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Coherent X-ray Diffractive Imaging Simulated by Monte Carlo Ray Tracing

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Introduction:

Coherent Diffractive Imaging (CDI) techniques [1]:

- lensless, require high degree of coherence
- provide high resolution and contrast
- can be combined with tomography

McXtrace [2]:

- a Monte Carlo based ray-tracing software package
- simulation of beamlines, optics, and experiments

McXtrace accounts for interference phenomena, which is a prerequisite to model CDI. Here, for the first time, we test this framework for CDI techniques. Being able to simulate a full CDI experiment in this way might prove helpful to pre-assess the feasibility and optimize performance of an imaging experiment on a given sample at a particular beamline.

Methods: Implementation. Diffraction is simulated in McXtrace with a Monte Carlo sampling scheme that reproduces Huygens' principle (Fig.1). We define a grid of sub-pixels in the detector's plane to compute the wavefield pointwise. Only the rays hitting the subpixels are traced.

Testing. We produced a ptychographic dataset according with the round scan depicted below, with the schematic of Fig. 2, using the following parameters:

- $\lambda = 1 \text{ \AA}$
- probe cSAXS beamline (@PSI)
1.2 μm wide
- sample size $\sim 3 \mu\text{m}$
- estimated overlap 60%
- detector width 35x35 mm, 200x200 pixels

