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USE OF EPICS IN SMALL LABORATORIES

H. Junkes*, W. Kirstaedter, A. Moshantaf, P. Oppermann[1]
Fritz Haber Institute, Berlin, Germany

A. D. Fuchs[2], J. A. F. Lehmeyer[2], M. Schieber[3], M. Krieger, H. B. Weber
Friedrich-Alexander-Universität, Erlangen-Nürnberg, Germany

[1]also at SLAC, Menlo Park, CA, US
[2]also at Humboldt-Universität zu Berlin, Germany
[3]also at Universität der Bundeswehr München, Germany

Abstract

Systems such as EPICS or TANGO are well-established solutions for instrument communication and data storage at large facilities (e. g. LIGO, ITER and Diamond Light Source). While these types of control systems have many inherent benefits such as time stamping, data archiving and timing solutions, they are also complex. The initial complexity and knowledge required to set up these systems is a high barrier to entry and often hinders adoption by new research facilities.

We demonstrate that such control systems can be used not only in highly sophisticated environments, but that it is possible to use and benefit from these systems in much smaller research labs and even in individual experimental setups. We present two separate use cases for which independent solutions have been developed.

The first use case demonstrates the use of an open-source configurable measurement software (NOMAD CAMELS) in a home-built Hall-effect measurement setup. Local instrument communication is combined with data acquisition from the laboratory infrastructure controlled by EPICS allowing flexible implementation of measurement protocols and automated recording of FAIR-compliant data and rich metadata.

The second use case presents the implementation of an all-EPICS environment in a catalysis laboratory allowing automated and standardized data acquisition and storage in a machine-readable and FAIR-compliant manner.

MOTIVATION

Distributed, scalable and robust systems like EPICS (Experimental Physics and Industrial Control System) [1] and TANGO (TAco Next Generation Objects) [2] proved to be beneficial and reliable for the control of large-scale facilities, e. g. synchrotrons, and are well established [3]. However, such control interfaces offer opportunities also for smaller laboratories and even standalone equipment through standardized instrument communication and automated collection of metadata. The reason why EPICS or TANGO are rarely used in small labs is mainly the lack of training, documentation and successfully demonstrated use-cases.

The particular challenge in research areas like experimental condensed matter physics, physical chemistry and material sciences is the heterogeneity of experiments. In these disciplines, experiments are often performed in individual and specialized ad hoc experimental setups, which offer the required flexibility. However, at the same time, in contrast to standardized equipment, such setups require the development of specialized measurement and control software tools. This is typically done by the researchers themselves and requires a deep knowledge of software development including the communication protocols of the huge number of available interfaces and instruments from various vendors and ages. This often results in redundant software development as each lab or even researcher has to (re-)write the code to implement new measurement protocols. Moreover, frequently not much attention is paid to FAIR-compliant [4] data and metadata acquisition. In fact, metadata such as instrument settings are rarely stored along with the raw data.

Here, standardized control systems (e. g. EPICS or TANGO) can provide solutions when additionally equipped with user interfaces that provide a low-threshold entry. Documentation and training should enable even students at the bachelor level to implement new measurement protocols.

In this paper, we report on two successfully implemented use-cases for EPICS in small laboratories developed within the FAIRmat [5] NFDI [6] consortium which serves as a blueprint.

NOMAD CAMELS AND THE DEMO LAB AT FAU ERLANGEN-NÜRNBERG

NOMAD CAMELS

The difficulties of implementing measurement and process control protocols for specialized experimental setups that enables the acquisition of FAIR data motivates the development of a software which allows the user to quickly and dynamically control measurement setups. Within the FAIRmat project we are developing the configurable measurement and experiment control system NOMAD CAMELS (or just “CAMELS”) [7]. This software aims to simplify the implementation of virtually any measurement and process control protocol without the needs of programming skills.

A core concept is the automatic recording of data and metadata that accurately documents the experimental proce-

* junkes@fhi-berlin.mpg.de

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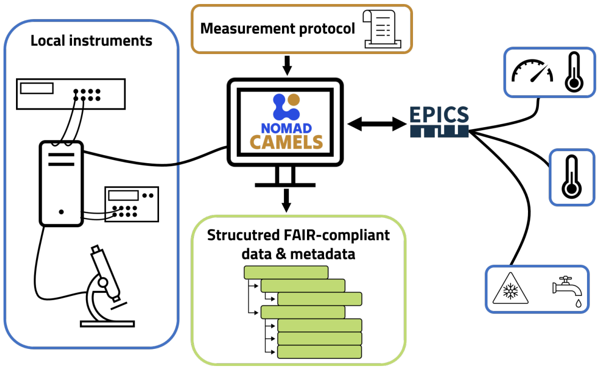

