GPU based data analysis on the example of time-of-flight spectroscopy

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Abstract and Motivation

Free electron lasers (FEL), such as FLASH in Germany [1], FERMI in Italy or LCLS in Stanford, improved the light brilliance by more than 9 orders of magnitude compared to synchrotron radiation sources [2]. This new light source allows to study non-linear multi-photon processes within one single FEL shot which is less than 50fs long and has a repetition rate of 120Hz at LCLS, for example. As a result, a huge amount of data is created in a very short acquisition time. Analyzing these data on a single shot level needs a lot of computing power but can be massively parallelized. In order to decrease the evaluation time, we created a GPU-based evaluation software for our electron time-of-flight spectrometer setup.

Experimental setup

In a cylindrical vacuum chamber (due to the compactness we call it 'cookie box') a number of electron time-of-flight spectrometers are mounted at various angles with respect to the horizontal polarization axis of the incoming light (see figure 1&2). All spectrometers point to the focal spot of the beamline into which various noble gas (or molecular) targets are introduced through a small needle in an effusive beam. The target gas is ionized by the FEL radiation and the generated photo electrons are detected at the end of the drift tubes of the spectrometers by micro channel plate (MCP) detectors. The flight tube of the spectrometers is divided into four segments (sections) of different length in order to apply a set of retardation voltages to slow down photo electrons and enhance the energy resolution. The ratio of the retardation voltages have been optimized by simulation as well as test experiments to preserve the transmission of the spectrometer when retarding. The MCP charge pulses are amplified and recorded by means of a multi-channel digitizer card system with a time resolution of 4Gsample/s (see figure 3) .

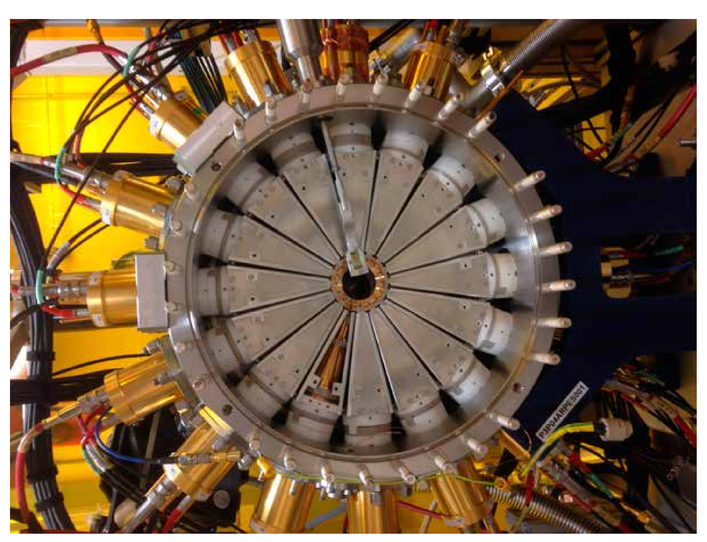

Figure 1: Photography of the opened 'cookie box' showing the 16 spectrometers with an angular difference of 22.5° between neighboring detectors and the interaction region of the FEL-light and the introduced gas target in the center.

