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A graphical user interface for real-time analysis of XPCS using HPC

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ABSTRACT

With the development of third generation synchrotron radiation sources, X-ray photon correlation spectroscopy has emerged as a powerful technique for characterizing equilibrium and non-equilibrium dynamics in complex materials at nanometer length scales over a wide range of time-scales (0.001–1000 s). Moreover, the development of powerful new direct detection CCD cameras has allowed investigation of faster dynamical processes. A consequence of these technical improvements is the need to reduce a very large amount of area detector data within a short time. This problem can be solved by utilizing a large number of processors (32–64) in the cluster architecture to improve the efficiency of the calculations by 1–2 orders of magnitude [1] (Tieman et al., this issue). However, to make such a data analysis system operational, powerful and user-friendly control software needs to be developed. As a part of the effort to maintain a high data acquisition and reduction rate, we have developed a Matlab-based software that acts as an interface between the user and the high performance computing (HPC) cluster.

1. Introduction

A partially coherent beam scattered by a disordered system produces an interference pattern called speckle. In a typical X-ray photon correlation spectroscopy (XPCS) experiment, the dynamics in the illuminated specimen, reflected by the temporal evolution of the corresponding speckle pattern, is quantified with the help of a normalized intensity autocorrelation function [2]:

$$g_2(\tau,q) = \frac{\langle I(t,q)I(t+\tau,q)\rangle}{\langle I(t,q)\rangle^2} \tag{1}$$

where $I(t,q)$ is the intensity scattered at the momentum transfer q at time t and $\langle\dots\rangle$ represents the time average. XPCS measurements yield detailed insights into the dynamic aspects of the measured sample. The analysis of the $g_2(\tau,q)$ functions, which often can be described in the form:

$$g_2(\tau,q) = \alpha e^{-(\tau/\tau_0)\beta} \tag{2}$$

allows one to determine the q-dependence of the characteristic time-scale for the dynamics τ_0 within the probed sample. The spatial and temporal heterogeneity of the dynamics is described with the help of the exponent β and α is the pre-factor describing the coherence of the experimental setup. A particularly powerful variation of XPCS, is so-called multispeckle XPCS, where an area detector is used to simultaneously collect data over a rage of wavevectors. Multispeckle XPCS has proven to be a well-established tool for the investigation of a wide range of systems, like colloidal suspensions, polymers and simple liquids [3].

In a typical XPCS experiment, the time series ranging from several hundreds to tens of thousands of CCD frames are collected. The shortest time-scale for the dynamics, which can be resolved using XPCS, is determined by the maximum frame acquisition rate. With the data collection speeds considerably improving nowadays, the experimenter faces a daunting task of processing a huge volume of data. The computation of the $g_2(\tau,q)$ functions for even a relatively short data set is a time consuming task, even with state-of-the-art workstations. Since fast data reduction is one of the key elements of a successful XPCS experiment, it is of high importance to develop the means of the rapid calculation of the autocorrelation functions from the collected speckle patterns.

A sophisticated acquisition/analysis system, developed at beamline 8-IDI at Sector 8 of the Advanced Photon Source (APS), offers an experimenter the possibility not only to probe the dynamics at the millisecond time-scales, but also to analyze the data at the rate it was collected. In this paper, we present one of the components of the system: a user-friendly graphical user interface software tool for data reduction and visualization using a high performance computing (HPC) cluster unit.

2. Architecture of the data acquisition/analysis system in Sector 8 at the APS.

The system architecture is presented in Fig. 1. The workload for the computing unit and the storage arrays is minimized by pre-processing

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(dark subtraction, running averaging, compression) of the acquired images, in real-time, using a field-programmable gate array (FPGA) on a frame grabber PCI based card [4]. The compressed images that are saved in real-time to a local storage disk are transferred to the data storage unit on the cluster, after the acquisition is done. Despite compression, the size of each data is large (typically several gigabytes). The problem of fast data transfer over the network was solved with the help of the GridFTP protocol [5]. The high data analysis rate has been achieved by performing the calculations in the parallel mode using multiple processors arranged in the cluster architecture. A parallel algorithm (MPICorrelator) [1], that computes the intensity autocorrelation functions, was written using the Message Passing Interface (MPI). Depending on the number of cores assigned, the HPC cluster usage reduces the data analysis time by a factor of more than 30, as compared to a single workstation [1]. The interface between the HPC cluster and the user is supported by a code, named XPCSGUI, which has been written in a Matlab environment.

