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

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\textit{McXtrace}
Outline

Introduction
   Statistical Optics
   Partial Coherence
   Open Questions

Approach
   Green’s Function + Monte Carlo Sampling

Status
   1D Gauss-Schell source

What’s next
   from 1D to 2D
   Hybrid Simulations
   To Do List
Correlation Functions

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

- **Cross-correlation Function:**

$$\Gamma(r_1, r_2; \tau) = \langle V^*(r_1, t) V(r_2, t + \tau) \rangle_t$$
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- **Cross-spectral density:**
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- **All measurable quantities can be related to correlation functions of the field.**
The propagation of cross-spectral density from an arbitrary closed surface can be achieved by:

\[
W(r_1, r_2; \nu) = \frac{1}{(2\pi)^2} \int \int S W(0)(r_1, r_2; \nu) \frac{\partial}{\partial n_1'} G^*(r_1, r_1') \frac{\partial}{\partial n_2'} G(r_2, r_2') d^2r_1' d^2r_2'
\]

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

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\]

- G is the Green’s function
- COMPUTATIONALLY INTENSIVE!
The Gaussian Schell-model (GSM) is a partially coherent planar source defined by:

\[ W^{(0)}(r_1, r_2) = A_0 \ e^{-\frac{(r_1^2+r_2^2)}{4\sigma_I^2} - \frac{(r_2-r_1)^2}{2\sigma_\mu^2}} \]

where \( \sigma_I \) refers to spectral density, \( \sigma_\mu \) to spectral degree of coherence and \( r_1, r_2 \) 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:

\[(r, k, P, \phi)\]

- \(k\)-domain propagation
- \(\phi\) can be used for coherent summation

two point sources out of phase
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

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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.

\[ U_k = A_k e^{i\phi_k} \]

\[ \mu_{k_c-k,k_c+k} = \frac{\langle U_{k_c-k} U_{k_c+k}^* \rangle}{\langle |U_{k_c-k}|^2 \rangle^{1/2} \langle |U_{k_c+k}|^2 \rangle^{1/2}} \]

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

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Which Path to Coherence in McXtrace?
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 algorithms 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.
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Problem: in order to propagate the same amount of information the accuracy of wavefront reconstruction must be matched at interfaces RT/WP.
Expand Mc-Xtrace capabilities by interfacing with specialized code for:

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

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- Wavefront propagation (PHASE).
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Identify suitable test geometries:

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

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

\[ U_k = A_k e^{i \phi_k} \]

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

\[ = \exp \left\{ -\frac{(2\pi m)^2}{6} \sin^2 \left[ \frac{\pi}{4} \left( \frac{2k}{k_{\text{max}} - 1} \right) \right] \right\} \]
Correlated sequence of $N$ speckle patterns

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