⇒ **Reconstructed Pixel Size**
14 nm

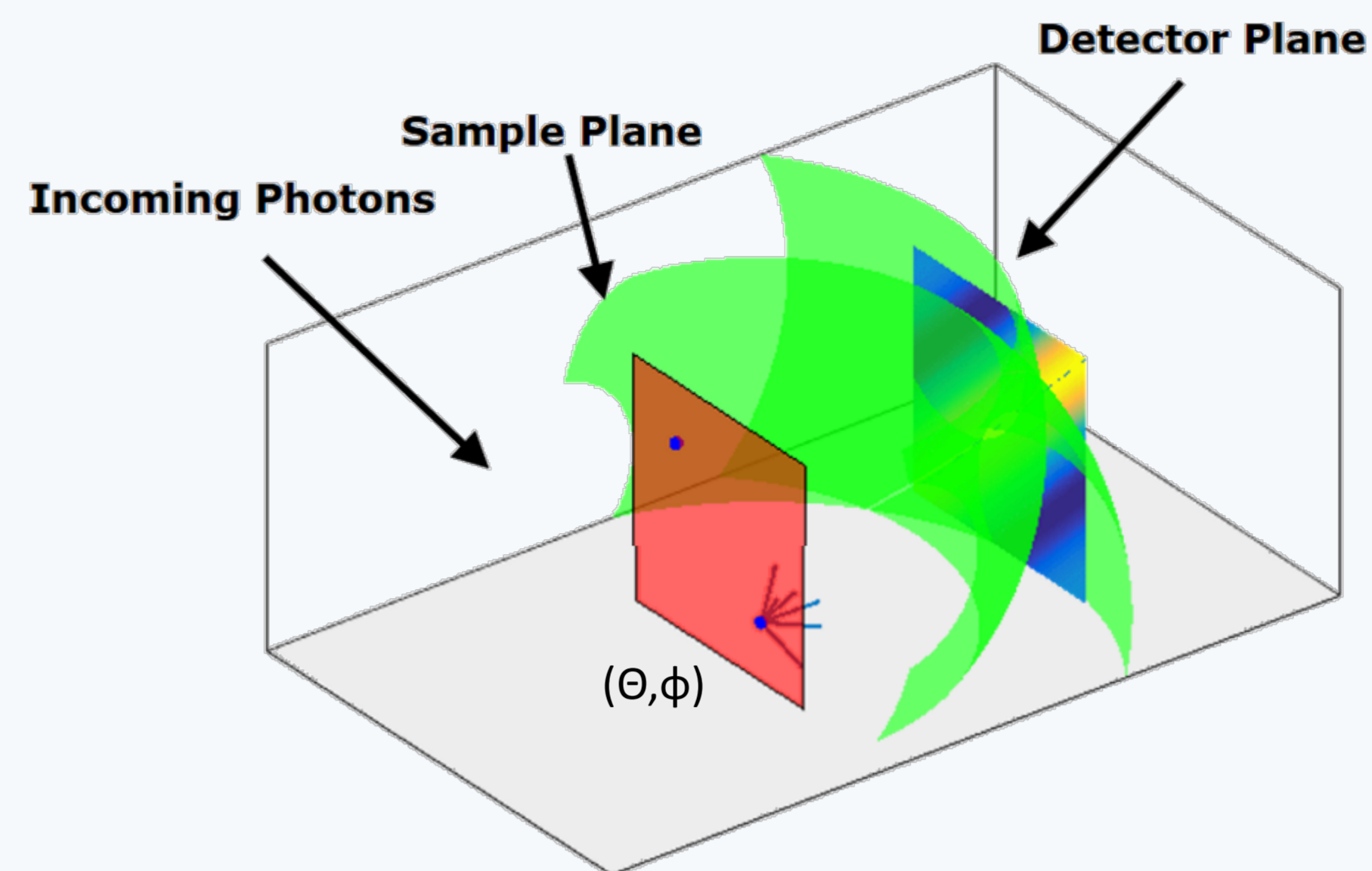
