The yaq project: Standardized software enabling flexible instrumentation

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ABSTRACT

Modern instrumentation development often involves the incorporation of many dissimilar hardware peripherals into a single unified instrument. The increasing availability of modular hardware has brought greater instrument complexity to small research groups. This complexity stretches the capability of traditional, monolithic orchestration software. In many cases, a lack of software flexibility leads creative researchers to feel frustrated, unable to perform experiments they envision. Herein, we describe Yet Another acQuisition (yaq), a software project defining a new standardized way of communicating with diverse hardware peripherals, yaq encourages a highly modular approach to experimental software development that is well suited to address the experimental flexibility needs of complex instruments, yaq is designed to overcome hardware communication barriers that challenge typical experimental software. A large number of hardware peripherals are already supported, with tooling available to expand support. The yaq standard enables collaboration among multiple research groups, increasing code quality while lowering development effort.

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I. INTRODUCTION

Instrumentation development is a key part of the scientific enterprise. Novel instruments are typically constructed of many individual components that are both purchased and home-built. Orchestration software must communicate with each hardware component in the course of a scientific experiment. Orchestration can involve the utilization of many interfaces: NI DAQmx, SCPI, 2 ModBus,³ PICam,⁴ and Thorlabs APT,⁵ among many others. The challenge of integrating all of these interfaces is a frustrating piece of the modern instrument development process. Weeks can be spent just integrating one new component into an existing project. In small academic labs, these software interfaces are typically created by student researchers without software development experience. Student researchers rarely focus on software reusability, and a lack of maintenance and documentation can make such software more difficult to use as time goes on. Scientists may struggle to rapidly innovate their experimental design when each hardware addition requires major software development.

Some large user facilities have addressed interface complexity via the adoption of unified standards, such as EPICS⁶ or TANGO.⁷ The unified standards define a network interface for any hardware component. Orchestration software can target these unified standards for reading and writing hardware states. Small background services are written to translate the myriad component interfaces into the standard EPICS IOCs and TANGO Devices. These programs are performant, open source, and have huge libraries of existing hardware interface support but require expert management to set up and provide descriptions via a separate server program. In our experience, EPICS and TANGO do not scale well to single-investigator lab environments.

As smaller research labs have grown in experimental complexity, many individual labs have created domain-specific orchestration software. In the last few years, several open-source projects by-and-for small-scale experimentalists have grown in popularity. ⁸⁻¹⁵ Although this growth is encouraging, many of these are limited by their focus on particular types of hardware or particular experimental domains. More work needs to be done to catalog, compare, and

contrast the large number of open-source projects that now exist. Most small custom research instrumentation continues to rely on monolithic software that has hard-coded interface support for each particular connected device. These monolithic applications tend to be inflexible and difficult to develop.

We have created a new network-based communication standard for scientific instrumentation, yaq (Yet Another acQuisition). This standard borrows the most important ideas from established projects used by large user facilities while retaining the simplicity appropriate for small research labs. We have built this standard to be self-describing, portable, and reusable wherever possible. Via the yaq interface, we provide easy-to-use hardware support for scientists to use with their choice of experiment orchestration software.

Here, we discuss the design of the yaq standard in the context of challenges facing instrument designers. First, we discuss how particularly challenging hardware interfaces can become seemingly insurmountable barriers to software control. Next, we discuss how inflexible orchestration software can limit experimental creativity. Then, we focus on challenges that arise when enhancing or modifying existing instruments with new hardware. Finally, we discuss the heavy software maintenance burden that many instrument designers face. In each case, we will highlight how the yaq project is designed to alleviate that challenge. Several case studies provide a view into the flexible ways that yaq can be applied to perform different scientific experiments. This paper provides an overview of the concepts and motivations behind yaq. Refer to the yaq website for a formal specification of the yaq standard. ¹⁶

II. HARDWARE INTERFACE CHALLENGES

In this section, we describe the architecture of the yaq framework in light of three major barriers that we have encountered in scientific instrumentation development. First barrier: Multiple interfaces are used to communicate with each component of the system. A fully automated system must be able to use all of these interfaces, a daunting task for scientists who do not specialize in software development. Second barrier: Certain specialty hardware has inconvenient interface requirements. A camera will only work with an obsolete interface card and drivers for Windows XP. A data acquisition manufacturer provides an Application Programmer Interface (API) that only works in Python 3.7. A graduate student wishes to drive several stepper motors using a Raspberry Pi. Third barrier: Some hardware interfaces are blocking. A graphical user interface stalls while waiting for a camera to collect data. Custom orchestration software needs to be closed before the manufacturer's configuration software can be used. A graduate student finds themselves needing to master advanced concepts in concurrency to orchestrate many motors performantly.

