SmartPhase – Real-time phase retrieval tool for X-ray near-field holography (NFH)

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In modern scientific research, understanding the operation of materials with multi-scale systems often involves observations that need to be carried out under in-situ conditions. This is the case in studies involving the degradation behavior of biodegradable magnesium implants for bone regeneration. In order to obtain information on the processes that occur on the sub-micrometer scale, the use of imaging techniques such as X-ray near-field holography (NFH) is widely used, especially in synchrotron radiation facilities such as PETRA III (DESY, Hamburg) as it offers the desired coherence of illumination. Being a method based on the propagation of phase contrast, however, the experiments carried out do not immediately provide conclusive information, i.e. the holograms (or images) obtained need to go through a phase retrieval process so that data can be analyzed and compared. A major challenge is that the lack of real-time feedback during these experiments can mean a vast amount of generated data which may be inconclusive due to experimental setup problems. To fill this gap, the Helmholtz Imaging Project SmartPhase, with cooperation from DASHH, proposes an online tool for visualization and phase retrieval of data from experiments based on the X-ray near-field holography technique. Moreover, the algorithm based on regularized project gradient descent is able to self-optimize its computation parameters, making the experience easier for the user.

Problem statement

Phase contrast techniques such as NHF can be employed when the x-ray attenuation or contrast is low, e.g., when accessing polymeric or biological materials or when accessing the 1 µm to sub-100 nm scale.

- Fresnel free-space propagator:

$$\mathcal{D}_{Fr}(\psi) = \mathcal{F}^{-1}[\exp(-i\pi/(2\,F_r)(k_x^2 + k_y^2))\,\mathcal{F}[\psi]]$$

- Intensity:

$$I_{det} = |\mathcal{D}_{Fr}(\psi)|^2$$

The actual image of the object is then given by the phases of the retrieved wavefield ψ from I, but this is a ill-posed problem.

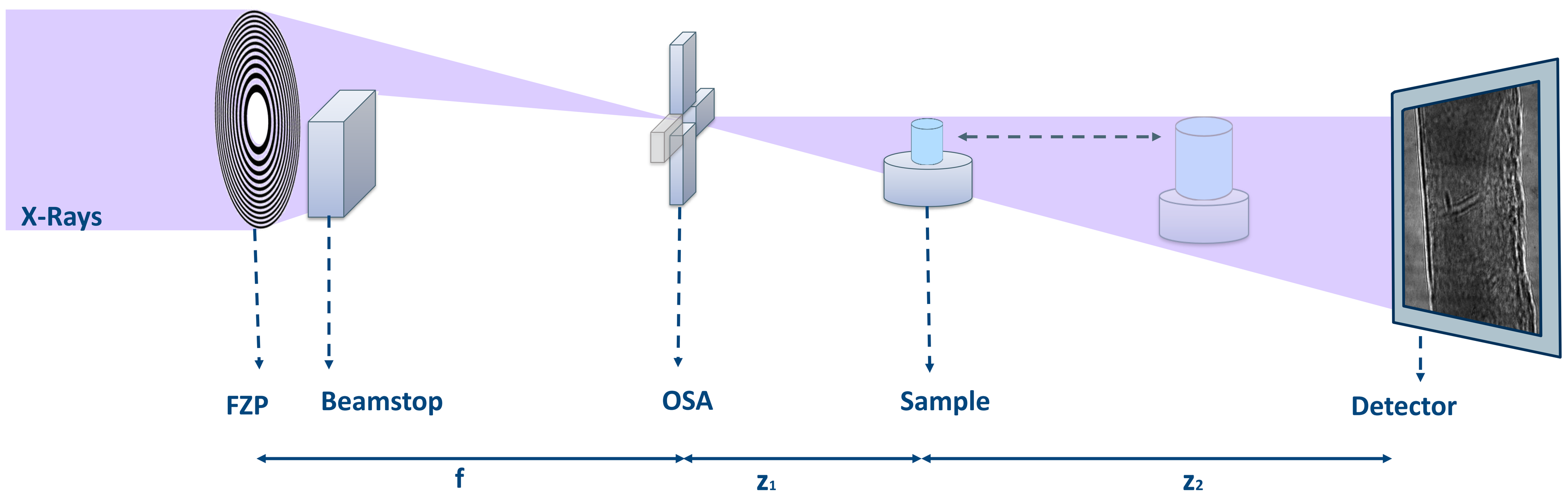

Fig. 1: X-Ray NHF setup at P05 (PETRA III, DESY): The Fresnel zone plates (FZP) focus the incoming beam, while the zero diffraction order are prevented by the beamstop. The order sorting apertures (OSA) filters the higher order comming from the FZP. The detector then captures the hologram, which has to be phase retrieved for further data analysis.

