Monte Carlo simulation of X-ray phase contrast and dark-field imaging for medical imaging and microscopy

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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 [1]. 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. More recently, X-ray Dark Field Imaging (DFI) has been proposed [2] as a complementary signal to X-ray PCI. The dark-field signal is due to small angle scattering (SAXS) in the sample, caused mainly by small porosity and the crystalline structure of the material. The dark-field signal has been demonstrated to reveal features in the sample that are not visible otherwise. For instance, it can reveal microstructure properties of the lung in case of chronic obstructive pulmonary disease that were not detectable with conventional techniques [3].

Currently, there is an increased interest in realistic simulators of X-ray phase contrast [4, 5]. 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. Dark-field imaging and its relation to the SAXS signal

Previously, we developed tools to simulate refraction using MC simulation in Geant4 [4, 6] as well as an analytical phase contrast simulator in GATE [7] and VIP [8]. A simple wave-optical simulator of X-ray phase contrast can trivially be implemented. Accounting for scattering is limited in this kind of approach, however. Advanced software for wave optics simulation exist, for example Novi-Sim [9], which takes into account most aspects of the imaging chain (source, optics, detectors, noise propagation). Scattering, cannot be trivially accounted for, however. Therefore, in this project, we propose the following tasks.

First, 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. 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. This part will be performed in collaboration with Novitom, Grenoble, and S. Rit and J.M. Letang, Creatis, Lyon.

Then, these tools will be applied to speckle-based imaging. Speckle-based imaging is a very promising new approach in X-ray phase contrast imaging in that the simplicity and stability of the set-up offers several advantages over the currently widely investigated grating-based DFI. For example, the speckle-based dark-field signal is intrinsically 2D, as opposed to the grating-based dark-field signal which is 1D. Grating-based imaging also requires very high stability to keep the gratings aligned. Clinical prototypes therefore require displacements of the patient rather than the imaging system. In speckle-based imaging, there is no need for such stability. The membrane can be integrated directly in a hospital source, thus greatly reducing complexity of the imaging apparatus and increasing convenience for patient and practitioner. Since this is a simpler case, because coherent effects are not necessarily taken into account, the existing code for refraction [10] will be used as a basis for the refinement of the model in the code, for example extending the implementation to voxellised objects, calculating reflections stochastically, and taking into account surface states. In order to maximise contrast, signal-to-noise and resolution for a given setup and application, aspects such as contrast from the membrane, qualitative aspect of the membrane contrast, placement of membrane, sample and detector, and composition of the membrane will be studied. Existing codes will be used to build tools that permit the simulation of specific imaging set-ups, for example laboratory microscopy and medical imaging setups. 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 will be performed in collaboration with E. Brun, Strobe, UGA Grenoble.

Finally, a DFI microscope will be simulated. This microscope is to be used in conjunction with SAXS and will serve as a pilot imaging system to permit precise investigation with SAXS in the most interesting regions of interest in a sample. The Monte Carlo simulator will be further developed to permit the study of the relationship between the dark-field signal and the SAXS signal. This tool will be used to optimise the study more general questions, such as ideal wave-front modulation for imaging, through simulation. This part will be performed in collaboration with Xenocs, Grenoble.

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