Figure 1 diagrams the yaq architecture. Here, we show three different computers connected via an Ethernet network. The top and bottom computers are connected to monitors for interactive use, whereas the middle computer is only accessible via the networks. This diagram might represent a complex scientific instrument involving several operator terminals as well as embedded computers. At the top, a single computer is connected to four hardware peripherals through RS232, TTL, USB, and PCI as indicated by the colored lines. That same computer is running four

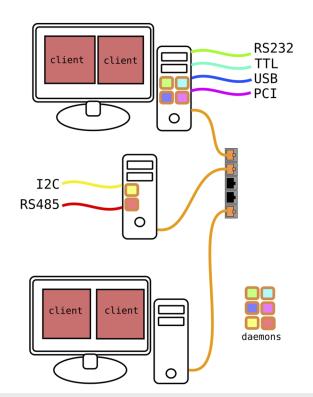


FIG. 1. A simplified network diagram for a hypothetical instrument. Three computers are connected via orange Ethernet cables and a network switch (middle right). Some of the computers are also connected to hardware peripherals via one of the six interfaces (colored lines). For each interface, the computer runs a yaq daemon (small colored squares). The top and bottom computers are also running yaq client applications.

separate programs, one for each peripheral. These small, targeted, programs are managed by the operating system and run in the background. It is conventional to call such programs "daemons." 17 The middle computer is connected to two additional peripherals and runs daemons for each. Besides communicating with the hardware peripheral, each daemon can communicate with other programs, "clients," through the network. The four client programs shown in Fig. 1 can each communicate with all six hardware peripherals shown. As an example, a client running on the bottom computer could communicate with the RS232 peripheral shown in green via the following path: client \leftrightarrow network switch \leftrightarrow top computer ↔ daemon ↔ hardware peripheral. This powerful architecture can be used on a single computer or used across many networked computers, including fully remote operator interfaces. This client-server architecture offers similar network capabilities to EPICS and TANGO. As we will show, the usage of standards and the creation of tooling make this architecture accessible to instrument builders outside of large facilities.

In yaq, communication between daemons and clients is performed over TCP/IP using Apache Avro RPC.¹⁸ Avro provides an agreed-on standard for efficient serialization of data and method calls from a remote (client) process. Practically, the yaq interface looks like a collection of methods or functions, which Avro

calls "messages." Each message has defined input parameters and output return types. A sensor might implement a message called "get_measured," which takes no parameters and returns a dictionary mapping channel names to the numeric or array data. A motor would implement a pair of messages for setting and reading back the motor position: "set_position(float position) \rightarrow null" and "get_position() \rightarrow float." Messages make up the lowest level functionality of the yaq interface. Each daemon supports a collection of messages for its unique functionality, called the "protocol." When a client first connects to a daemon over TCP/IP, the daemon provides a complete description of its own protocol. We, therefore, refer to the daemons as "self-describing."

Each individual communication between the client and the daemon involves one message being requested by the client and the response returned from the daemon. If multiple messages are sent simultaneously, the daemon processes one message at a time. The protocol is preemptive: in the case of a conflict, the daemon will obey the last message to arrive. By being completely open to messages from multiple clients, yaq makes it possible to accidentally supersede a message. This has not become a problem for our usage where instruments are controlled by single scientists who can clearly see all of the clients interacting with their system. Typically, there is just one client sending "set_position," and many clients polling "get_position" to record data or display real-time information. Users may choose to implement access control systems, but we do not foresee building access control into the yaq protocol. This is similar to how access control works, in practice, at some large facilities.

yaq introduces a concept called "traits," which are collections of related messages that are shared among multiple protocols. Motors implement the "has-position" trait, which defines "set_position," "get_position," and "get_units." Sensors would implement the "is-sensor" trait, which defines "get_measured," "get_channel_names," and "get_channel_units." Protocols that implement a trait must support all of the messages from the trait. Traits are compositional: a given protocol may implement several traits at once. For example, a protocol representing a monochromator with several gratings might implement both "has-position" and "has-turret," where the latter defines special messages for choosing which grating is used. Importantly, specific protocols can also implement arbitrary additional messages that are not defined by any trait.

