2020 HGF – OCPC – Programme

for the involvement of postdocs in bilateral collaboration projects

Title of the project:

Machine Learning on Fiber-based SAXS-CT data reconstruction pipeline

Helmholtz Centre, division/group:

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Department/Group: (at the Helmholtz centre or Institute)

Photon Science / FS-PETRA-D

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Description of the project (max. 1 page)**:**

Fiber-based materials are commonly categorized based on the fiber origin: natural (plant, animal or mineral) or man-made (semi-synthetic or synthetic) (Pickering, 2016). These materials abound in everyday life finding use in areas as diverse as fashion textiles, medicine, energy, aerospace and construction composites. In medicine, the arrangement of the mineralized collagen fibrils in bone (Groetsch, 2019) (Fratzl, 2004) and teeth (Nalla, 2003) has been associated with fracture risk as well as the non-mineralized one as playing a key role on the growth and progress of breast cancer (Conceição A. A., 2009) (Conceição A. A., 2014), while natural fiber-based materials have been used to fabricate functional tissues to repair those damaged (Tamayol, 2013). Fiber-based solar cells have the performance much less dependent on variations in illumination angle (O'Connor, 2008), presented higher efficiency whereas reducing the effective cost of fabrication (Martinsen, 2015) are able to generate electrical power from absorbed solar irradiance and mechanical motion (Chen, 2016). Likewise, rapid growth in research and innovation on natural fiber composites encouraged by government legislation due to its lower cost and eco-friendly characteristics to replace their synthetic counterpart in cars (Faruk, 2014), aircraft (Ho, 2012) and construction industry (Dweib, 2006) has been observed.
X-ray fiber diffraction/scattering has made critical contributions to our understanding of

biomolecular and synthetic fibrous systems, which includes both the structure of the individual structural unit and qualitative and quantitative information about the preferred orientation state of the ensemble, and it will undoubtedly continue to do so as new resources and instrumentation become available to the scientific community (Squire, 2003). A good example is the Small-angle X-ray Scattering Computed Tomography (SAXS-CT) technique which offers the possibility to probe nanoscale structures in three-dimensional macroscopic samples, generating six-dimensional information (Liebi, 2015). For SAXS tomography, 2D SAXS data must be collected at each position of the x–y plane and at many rotation angles, not just around one axis but around many axes. However, this technique relies on a massive computational power for modelling the three-dimensional reciprocal-space map using spherical harmonics and minimizing error between the measured and modelled intensity. Generally, for a millimetre size sample more than one million SAXS patterns are collected, equating to terabytes of data, and the computations needed for one tomogram require several days of computing time. In this sense, a computer vision algorithm to automate the process of scattering pattern modelling based on a deep-learning multiclass fiber-orientation classification would speed up this task and minimize computational efforts.

Therefore, in this project, we aim to develop a Convolutional Neural Network to enable SAXS fiber signal modelling and using simulated and measured patterns, which includes feature extraction tools and image classification to be part of the SAXS-CT pipeline.

References

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Description of existing or sought Chinese collaboration partner institute (max. half page)**:**

Although currently there is no active collaboration between our group and a Chinese research Institute, we are interested to establish such collaboration with a group with expertise in machine learning applied to modelling data and image classification. Additionally, it would be more attractive whether this group/partner institute has strong interested in three-dimensional spatial resolved nanostructure characterization of materials using computed tomography techniques such as Small Angle X-ray Scattering computed tomography.

Required qualification of the post-doc:

- PhD in physics, chemistry, or equivalently disciplines
- Extensive knowledge and experience with scientific programming (Python or C++)
- Additional knowledge of X-ray scattering technique and machine learning beneficial
- Language requirement English