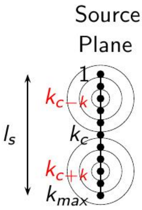
Stochastic Source + Monte Carlo Sampling of the Green's Function

1. A GSM Stochastic Source with arbitrary spatial coherence is synthesized by means of the "Gaussian copula" statistical tool.
2. The Green's function is obtained by sampling Huygens–Fresnel waves with Monte Carlo methods.

Stochastic Source + Monte Carlo Sampling of the Green's Function

1. A GSM Stochastic Source with arbitrary spatial coherence is synthesized by means of the "Gaussian copula" statistical tool.
2. The Green's function is obtained by sampling Huygens–Fresnel waves with Monte Carlo methods.
3. Propagation.
4. Coherent summation of generated rays is performed at the detector.

The gaussian copula is at the heart of the algorithm for synthesizing a source with desired partial correlation properties.



$$U_k = A_k e^{i\phi_k}$$

$$\mu_{k_c-k,k_c+k} \equiv \frac{\langle U_{k_c-k} U^*_{k_c+k} \rangle}{\langle |U_{k_c-k}|^2 \rangle^{1/2} \langle |U_{k_c+k}|^2 \rangle^{1/2}}$$

$$= exp\left\{ -\frac{(2\pi m)^2}{6} sin^2 \left[\frac{\pi}{4} \left(\frac{2k}{k_{max}-1} \right) \right] \right\}$$

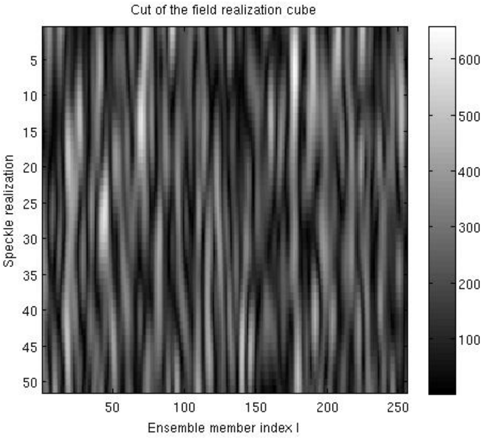
Propagation of the individual field realizations

The matrix form of Eq. 1 is given by:

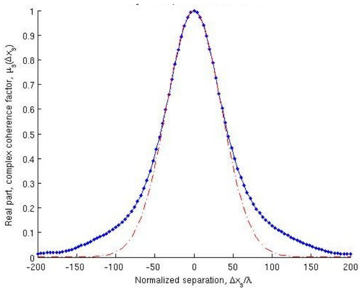
$$W = GW^{(0)}G^{\dagger}$$

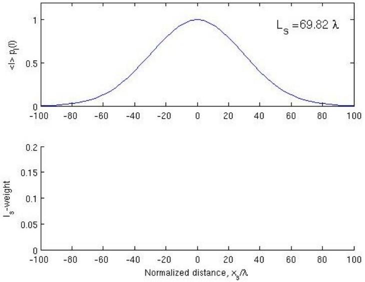
where the G_{ij} element is the coherent sum of all fields starting at the j-th source element and reaching the i-th detector element.

Correlated Speckle Sequence generation



1D Gauss-Schell source





The real challenge: from Cylindrical (1D) to Spherical Wavefronts (2D)

Computational complexity involved:

- Generate a 2D source using a similar correlated speckle pattern sequence
- Matrix representation of Green function is 4-dimensional
- Fully parallelizable and independent algorythms for:
  - generation of field realizations
  - ray generation

Towards a Hybrid Simulation Engine: Ray Tracing + Wave Propagation when needed

Let them both do what they do best !

- Ray tracing: easier to model optical elements and aberrations.
- Wave propagation: diffraction from slits, interference effects.

Towards a Hybrid Simulation Engine: Ray Tracing + Wave Propagation when needed

Let them both do what they do best !

- Ray tracing: easier to model optical elements and aberrations.
- Wave propagation: diffraction from slits, interference effects.

Problem: in order to propagate the same amount of information
the accuracy of wavefront reconstruction
must be matched at interfaces RT/WP.