Figure 1: NOMAD CAMELS is a configurable open-source software tool for measurement, experiment and process control. It allows for configuration of virtually any measurement protocol without the needs of programming skills. CAMELS communicates with local instruments or distributed laboratory environments through community-built instrument drivers and collects all data and metadata finally stored in a structured FAIR-compliant file format.

dure, including all instrument settings. The data and metadata are stored in a structured FAIR-compliant file format (cf. Fig. 1). The metadata can include links to electronic lab notebooks (ELNs), e. g. sample history, equipment, operators. A native connection to the NOMAD Oasis ELN and repository is provided. CAMELS provides a user-friendly graphical user interface (GUI), a setup wizard, and documentation so that researchers and students can easily get started in just a couple of minutes. The GUI generates Python code that interfaces with bluesky [8] to communicate with the instruments and orchestrate the measurement. CAMELS can also be used to seamlessly communicate with large-scale, distributed systems implemented with EPICS.

Using NOMAD CAMELS and EPICS in a Hall-Effect Measurement Setup

The Hall-effect measurement technique is an important characterization tool in semiconductors physics. At the Chair of Applied Physics, we use a specialized home-built setup allowing for advanced semiconductor sample and device characterization using electrical currents from the pA to the mA range in a magnetic field of approx. 0.6 T and at sample temperatures from 20 K to 700 K. An additional gate voltage source allows for Hall-effect measurements in the channel of metal oxide semiconductor field-effect transistors. The core of the setup is an Agilent E5270B multi-channel atto-level source-measure unit. Additional instruments are used for magnet and temperature control.

The Hall-effect setup is embedded in our laboratory infrastructure including a vacuum system for the cryostat and cooling water for the electromagnet. The operating conditions of these systems as well as the room climate can sometimes have influence on ultra-sensitive measurements. Thus, recording of these complementary data is important in order to fully document the experiments.

We use NOMAD CAMELS for the measurement and experiment control. For instrument communication, we decided for a two-fold approach: (i) All lab infrastructure instruments (vacuum, cooling water, climate sensors) were connected to an EPICS input-output controller allowing for direct access to the measurement values via IT network. In addition, an EPICS ArchiverAppliance [9] continuously logs the lab infrastructure status enabling the researchers to monitor all parameters and their evolution over time from their desks via a graphical web interface. At the same time, NOMAD CAMELS accesses the relevant parameters via the EPICS protocol and stores them alongside with the measurement data. (ii) The dedicated instruments for the actual Hall-effect measurement are connected directly to the measurement computer running NOMAD CAMELS allowing for fast real-time measurement data recording and visualization. Here, NOMAD CAMELS uses device commands exchanged via the VISA protocol with the instruments.

Table 1 summarizes the instruments used and the communication type.

Table 1: Overview of the Used Devices and the Way NOMAD CAMELS Communicates with Them

Instrument	**Communication**
Agilent E5270B	local / GPIB
NI-DAQ card	local / USB
Voltcraft PPS	local / USB
Agilent 34401A	local / RS232
WIKA CPG1200	EPICS
Turbovac SL80	EPICS
Arduino climate sensor	EPICS

In conclusion, the use of NOMAD CAMELS as measurement and experiment control software gives us the following benefits:

- Flexible implementation of measurement protocols including newly conceived non-standard protocols
- Fast communication with local measurement instruments allowing for real-time visualization of the recorded and time-stamped measurement data
- Retrieval and recording the time-stamped lab infrastructure status
- Automatic storage of FAIR-compliant data and rich metadata as a complete documentation of experiments allowing for detailed data evaluation and understanding as well as reproducibility of experiments

After the successful implementation of NOMAD CAMELS and EPICS in our Hall-effect measurement setup, our target is to embed all our laboratory infrastructure into the EPICS control network and using NOMAD CAMELS on all setups for measurement and process control. The combined approach of fast local communication with instruments and network access to lab infrastructure parameters is an excellent solution for small laboratories with specialized and constantly changing measurement setups and measurement

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protocols as it is often found not only in condensed-matter physics.

EPICS ENVIRONMENT AT CATLAB

General Setup

The Fritz Haber Institute, the Max Planck Institute for Chemical Energy Conversion and the Helmholtz-Zentrum Berlin are building a research platform for catalysis named CaTLab [10] to achieve leaps of innovation in hydrogen research. CaTLab is intended as a bridge between pure research and industry.

To solve the current challenge in catalysis research in the development of new, scalable catalysts for hydrogen-based future technologies, a better integration of theory and experiment is required. The necessary data exchange demands extensive digitization in catalysis. Experimental data must be generated reproducibly and with sufficient diversity, and must be available in machine-readable form. Artificial intelligence can then contribute to the discovery of correlations [11].