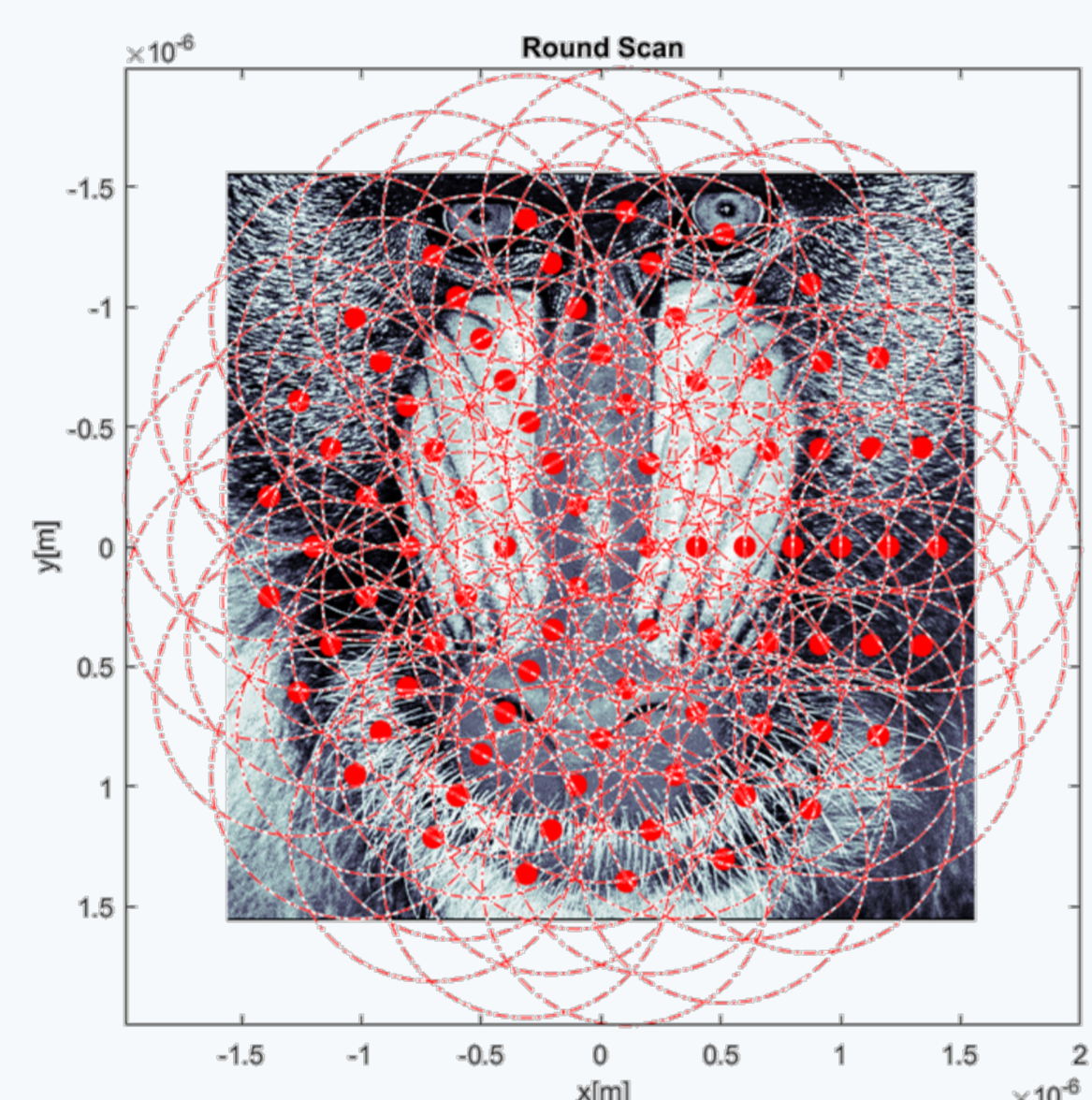