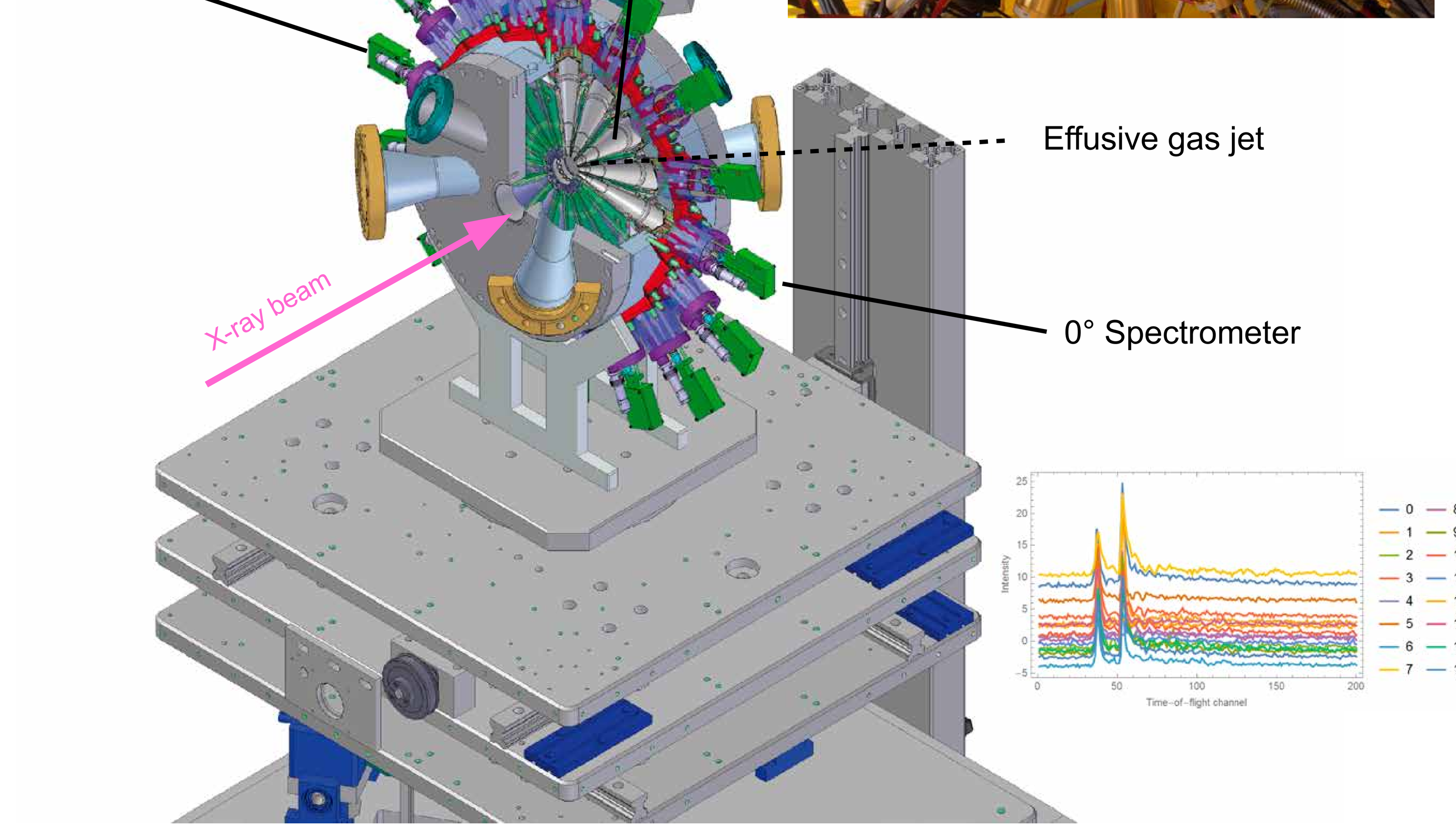

Figure 2: Sketch of the experimental apparatus 'cookie box' used in our measurement campaigns at the free electron laser (FLASH, FERMI, LCLS) and synchrotron (PETRA III) facilities. The inset figure (bottom right) shows an example of recorded single shot data.

Where the GPU comes into play

An enormous number of time of flight spectra is created. For instance, during an acquisition time of 30 minutes and with a repetition rate of 120Hz we record 3,456,000 spectra. In general, the idea is to interpret these spectra as vectors (and combinations of them as matrices) and to perform the data evaluation as matrix/vector-operations on the GPU.

Task	Operation on GPU
Sum spectra of single shots	Adding vectors
Covariance analysis (coincidence)	Matrix multiplication, scalar products
Intensity filter	Numerical integration
Single shot fitting	Parallel least square fits
Detector ringing removal	Matrix multiplication