We have carefully defined yaq traits to maximize interoperability while not excluding hardware with unusual features. New traits can be discussed by the community through the yaq enhancement proposal system. It is crucial that multiple hardware interface examples be considered when defining traits. Configuration that is unique to a single interface is best handled through protocol-specific messages. For example, our protocol for interfacing with a specific data acquisition card provides a message for setting the segment count. Unique messages are available through script-based and graphical clients, but the usage of such messages in scripts naturally limits portability.

We now describe how the yaq architecture addresses the three hardware interface barriers described at the beginning of this section. The first hardware interface barrier: Multiple incompatible interfaces are used to communicate with each component of the system. yaq provides a unified TCP/IP interface to all hardware peripherals based on the well-described Avro RPC protocol. The

trait system was introduced in pursuit of our primary goal of easing the client development process. Clients can trust that protocols that implement a given trait will behave in similar ways. The standardized yaq interface presents the same set of interactions for client-side scientific code, simplifying the experience of using hardware.

The second hardware interface barrier: Certain specialty hardware has inconvenient interface requirements. Since yaq enables multiple machines, any hardware requirements can be addressed by putting a machine for that specific hardware on the network. The Raspberry Pi, which drives several stepper motors, can be placed onto a private network to communicate with the primary instrument computer using yaq. Because each yaq daemon is running in its own process, the software environment can be tailored to its needs. A client running up-to-date Python 3.11 communicates seamlessly with a daemon running Python 3.7.

The third hardware interface barrier: Some hardware interfaces are blocking or slow. Experimental orchestration often means doing several things at once, e.g., simultaneously moving several motors. To accomplish this task performantly, monolithic orchestration software often necessitates separate threads for each component hardware interface, a fragile pattern in which small mistakes become both critical and elusive errors. When writing orchestration software using yaq, slow hardware interfaces are replaced by fast Avro-RPC. In our experience, the yaq interface is responsive enough to give good performance when orchestrating tens of motors using a singly threaded client. There is a limit where using TCP becomes a bottleneck for large responses, such as those from cameras or other highthroughput sensors. In our experience, this limit is ~1 megapixel. For larger sensors, a pure yaq approach may not be appropriate. There is a longer discussion of timing and order-of-operations control details using yaq in the supplementary material.

III. EXPERIMENTAL FLEXIBILITY

Existing experimental orchestration software is often highly inflexible. An experimentalist will spend many hours in the lab manually repeating acquisitions because it is too challenging to add repetition functionality to their software. A laser lab needs to spend weeks on software development when introducing a single new step into its experimental procedure. Researchers are disappointed to realize that they are forced to start from scratch when developing software for a similar instrument built with trivially different hardware.

Unique experiments will always need custom orchestration and user experience. We believe that novel instrumentation development naturally and necessarily includes the creation of targeted software. Developing experimental software is an iterative process tied to the scientific goals of the instrument. Often experimentalists must apply their specialty scientific knowledge to develop this software.¹⁹

In our view, software inflexibility is a natural consequence of the typical software development practices used by custom instrument builders. Instrumental software is often built as one monolithic program that does everything from providing a graphical interface, through hardware interfacing, and writing data files. Such software is typically impossible to debug without access to real hardware, often requiring all of the hardware to be available to simply start the program. As such, instrumentation software development time is in conflict with valuable data acquisition time. The hardware interfaces that these programs implement are typically made quickly and without regard to standardization with similar hardware. The orchestration routines are intimately tied to the particular hardware configuration of one instrument.

yaq is architected to encourage better software development practices when creating such programs. In a yaq context, orchestration code and graphical control interfaces are implemented as clients. These clients are automatically simpler because they only need to implement the yaq standard and do not need to include the vast array of hardware-specific communication interfaces. Beyond this, clients can use traits to interact with similar hardware identically. A client written to perform a two-dimensional fluorescence experiment using two Acton monochromators will also work with Horiba monochromators without any modification.