To Do List

Expand Mc-Xtrace capabilities by interfacing with specialized code for:

- SR emission spectra (SPECTRA, WAVE,..).
- Wavefront propagation (PHASE).
- Fourier Optics libraries.

To Do List

Expand Mc-Xtrace capabilities by interfacing with specialized code for:

- SR emission spectra (SPECTRA, WAVE,..).
- Wavefront propagation (PHASE).
- Fourier Optics libraries.

Identify suitable test geometries :

- to choose optimal interface param. when switching methods.
- to establish confidence levels for statistics of MC sampling.

Conclusions

- We are working on a scheme for partial coherence which exploits the Monte Carlo engine of Mc-Xtrace.

Conclusions

- We are working on a scheme for partial coherence which exploits the Monte Carlo engine of Mc-Xtrace.
- Results on 1D Gauss-Schell model source are encouraging.

Conclusions

- We are working on a scheme for partial coherence which exploits the Monte Carlo engine of Mc-Xtrace.
- Results on 1D Gauss-Schell model source are encouraging.
- Mc-Xtrace's bigger goal is to become a general framework for implementing new ideas and interfacing existing ones.

Partial list of References

1 Born & Wolf, *Principles of Optics*, cap. 10.
2 Fisher *et al.*, J. Opt. Soc. Am. A 25, 2571 (2008).
3 Prahal *et al.*, J. Opt. Soc. Am. A 26, 1533 (2009).
4 Zysk *et al.*, Phys. Rev. Lett. 95, 043904 (2005).
5 Zysk *et al.*, Proc. of SPIE Vol. 7078, 70781A-1 (2008).
6 Saldin *et al.*, Optics Comm. 281, 1179 (2008).
7 Singer *et al.*, Phys. Rev. Lett. 101, 254801 (2008).

Partially Coherent Source: Gaussian Copula algorithm

In statistics, a Copula C links two marginal distribution functions $F(x)$,$G(x)$ into a prescribed joint distribution function:

$$H(x,y) = C[F(x), G(y)]$$

Given two S.I. uniformly distributed random variables X_1, X_2:

$$Y_1 = \sqrt{-2 ln X_1}\, cos(2\pi X_2);\, f_{Y_1} = \frac{1}{2\pi} exp\left\{-\frac{1}{2} y_1^2\right\}$$

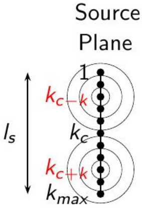
the Gaussian copula linking f_{Y_1}, f_{Y_2} involves rotation and scaling:

$$f_{Z_1,Z_2} = \frac{1}{2\pi\sqrt{1-r^2}} exp\left\{-\frac{1}{2(1-r^2)}(z_1^2 - 2rz_1z_2 + z_2^2)\right\}$$

where Z_1, Z_2 are bivariate normal with correlation coefficient r

Stochastical source (1D) with Gaussian spatial correlations

The gaussian copula is at the heart of the algorithm
for synthesizing a source with desired partial correlation properties.

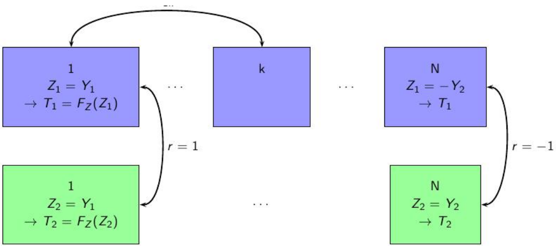


$$U_k = A_k e^{i\phi_k}$$

$$\mu_{k_c-k,k_c+k} \equiv \frac{\langle U_{k_c-k} U^*_{k_c+k} \rangle}{\langle |U_{k_c-k}|^2 \rangle^{1/2} \langle |U_{k_c+k}|^2 \rangle^{1/2}}$$

$$= exp\left\{ -\frac{(2\pi m)^2}{6} sin^2 \left[\frac{\pi}{4} \left(\frac{2k}{k_{max} - 1} \right) \right] \right\}$$

Correlated sequecence of N speckle patterns



$$r_{1k} \equiv \frac{E\{(T_{11} - \mu_{11})(T_{1k} - \mu_{1k})\}}{\sigma_{11}\sigma_{1k}} = \sqrt{\frac{1+r}{2}}$$