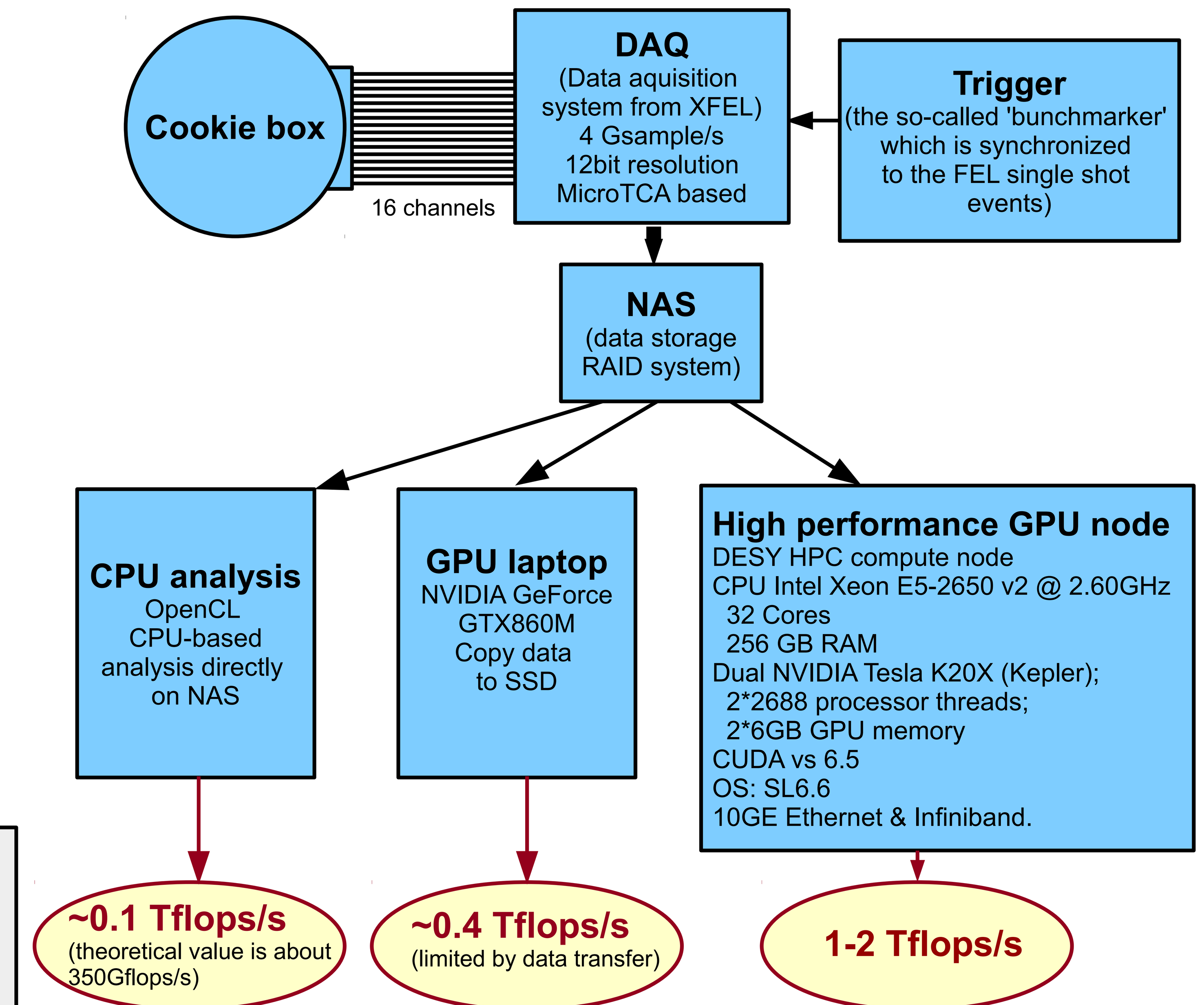

Figure 3: Schematic depiction of the data recording and analysis; the 16 MCP traces are recorded with a digitizer system equipped with powerful FPGAs capable of pre-processing and data streaming (http://spdevices.com/index.php/adq412) and stored on a NAS. The data can then by analyzed directly on the NAS on CPU level or on a different device as a GPU laptop or a new GPU performance node (http://it-hpc-web.desy.de/).

Sideband experiment at FLASH

Very recently, we performed a two-color photoionization experiment [3] in a noble gas target. An optical laser was overlapped in space and time synchronized with the extreme ultra-violet (XUV) FEL pulses. Electrons, born in the overlapping electric fields, can in addition to the XUV photon absorb or emit additional optical photons. This results in a splitting of the photo electron line into a multiplett of lines, the so-called sidebands. In addition the tilt angle of the linear polarization of the optical laser was tunable. The detector signals showed ringing and cross talks which could be removed by a covariance mapping analysis in addition with sideband intensity filtering performed on the GPU which decreased the calculation time of these many matrix products by the factor of ~40. The preliminary results are shown in figure 4 and compared to theoretical predictions of Nikolay Kabachnik et al. [4].

