Monte Carlo simulation of phase contrast imaging

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X-ray phase contrast imaging permits to reach nanometric resolution in tomographic imaging with several orders of magnitude higher sensitivity than using the attenuation. The main drawback is that it needs an additional reconstruction step, known as phase retrieval, to yield quantitative images. Several methods for generating phase contrast have been developed, the most recent one being X-ray speckle-based imaging.

Currently, there are no realistic simulators of X-ray phase contrast. This would have several benefits: optimisation of imaging conditions and reconstruction, planning of experiments, investigation of artefact sources, as well as providing data for machine learning algorithms. Therefore, the aim of this project is to combine simulation of phase contrast with simulation of scattering. Phase contrast is usually modelled from a wave perspective using the Fourier transform, while scattering is usually modelled from a particle perspective using e.g. Monte Carlo simulation.

The main challenge of this project is therefore to combine the two perspectives.

The main objective is to develop new Monte Carlo based methods for the simulation of phase contrast imaging. Since the physics of phase contrast imaging remains the same, the scope for application is vast. Here, three modalities are envisaged:

1. X-ray propagation-based imaging
2. X-ray speckle-based imaging
3. Holographic microscopy

Previously, 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].

In a first step, these tools will be applied to speckle-based imaging [4]. Since this is a simpler case, because coherent effects are not necessarily taken into account, the existing code for refraction will be used as a basis for the refinement of the model in the code (voxellised objects, stochastic reflection, real surface...). A numerical emulation of the random mask will have to be defined to simulate speckle imaging. A validation study will be conducted against existing experimental data. This part of the project will be performed in collaboration with E. Brun, Strobe (INSERM UA07), Grenoble.

Second, the existing tools will be extended to study the possibility of combining the different signals (diffraction, refraction, scattering). Possibilities range from incoherently summing the contributions from each process, to 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.

The simulator will be applied to X-ray propagation based imaging, and Holographic microscopy. 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. 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 [5], 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. This part of the project will be developed in collaboration with F. Momey, Laboratoire Hubert Curien, St Étienne.

In propagation based imaging, envisaged applications include increased understanding of sources of artefacts, 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 (MSc project, WP4).

Finally, possibility for use of the code for the simulation of mammographic imaging with the aim of optimising image acquisition protocols and phase reconstruction algorithms will be investigated. This part of the project will be developed in collaboration with Institut Bergonié and AlphaNov, Bordeaux. Future work includes planning of synchrotron experiments to optimise image quality and beam time use, and use of realistic simulated images as training data for machine learning based reconstruction algorithms.

There is currently no realistic simulator of phase contrast imaging. Such a tool would be very valuable in a host of applications, from the theoretical all the way to the clinical. Further, it would be useful for several modalities, further indicating the probable impact.

The simulator will be applied in mammographic using X-ray propagation based phase contrast. This part of the project will be developed in collaboration with X. Orrade, Inistitut Bergonié, Bordeaux, and A. Bakkali, Alphanov, Bordeaux.

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