Advanced simulation of near-field holography using Monte Carlo

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X-ray phase contrast imaging permits to reach nanometric resolution in tomographic imaging. Further, phase contrast offers several orders of magnitude higher sensitivity than standard, attenuation-based x-ray imaging. The main drawback is that it needs an additional reconstruction step, known as phase retrieval, to yield quantitative images. Phase information is directly linked to the optical path in objects crossed by incident light, and then to the difference of refractive index with their surrounding medium. Reconstruction of phase objects is also a central problem in digital holography, an interferometric imaging technique under visible coherent illumination, whose various applications include microscopy, biomedical imaging, and fluid mechanics.

A common problem with phase retrieval is the presence of low frequency noise in the reconstructions. The sensitivity to noise in the low spatial frequency range is due to low transfer of contrast by the imaging system. The origin of the noise is not known, however. One hypothesis is that it originates from the scattering that occurs inside the imaged object.

X-ray phase contrast is usually modelled deterministically from a wave perspective using the Fresnel transform. This deterministic model makes a number of assumptions on the object, for example that the object can be considered thin, i.e. that it can be represented by a 2D aperture function. In other words, this means that diffraction is assumed to occur in the same plane in the object, and that no secondary diffraction (diffraction of the diffracted wave) occurs (Born approximation). These inner scattering effects can be modelled from a particle perspective using Monte Carlo simulation, which can include refractive effects; the deflection of electro-magnetic radiation at the interface between media.

A similar imaging problem arises in holographic microscopy with visible light. Therefore, we expect strong synergies between the two modalities. Current state of the art in holographic microscopy uses deterministic simulation tools based on Lorenz-Mie theory. The Lorenz-Mie model allows the calculation of the complete electro-magnetic field scattered around simple diffracting objects such as spheres [4]. The domain of validity is when the scattering particles are of comparable size to the wavelength of the light. This model is currently used for imaging of isolated particles, for example of bacteria and in droplet tracking. The model is used either as validation or included directly in reconstruction algorithms [5,6]. The Lorenz-Mie model is limited to simple objects, however. There is a strong need of advanced simulation tools adaptable to more complex objects. This is of particular importance in the field of diffractive tomography [7], a multi-view extension of holography where the goal is to reconstruct the 3D refractive index of micrometric objects distributed in a medium. In this modality, the Born approximation is not valid. Therefore, reconstruction algorithms will have to explicitly model multiple scattering inside the imaged object.

Objectives

The aim of this project is to develop advanced simulation tools with the main aim to increase the understanding of origin of artefacts in phase contrast imaging and to improve the accuracy of existing models used for reconstruction algorithms, both for X-ray and visible light phase imaging.

Methodology

The thesis can be divided into a series of experiments mimicking progressive refinements of the considered phenomena, namely: 1) the inclusion of scattering in the simulation of phase contrast, 2) the effect of refraction, first in simple objects, on the resulting contrasts, and 3) the effect of taking into account a thick object, for example through successive propagation through consecutive planes, to model higher order scattering and diffraction.

In a previous Master project, we developed tools to simulate refraction using MC simulation in Geant4 [1] as well as an analytical phase contrast simulator in GATE [2] and VIP [3]. These tools will be extended to study the possibility of combining the different signals (diffraction, refraction, scattering), either incoherently by directly summing the contributions from each process, or first calculating the exit wave-field analytically and calculating the MC probability for position and momentum of the corresponding particles by sampling the Wigner transform of the wave-field to generate the scattering signal. Particular attention will be paid on the domains of validity of the hypotheses made for both modalities.

The developed simulations will be validated using experimental data acquired at synchrotron radiation facilities, laboratory X-ray sources and visible light holographic imaging devices.

Envisaged applications include increased understanding of sources of artefacts in phase contrast imaging, the generation of realistic phase contrast images for development of reconstruction algorithms as well as experiment planning (synchrotron radiation beam time is expensive, i.e. it has either to be bought or won in competitive call for proposals); and in the longer term the simulator could be included in an iterative reconstruction scheme or be used to generate training data for a deep learning based phase retrieval algorithm.

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