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Taking into account wave effects in Monte Carlo simulation of phase contrast imaging using the Wigner Distribution Function.

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X-ray phase contrast imaging techniques have revolutionised the field of biological imaging, enabling the visualisation of subtle structural details that are otherwise challenging to detect using conventional absorption-based methods. It is an imaging technique based on coherence that holds the potential to provide significantly higher contrast sensitivity, potentially spanning multiple orders of magnitude. When combined with computed tomography, it enables three-dimensional imaging at nanometric resolutions.

The aim of this study is to present a simulation framework for phase contrast imaging, aimed at improving image analysis and interpretation; it would need to accurately model the complex physics involved in phase contrast imaging, including the interactions of X-rays or other incident particles with the sample: reflection, refraction, absorption, scattering and more. By incorporating the principles of the Monte Carlo method, it will allow generating realistic synthetic data, simulating the propagation of phase-shifted waves through the sample and their subsequent detection.

However, the current simulations that take into account wave effects calculate the interference at the detector; calculating the interference at the exit plane of the sample would allow incorporating further interactions, such as including scattering.

To bridge the gap between wave and particle-based simulations, we will use the Wigner Distribution Function (WDF).

*Speaker

The WDF represents simultaneously information both on the wave nature and particle nature of light. It is a mathematical transform used in quantum mechanics that bridges the gap between classical and quantum mechanics by providing a way to represent the quantum state in terms of both position and momentum variables. The WDF results in a Wigner quasi probability distribution. The Wigner distribution possesses the capability, and typically exhibits, negative values for states that lack a classical model: this serves as a useful indicator of quantum-mechanical interference. In the context of the double-slit experiment, it is possible to calculate the intensities at both the slits and the detector analytically. Furthermore, a crucial aspect is that the WDF can also be analytically calculated. This enables us, at least for now, to bypass the most challenging numerical difficulties. The framework aims to combine the contributions of diffraction (wave-effect aspect) and incoherent scattering (particle effect) in a single simulation.

The current stage of the framework is a validated use of the WDF for the double-slit experiment. Firstly, the photon probability is calculated at the object's exit plane utilising the WDF to incorporate interference effects by projecting the modulus of the WDF; secondly photon positions are then generated based on this distribution; lastly the photons are simply diffracted for the moment. This diffraction is done by computing the distribution of diffraction angles at the corresponding position and select an angle from the WDF using its modulus at that point as a probability density function; the sign of the photon is determined based on the WDF at that specific position and angle; the position on the detector is then calculated using geometric methods. The detection of the photons depends on the sign of the photon: the negative potential is increased or decreased at a given pixel on the detector. The final photon (the potential if positive, zero otherwise) is displayed at the detector once the simulation is complete.

The results presented here showed that the WDF is capable of taking into account wave effects using Monte Carlo simulation in the case of the double-slit experiment. The following stage for the framework is to incorporate a scattering object in order to include accurate particle interactions during x-ray phase contrast imaging.

Keywords: wigner, young, analytique, monte carlo, imagerie à contraste de phase, double, slit, phase contrast imaging