Smartphase solution

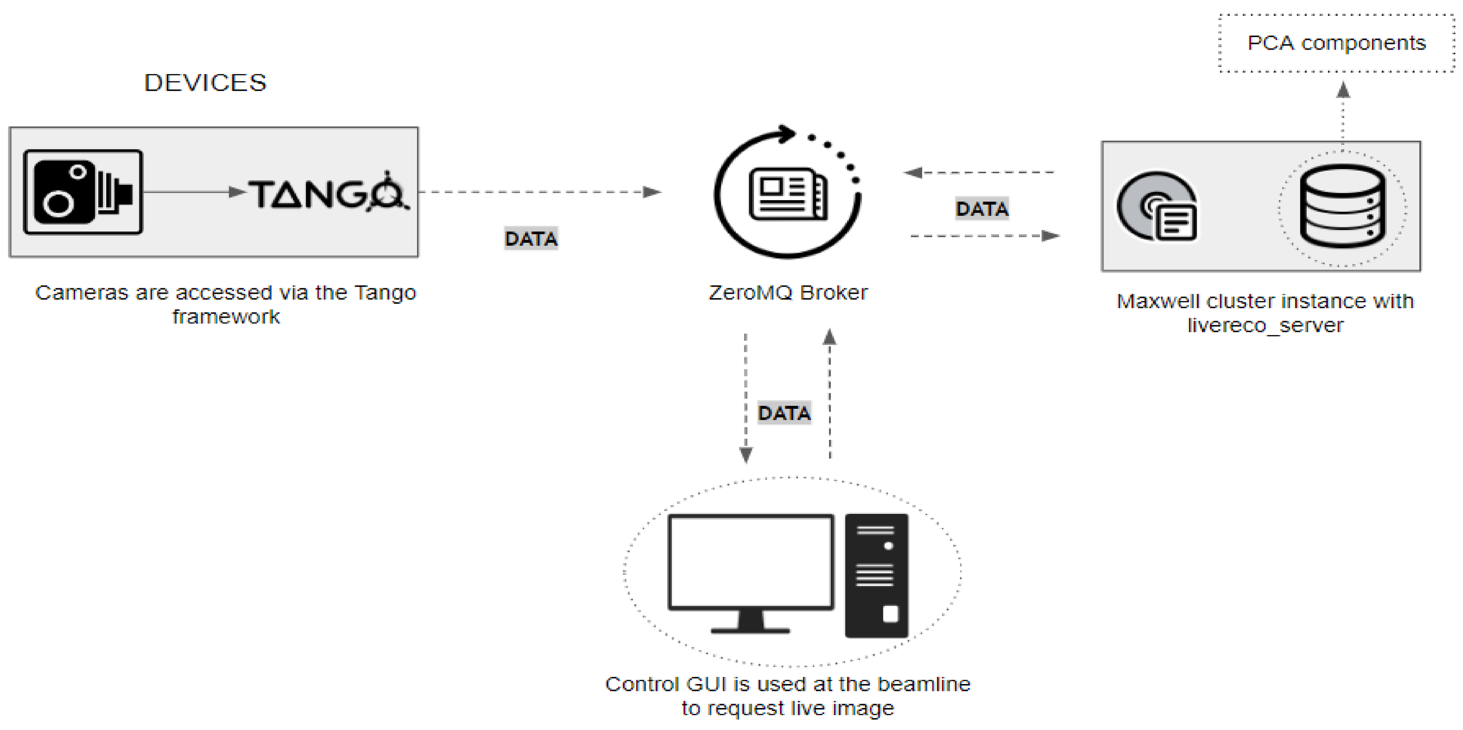

Fig. 2: Proposed software archictecture.

Implementation:

- The phase retrival reconstruction algorithm is based on regularized projected gradient descent (Nesterov) with self-optimizing parameters;
- The current running version is implemented in Python, already GPU, using basic CUDA libraries via PyTorch;
- The online reconstruction is made possible through the communication between software modules, using ZeroMQ protocols.

Results & Outlook

Online view at beamline P05 :

- A first version of the phase retrieval tool could already reconstruct sharp phase retrieved holograms of data from *in-situ* degradation behavior studies of biodegradable magnesium wires, used for implant fabrication;
- The software optimizes the focal plane of a single shot image fast enough to operate the live view at the beamline;
- The reconstruction parameters are independent from the measured object.

In development:

- Currently, an machine learning based phase retrieval module is being implemented;
- A new user interface is in development to facilitate the user interaction.

Fig. 3: Current user interface from P05 beamline. Showing the phase retrieved hologram. The phase retrieval algorithm takes approximately 40 seconds to obtain this result.

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Collaborators: DASHH, TUHH Hamburg University of Technology, UKE Hamburg

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