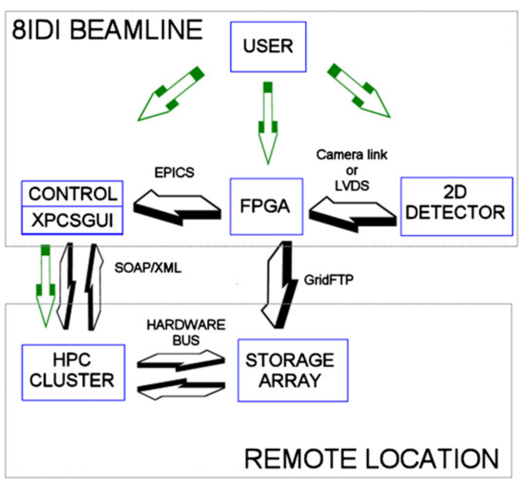

Fig. 1. The architecture of the data acquisition/reduction system at beamline 8-IDI at Sector 8 of the APS. The data and the control flows are marked with blue and green arrows, respectively. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

3. XPCSGUI

The XPCSGUI software is a sophisticated tool providing the experimenter with an easy way to perform a rapid analysis of the speckle patterns collected in various scattering geometries. It supports calculations on a local workstation (efficient for very small data sets) as well as the parallel computations on the cluster in the case of voluminous data sets. With the addition of the settings for the cluster (Fig. 2), there is no difference noticeable for the user in the GUI and the data reduction procedure between the local and the cluster-based analysis. Further, in the absence or the unavailability of the cluster, the calculations are carried out automatically on the local computer. When set to the remote/cluster mode, XPCSGUI utilizes Matlab's timers to periodically monitor the progress of the computations. Such an approach significantly reduces the usage of the local computer resources, making them available for other tasks.

To commence the data analysis, the user is given a set of tools for visualization of the subset of the measured data to aid in making decisions about binning and region of interest (ROI). For example, the ROI is defined and divided into user selectable number of partitions, each corresponding to the same momentum transfer value q. In the case of the cluster-based analysis, such a partition map convoluted with the ROI, is saved in a library folder on the cluster. The same partition map can be assigned by the user to multiple data sets. The scattered intensity is correlated individually for each pixel as a function of time using the multi-τ algorithm [6]. In the final part of the calculations, autocorrelation functions computed for the pixels belonging to the same q partition are averaged and normalized. Besides returning the autocorrelation functions, the software also performs basic fits based on Eq. (2). Additionally, the time series of the scattering patterns, calculated from the averaged speckle pattern, are displayed to detect any evolution of the sample structure due to non-equilibrium aspects of the dynamics or beam damage.

XPCSGUI provides an intuitive way for the user to interact with the HPC via web-based services without the user being aware of the complex processes occurring on the HPC system remote from the beamline. Before launching the parallel computation, XPCSGUI configures MPICorrelator by optimizing the number of processors

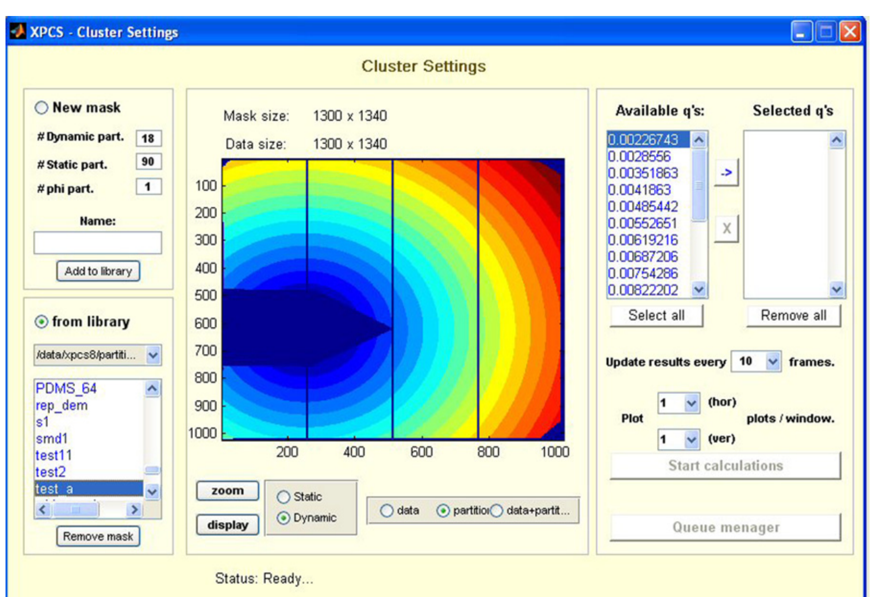

Fig. 2. The part of the XPCSGUI devoted to the setting of the analysis using the HPC cluster. An example ROI superimposed on the dynamic partitions mask is shown in the middle of the window.

used, and sets the frequency (number of frames), with which the partial correlation functions are saved and displayed for the user. All the settings used for the cluster operation are saved for future reference. The outcome of each analysis run is also saved in ASCII format in the separate folder, enabling the user to compare the results obtained under different experimental conditions and input parameters. In addition to the interactive mode of operation, the GUI can use a queuing system that allows for processing multiple data sets in a time efficient manner.

4. Future direction

The ultimate goal of this work is to extend our XPCS data acquisition system to support real-time data analysis, allowing a user to preview the intensity autocorrelation functions as the CCD images are being collected. XPCSGUI is an important component in that direction. Although, the current version of the GUI supports the real-time operation mode, the existing code needs to be further optimized to provide user-friendly tools to manage the data and queuing systems.

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