Figure 2 shows that yaq supports a diverse array of client types. At the top, we represent the most lightweight interface to yaq, Python scripting. yaqc²⁰ is a Python client that is excellent for using in scripts or any other Python program. The code shown creates three client objects that could be used directly through an interactive Python prompt or in a reusable script. Each client object provides Python methods for each Avro message specified by the associated protocol.

FIG. 2. Representations of three very different yaq client experiences. Top: lightweight scripting. Middle: graphical user interface. Bottom: integration with Bluesky for data collection. In all three cases, the same daemons are addressed.

In the middle, the same three hardware peripherals are represented in an interactive, graphical form. yaqc-qtpy²¹ is a graphical application that builds interactive controls based on traits for any conceivable yaq protocol. The self-describing yaq interface is used to provide graphical elements for the most commonly used messages. yaqc-qtpy is an invaluable tool that provides a "free" graphical user interface (GUI) to any daemon.

At the bottom, we graphically represent the integration between yaq and the Bluesky project. ²² Bluesky provides a powerful orchestration layer for conducting and recording data for a wide variety of experimental procedures. Bluesky has no built-in hardware interface support, instead relying on packages to create hardware interfaces that are compatible with their Hardware Protocol definitions. yaqc-bluesky²³ is a specialized client that adapts any yaq protocol into Bluesky. Similar translation layers could be built for a variety of orchestration software such as PyMoDAQ,⁸ PyMeasure,¹³ or TRSpectrometer.¹⁰

All three types of clients represented in Fig. 2 have been shown addressing the same three hardware peripherals. All types of clients can be used simultaneously to interact with the same instrument in different modes. Client sophistication can be introduced naturally, as novel experiments are tested and refined. Different clients can specialize in different requirements of a custom instrument. For example, yaqc-qtpy can provide a quick interface for setting and viewing hardware positions, whereas Bluesky can focus on experimental data acquisition.

The Landis Group at UW-Madison is currently working on a new type of flow reactor: the Wisconsin Quench Kinetics Reactor (WiQK). This reactor incorporates several computer-controlled valves and syringe pumps as well as various sensors. The set of hardware peripherals is rapidly changing as researchers continue to test and refine their design. Only a few researchers are actively using the reactor during this prototyping stage. These researchers are experimentalists who have limited background in software development. The Landis Group has written basic Python scripts to orchestrate hardware for their reactor. These lightweight scripts can be extensively refactored by the experimentalists as the hardware and orchestration strategy changes dramatically during WiQK development. This approach ensures that the Landis Group is not slowed down by complex, inflexible orchestration software. Once the reactor is complete, more sophisticated graphical clients will be created to accommodate end users who were not involved as the reactor was built.

The Wright Group at UW-Madison needs to orchestrate a large variety of hardware in multidimensional scans for their complex spectroscopy experiments. ^{24,25} This need for exquisite hardware control has resulted in several prior attempts at "home-built" orchestration software. ^{26–30} Now, using yaq, the Wright Group has been able to move to Bluesky rather than inventing their own sophisticated control software "from scratch." The Wright Group uses simulated hardware to enable client development away from active laboratory computers. Hardware simulation allows Wright Group researchers to create polished client interfaces without interrupting ongoing experiments. Clients developed by the Wright Group have proved flexible enough to be used on four laser systems, each with different complements of hardware. Moving forward, the Wright Group will spend less energy developing control software and more energy developing creative spectroscopy experiments.

