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APT_PyControl, an Open-source Python Atom Probe Tomography Control Software Package

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Atom Probe Tomography (APT) is a fast-growing domain where the vast majority of systems are marketed with proprietary software. Closed instrument hardware and locked-in control algorithm on these systems limit many aspects of the experiment where low-level access to machine control or experiment results data is required. Over the past decade, the emergence of off-the-shelf detector systems with a fast data bus such as USB 3.0 have made it viable to design and build atom probe systems without sophisticated electronics engineering skills. In spite of these significant hardware improvements, the number of measured atoms over the last few years has not increased significantly [1]. For many projects in this direction, the need to develop control software and the associated time commitment continued to be a significant impediment.

Here, we present a modular open-source atom probe control software package written in Python, which allows full control of the experiment and data collection [2]. This software takes the detection events from a commercially available delay-line detector Surface Concept DLD 8080 (Surface Concept GmbH, Mainz, Germany) via a USB 3.0 connection from the time-to-digital converter (TDC). It also includes a module for connecting to the RoentDek hexanode delay-line detector (RoentDek Handels GmbH, Kelkheim-Ruppertshain, Germany) through a PCIe connection. As an initial step to directly digitize the detector signal, a Domain Sampling Chip (DRS) digitizer module (RDEC GmbH, Villigen, Switzerland) was implemented in this project. In an atom probe control system, several devices must be controlled simultaneously, and data must be collected without interruption. This package used multithreading and multiprocessing in device communication, graphical interface, and detector reading to attain this subjective.

Python program execution is notoriously slow, mainly because of the way that the language is built; however, because of the vast library support and productivity in Python, we are able to implement versatile software in an easily readable format [3]. As a result, detector readout functions run in C++ through the Dynamic Link Library (DLL) to resolve the performance problem. In Figure 1, the modules in the package are illustrated. The project consists of seven main modules, three of which are intended to collect detector or TDC data. The device module contains all the scripts for controlling and monitoring devices such as gate valves, gauges, or cameras.

As the control algorithm, a proportional control has been implemented based on the number of results detected since the last TDC or detector reading. The effectiveness of the control algorithm was verified with multiple simple and complex samples such as Aluminum, Nickel, and Tungsten [4]. Figure 2 shows the user interface of the control software, which shows how the user can adjust the settings of the experiments and monitor the flight time histogram and detector map. At the end of the experiment, the data are then stored in a Findable, Accessible, Interoperable, and Reusable (FAIR) data format (HDF5), containing all data collected during the experiment, with the possibility of raw detector data. Therefore, this controlling system forms the basis of a fully FAIR atom probe data collection and analysis chain [5].