Fig. 1. Diffraction in McXtrace. A ray is allowed to change direction by drawing a new one from a random uniform distribution. That produces a spherical wavefront.

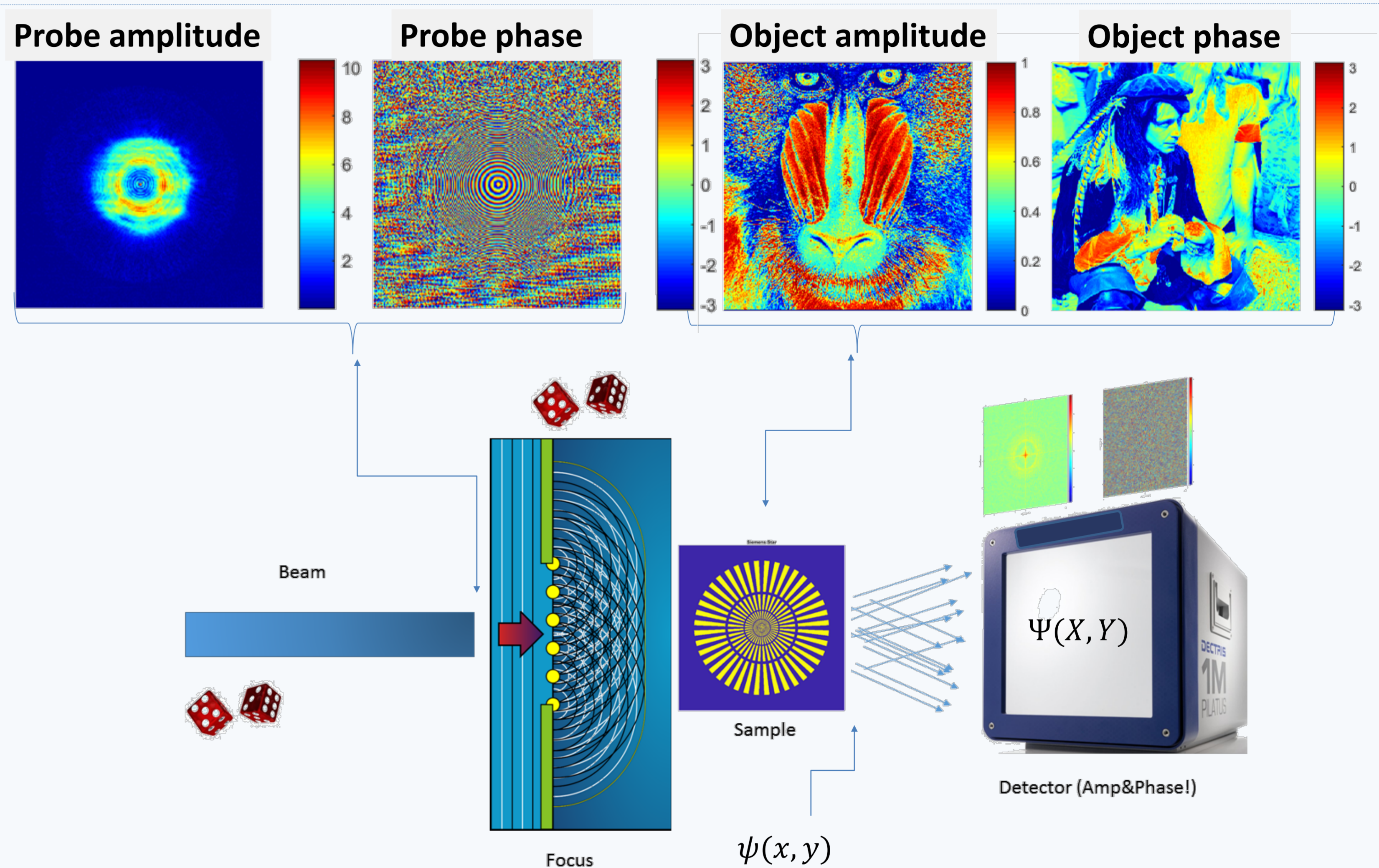
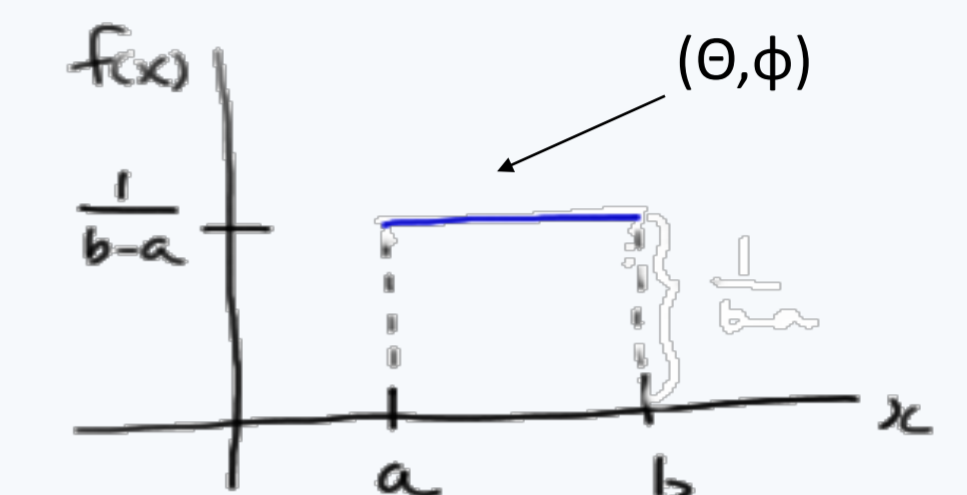
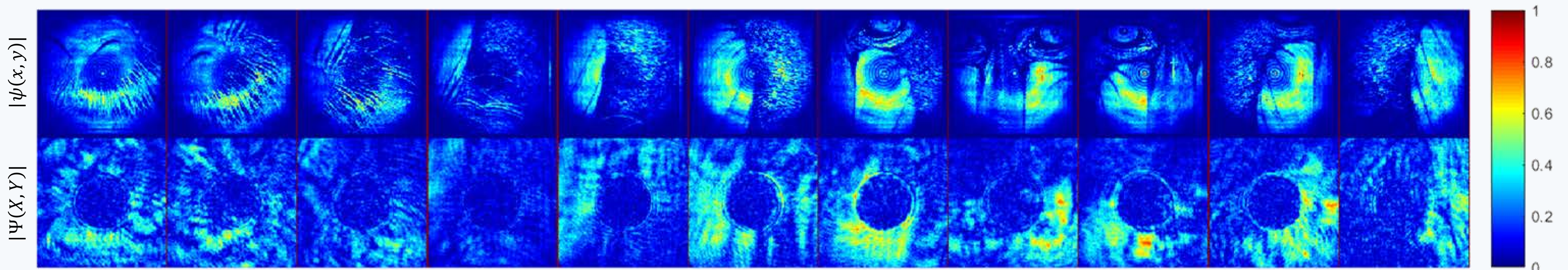
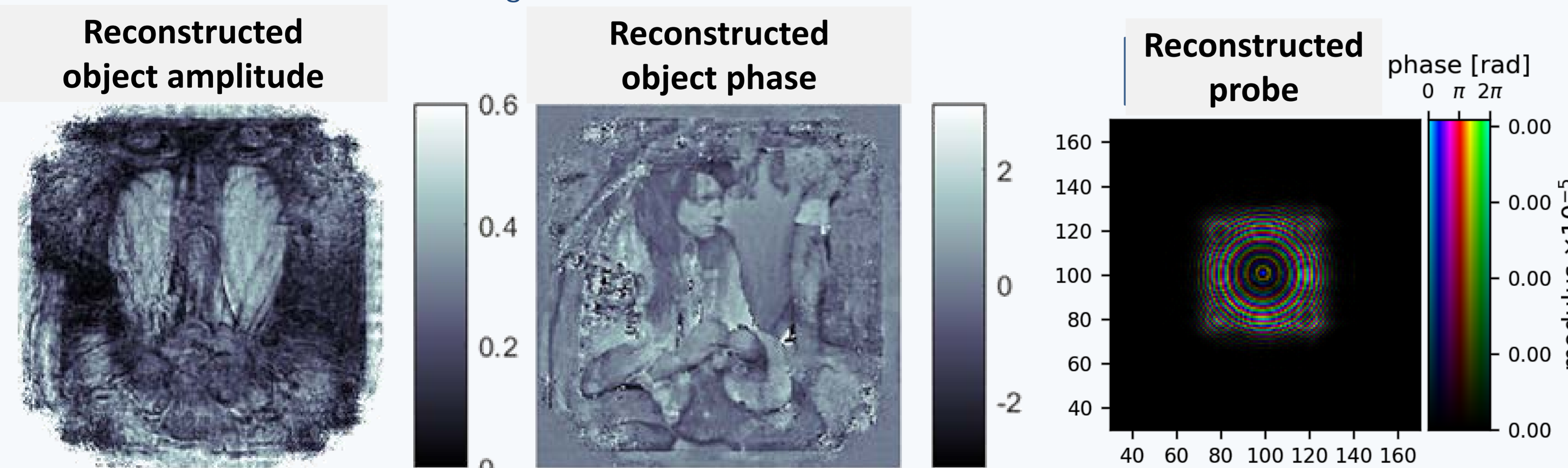


Fig. 2. Schematic of a simulated experiment. The dice indicate where a Monte Carlo process takes place. Differently from a real experiment, the detector records also the phase of the wavefield.



Results: Some diffraction patterns of the simulated ptychographical dataset are shown above. Amplitudes of the wavefield immediately after the sample in the first line, and the corresponding diffraction patterns in the second. Each of the 84 diffraction patterns was run with $1e10$ rays and took around 20 min on a 16 nodes cluster. Below, the results of the reconstruction run through ptypy [3] with 200 iterations of the EPIE algorithm.



Conclusions and Outlook: We suggest a scheme for simulating coherent diffractive imaging in a ray-tracing framework. The scheme was implemented and tested on McXtrace with a 2D toy problem. Proper encoding of amplitude and phase of the exit wavefield into the diffraction patterns is finally assessed by a correct ptychographical phase retrieval. Tomography can be simulated with the aid of the ASTRA toolbox, which can perform the line integration through a 3D object for different angles yielding a set of masks to simulate in McXtrace. Our ongoing work aims at verifying quantitiveness of these simulations, by comparison to real data, and at simulating partial coherence.