OPTIMIZED WORKFLOWS FOR SYNCHROTRON-BASED X-RAY TOMOGRAPHIC MICROSCOPY: FROM ACQUISITION TO ANALYSIS

Federica Marone*[1], Christian M. Schlepütz[1], Alain Studer[2] & Marco Stampanoni[1,3]

[1]Swiss Light Source, Paul Scherrer Institute, Villigen, Switzerland
[2]Information Technology Division, AIT, Paul Scherrer Institute, Villigen, Switzerland
[3]Institute for Biomedical Engineering, University and ETH Zurich, Zurich, Switzerland

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Summary: The investigation of dynamic processes in 3D with micrometer resolution is a reality. These new possibilities are coupled to a tremendous increase in data rates as well as experiment complexity asking for an optimization of the entire workflow from data acquisition to analysis. We will discuss latest developments at the TOMCAT beamline including a new reconstruction pipeline and advanced preview capabilities.

1. INTRODUCTION

In recent years, tomographic microscopy beamlines have experienced a tremendous increase in data rates. Technological developments, in particular in the detector field, pushed the time resolution to the sub-second regime opening up new scientific possibilities, including the investigation of dynamic (in-situ, in-operando and in-vivo) processes in 3D with micrometer resolution (Fig. 1) [1, 2]. In parallel with the data rates and the related new opportunities, also the general experiment complexity at beamlines has been steadily increasing, with complex sample environments, multiple triggers and complex time sequences. The typical amount of data generated during such studies in a few days is in the order of tens of Terabytes (TBs).
To optimally exploit the latest hardware advancements for new opportunities, the entire workflow from data acquisition to the analysis needs to be completely rethought and redesigned. The acquisition framework needs to be flexible and user-friendly to be able to best adjust the acquisition scheme to the peculiarities of each single experiment. Advanced preview capabilities are essential to monitor and tune in real-time the investigated processes. The reconstructed data or a subset thereof should be available few seconds after the end of the experiment to at least semi-dynamically control the experiment and beamline parameters for optimal image quality. Finally, the visualization, characterization and quantitative analysis of the obtained reconstructed volumes becomes not trivial in particular for their large size. New semi-automated and scalable solutions are needed to ensure full success of the experiments.
At the TOMCAT beamline [3] at the Swiss Light source, a dedicated ultrafast tomographic microscopy endstation has been recently established [4], featuring an in-house developed detector system (GigaFRoST [5]), which can be read out continuously leading to sustained data rates as high as 7.7 GB/s. To fully exploit the potential provided by this innovative system, different aspects of the entire data workflow have been (or are in the process of being) redesigned and optimized.

2. RECONSTRUCTION PIPELINE

Particular efforts have been put towards a fast, flexible and user-friendly post-processing pipeline [6]. It delivers reconstructed tomographic datasets just few seconds after the data have been acquired, enabling fast parameter and image quality evaluation as well as efficient post-processing of TBs of tomographic data. It can handle raw data exploiting different contrast mechanisms and it is based on a modular framework easily allowing extensions even by non-expert programmers thanks to its implementation in Python. It is optimized for a CPU architecture and can be deployed in a transparent way on single and multi-node systems as well as high performance computing facilities. It includes a user-friendly graphical interface easing the tomographic reconstruction work

* e-mail: federica.marone@psi.ch

mostly running in parallel with the actual experiment.

3. OUTLOOK

Ongoing work focusses on the design and implementation of a flexible and user-friendly acquisition framework, including a modular description of the beamline components enabling customized scripting optimally capturing the complexity of each single experiment. Automatic collection of richer metadata is also foreseen. The experiment experience is also going to be augmented by advanced preview capabilities supported by direct data streaming possibilities from the detector to the reconstruction pipeline [6]: few selected tomographic slices are available in less than half a second, paving the way to new concepts for on-the-fly control of dynamic experiments. The optimized workflow will also include an extended reconstruction platform featuring a flexible and customizable iterative reconstruction framework in addition to the standard analytical routines, so to guarantee highest quality tomographic volumes even for noisy and undersampled datasets common for ultrafast experiments. Finally, flexible, scalable and semi-automated solutions for the quantitative analysis of sheer volumes of tomographic data are also under investigation.
Such workflows will be fundamental at the new diffraction limited sources currently coming into operation, where sustained data rates of several GB/s will become even more routine.

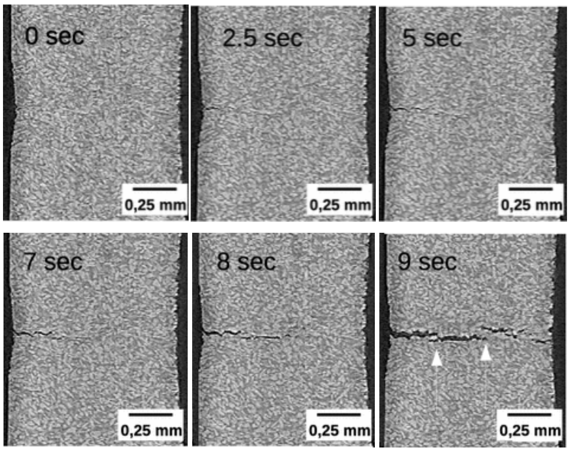

Figure 1: Fracture mechanics – 20 Hz Tomography - Reconstructed slice extracted from the same region in the middle of the sample at different instants during the fracture experiment. The tensile axis is vertical in the figure. The crack nucleates at the notch and then propagates from left to right. The white arrows at t = 9 s indicate a change in propagation plane [1].

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