IV. INCORPORATING NEW HARDWARE

In a yaq context, new hardware can be incorporated into an instrument through the addition of a new daemon. The yaq architecture simplifies hardware interface development in several ways. First, because daemons are separate and portable programs, the development effort can be spread across the community of yaq users. Often, researchers can download an existing daemon rather than writing a new one. Second, yaq daemon development can be performed separately from the particulars of any individual client. Often, this separation allows initial hardware enablement work to be done on a researcher's personal machine before the new hardware peripheral is installed in the instrument. Separability, portability, and distributed development are advantages common to many open-source hardware interface projects. Third, when developing trait-compliant protocols, it becomes easy to design and fully test your hardware interface. Traits are unambiguous and well described, making an obvious target for development. Tooling exists to verify full trait compliance, for example, you can use yaqc-qtpy to provide a graphical program to interact with your hardware immediately. Finally, as discussed in Sec. II, yaq provides options to design using remote hardware or unusual interfaces when necessary.

We have created several tools to aid in daemon development. First, a Python library, yaqd-core, 31 which implements shared functionality. Second, yaq-traits 32 is a command line application that allows the description of messages provided by a yaq protocol to be written in a human-readable fashion and translated into a more fully described machine-readable format. The format it generates is an important part of how yaq protocols are self-describing. This shields developers from the details of Apache Avro, which can be somewhat esoteric.

Figure 3 shows the distribution of unique lines of Python code written to implement each of the daemons in our current ecosystem. Although lines of code are an imperfect metric, we use it here to represent the amount of work required to create a daemon for

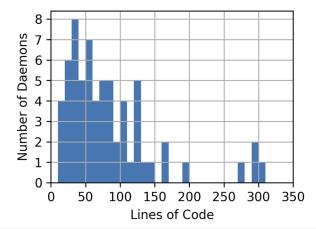


FIG. 3. Histogram of the number of lines for each implemented daemon. Some daemons are implemented in ways that share code, resulting in apparent line counts of less than 10. For example, the Thorlabs APT⁵ motor implementation supports at least eight different daemons with each specifying only a handful of constants. These are extreme examples that are not representative of most hardware interfaces; hence, we omit them here.

a new hardware peripheral. Most interfaces, such as Brooks MFC,³³ have been implemented in fewer than 100 lines of Python code. Even the most complicated daemons are implemented in about 300 lines. Implementing yaq daemons using Python is enabled through our own tooling mentioned above and the large and growing ecosystem of hardware interface libraries that Python now provides.^{34–37} In our experience, the process of creating a new daemon involves about a day of work after mastering communication with the hardware. There are currently 72 daemons in the yaq project supporting at least 66 types of hardware, noting that some daemons support the same hardware and others are software only. Because yaq is standardsbased, anyone can design and publish new daemons extending our hardware support. A living list of all daemons and supported hardware can be found on the yaq website.³⁸

The Stahl Group at UW-Madison created a custom reactor that monitors gasses being produced or consumed in the reaction head space. ³⁹ This reactor incorporates a collection of sensitive pressure transducers and a single-heating process value under computer control. yaq daemons are used to interface with each sensor and the heater controller. Recently, experimentalists have been attempting reactions involving smaller, slower, pressure changes. A fundamental flaw in the initial analog-to-digital converter board was revealed by these attempts. As a result, a new digitizer has been purchased. This new digitizer will be incorporated into the existing reactor without modifying the existing graphical user interface and data recording program, minimizing downtime.

V. TECHNICAL DEBT

Years after the original researchers leave, large monolithic acquisition programs become unknowable, undocumented, and unmaintained. A graduate student discovers a hard-coded conversion factor that is incorrect years after implementation. Scientists resort to sourcing an exact replacement for an old, broken oscilloscope due to their software's reliance on that particular interface—newer, cheaper oscilloscopes are readily available. A graduate student is forced to meticulously reverse engineer the LabVIEW codebase that they inherited to understand the details of their experiment. Software developers refer to the extra effort required to modify or fix large unmaintained codebases as "technical debt." Technical debt grows especially fast in academic environments where graduate students are involved in projects for a limited time.