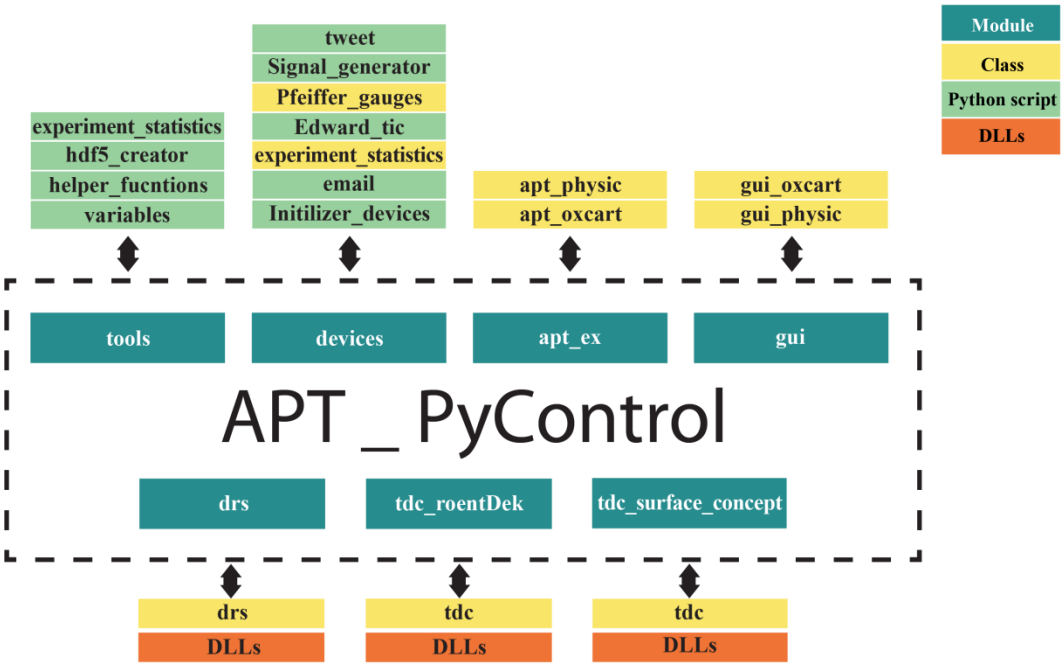

Figure 1. The APT_PyControl package consists of seven modules. TDCs & DRS modules are used to collect detector data. The remaining modules contain functions for controlling the machine's devices, such as the signal generator, gauges, etc. The C++ DLLs were used under Python wrappers to achieve fast data acquisition.

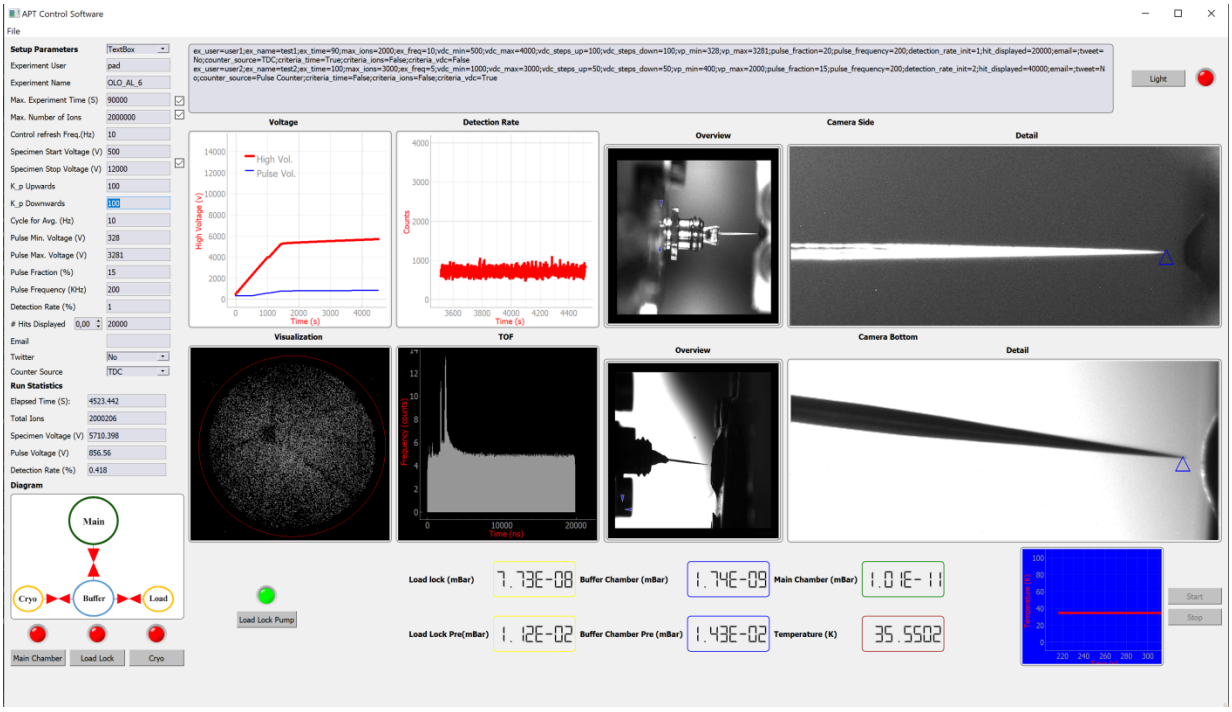

Figure 2. The user interface of the atom probe control system, including data visualization. The valve and pump controls, as well as the camera view, allow the user to insert and align the sample.

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