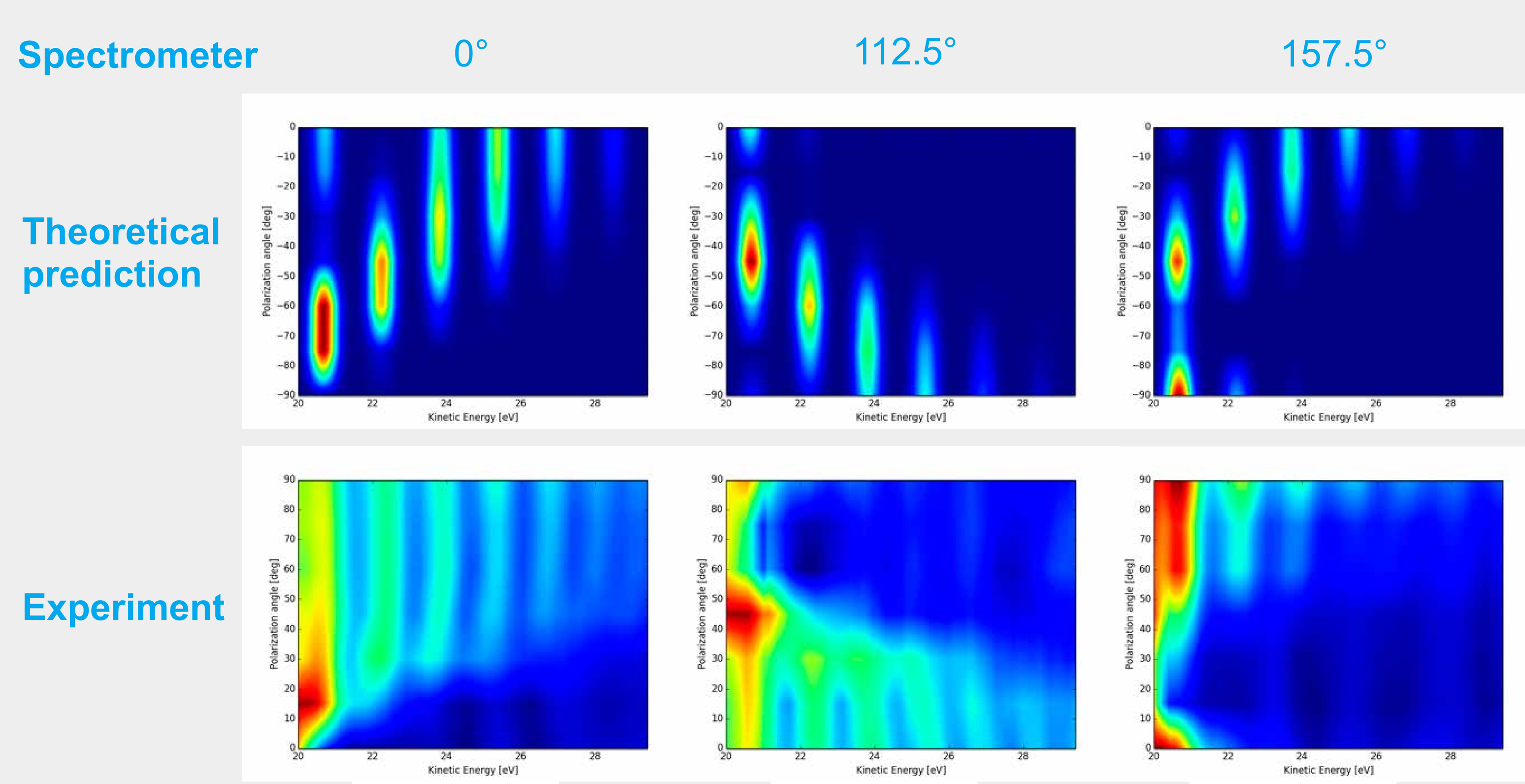

Figure 4: Comparison of theoretical predictions with our experimental results for 3 detectors examples. The density plots show the electron intensity as a function of electron kinetic energy (x-axis) and polarization angle (y-axis, the angle between FEL- and optical laser-polarization is meant). The analysis was performed by the use of a GPU in order to perform numerous matrix multiplications.

Conclusion and outlook

Our setup was already used for various scientific investigations of atomic and molecular photoionization processes at synchrotron and free electron laser facilities [5] as well as beamline commissioning at FERMI [6], FLASH and LCLS. The online feedback of the cookie box (as for instance the degree and tilt angle of linear polarization, intensity monitor, beam position, etc.) is very particularly interesting for the undulator crew of the specific beamline. The parallel calculation-power of NVIDIA GPUs opened a new set of evaluation methods of the large amount of data recorded at the experiment. Our new high performance GPU node (see figure 3) will enable highly complex evaluations even in an online analysis mode improving the direct feedback of our setup in a whole new way. Additionally, the European XFEL data acquisition group is working on data streaming interfaces in order transport the data to the processing systems in real-time. This will completely remove the NAS system out of the data recording and evaluating process.

References:

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