The yaq approach favors many small single-purpose applications above the large monolithic ones. For daemons, the purpose of each application is obvious and unambiguous. There is a strict, well-defined interface that explicitly limits the kinds of interactions that are provided to the hardware, thus limiting the opportunity for unintended consequences. The lack of hardware interface code makes yaq clients much simpler and easier to describe and maintain. Tools like yaqd-fakes⁴¹ allow clients to be tested and improved outside of their instrument, including the possibility of fully automated testing. Simple, script-based clients written using the expressiveness of Python can be read and understood in hours rather than weeks. Integrations with communities like Bluesky offer powerful features that are actively maintained across many institutions.

In yaq, each component of an instrument can be developed and distributed separately. For example, two different instruments might

happen to use the same temperature sensor. Because the temperature sensor daemon is its own independent program, both instruments can benefit from the same daemon. The growing "ecosystem" of yaq daemons makes future instruments easier and easier to develop. Growing this ecosystem is a collaborative effort where many yaq users create portable daemons that they need and share them with the community where they will be used and improved. yaq components can be incorporated seamlessly into existing software projects, including languages other than Python. For example, an existing LabVIEW project may provide additional hardware support via yaq. In this way, a more modular instrument can be built gradually without needing to overhaul all of the software simultaneously.

Software built by scientists often has incomplete and inadequate documentation. ⁴² yaq attempts to automate daemon documentation as much as possible. Our website, https://yaq.fyi, automatically builds generated reference pages for all known protocols. These pages are automatically updated when new versions are published. Our website also contains written and video tutorials on yaq usage and development.

We have designed yaq to be easier to deploy and maintain when compared with EPICS and TANGO. yaq daemons are Python packages that can be installed on any platform using pip or conda. There is no need for centralized management servers or databases when using yaq. The Avro RPC standard unambiguously describes the message signatures for any protocol; hence, users are always aware of the capabilities their hardware supports. Traits enable interchangeability where possible. yaq can easily be used alongside other experiment control software. We provide tooling (yaqd-control) that makes it easy to configure, list, and manage daemons as background services on Windows, MacOS, or Linux (see supplementary material for more details).

yaq is open-source software. Anyone can view, install, edit, and suggest changes to our growing collection of daemons and clients. Furthermore, anyone can create their own totally custom client or daemon software separately by following the specified yaq standard. Thirteen individuals have contributed code to the development of yaq. Open-source development can be a powerful approach for research communities looking to share software development and maintenance burdens.⁴³ It is our hope that a vibrant open-source community will form around yaq. Although open-source development is not a panacea,⁴⁴ we hope that by maintaining a distributed development strategy with a strict focus on only hardware interfaces, the yaq project might prove sustainable.

VI. CONCLUSION

The yaq project defines a new general-purpose standard for hardware control in the context of scientific instrumentation. This standard has some of the powerful features of facility-scale standards while remaining simple enough for feasible implementation and maintenance in small research labs. We have shown how this approach alleviates common problems through discussion and case studies. Designing around self-describing protocols is a productive approach that has great promise in scientific software development.

SUPPLEMENTARY MATERIAL

See supplementary material for full set of line-count data and script used to produce Fig. 3. More detailed examples of orchestration using yaq, including scripts and graphical user interfaces. Detailed description of yaqd-control. Discussion and quantitative analysis of the yaq interface's performance with large arrays.

See supplementary material for a full description of the name "yaq."

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AUTHOR DECLARATIONS

Conflict of Interest

The authors have no conflicts to disclose.

Author Contributions

Kyle F. Sunden: Conceptualization (equal); Data curation (lead); Software (lead); Writing – original draft (equal); Writing – review & editing (equal). Daniel D. Kohler: Conceptualization (equal); Software (supporting); Writing – original draft (supporting); Writing – review & editing (supporting). Kent A. Meyer: Conceptualization (equal); Software (supporting); Writing – original draft (supporting); Writing – review & editing (supporting). Peter L. Cruz Parrilla: Conceptualization (equal); Software (supporting); Writing – original draft (supporting). John C. Wright: Conceptualization (equal); Funding acquisition (lead); Supervision (supporting); Writing – original draft (supporting); Writing – review & editing (supporting). Blaise J. Thompson: Conceptualization (equal); Software (equal); Writing – original draft (equal); Writing – review & editing (equal).

DATA AVAILABILITY

The data that support the findings of this study are available within the article and its supplementary material.

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