We have developed and implemented a concept for a local data infrastructure (cf. Fig. 2) for such a modern catalyst laboratory. In the field of catalysis research, handbooks are written (preferably in machine-readable form) detailing how experimental data are obtained, including the definition of benchmark catalysts. The implementation of the concept of manuals can only be realised through a fully automated system for data collection and storage. Our developed system uses EPICS for communication with devices and for data acquisition. The archiving appliance for storing time series, Phoebus for creating graphical user interfaces, Python/Bluesky/Jupyter notebooks for creating automations and evaluations, and an S3 storage system [12] for storing the complete data sets (including image data). An in-house developed data management system ("*archive*" [13]) is used to document and link the metadata. This system can be seen as a kind of ELN combined with a Laboratory Information Management System (LIMS).

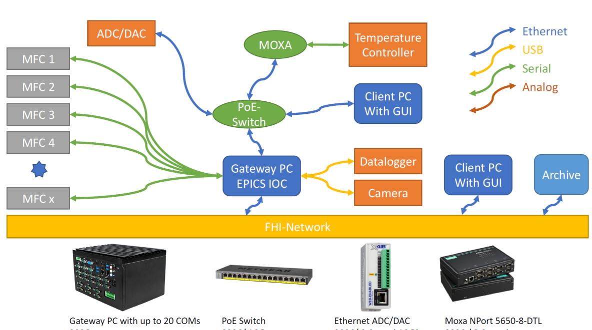

Figure 2: A standardized system layout (here to control a Chemical Reactor) enables an infrastructure that is uniform and flexible as possible and meets today's security requirements.

Each experiment setup (comparable to beamlines at synchrotrons) is equipped with a so-called edge computer . This is usually a passively cooled computer [14] with two network interfaces and some serial ports (these are available in various expansion stages, RS232, RS485), see Table 2.

Table 2: Hardware Specifications, Edge Computer

Component	Purpose
Fanless Box PC [14]	Gateway/DNS TFTP/Serial/Storage
Network Switch [15]	Experiment–Network/PoE
Serial Device Server [16]	Further serial interfaces (if required)

The edge computer hosts a device IOC, CA/PVA - gateway, DHCP, DNS, NAT and thus provides the basis for a data acquisition system, see Table 3.

Table 3: Software Specifications, Edge Computer

Component	Purpose
debian/procserv	OS/Start wrapper
ca-gateway	Channel Access gateway
epics-base(7)	Base software, incl. pv-access
seq/sscan/calc/asyn	sequencer/device interfacing
StreamDevice	support for stream based devices
autosave/busy	IOC save and restore PVs
recsync/client	record synchronizer
motor/modbus	motor support, industrial control

Data Acquisition System

We also use components of the Bluesky [8] project for these systems. EPICS is used as control layer to allow the communication with the measurement hardware. This is realized by a device IOC running on the edge computer. The connection to the Bluesky system is made by the Ophyd layer. Ophyd can represent the hardware devices into logical Devices. Signals from Ophyd can be inserted into plans and used in the Bluesky run engine. A plan in Bluesky can consist of more then one run. A run is a sequence of instructions for controlling the instrument equipment. The Bluesky run engine can subscribe to the Databroker. While Bluesky is processing a run the Databroker is collecting the raw data and storing then in the local storage of the executing computer. Each run has a unique ID. The UID is used as a filename for the saved raw data from each run. The Databroker can be used again to read the data and export them e.g. into a pandas data frame. The data frame can be processed and analyzed to generate different types of file formats and reports. Our preferred storage file format is NeXus [17] (uses HDF5) and contains roughly 4 groups: (i) header, (ii) analysed data, (iii) raw data and (iv) a pdf. Every method has its own sub-group in the main groups. The data from each stage are saved seperately. This allows us to store

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the data according to the FAIR principles, but also to give the users the possibility to directly retrieve a PDF report, for example. All raw data collected from the experiment is also stored in a csv file. This is a convinient step to give the users the possibility to edit the data with their usual software tools.

Automated Sequencing

To make these systems usable for users without programming and/or IT knowledge, we created a graphical method editor (with Phoebus [18]), which made it possible for users to select the methods described in the catalysis handbook and to develop a recipe from it which can be executed by a DAQ runner on the edge computer. This recipe is stored in our *archive* along with a sample-id as a JSON script. The script can also be edited in the *archive*.

To automate the process as described above, the following Python-based components are additionally installed on the edge computer:

- **Meta IOC** : IOC that holds machine metadata and controls the Runner, and can be controlled from any CA client like Phoebus
- **DAQ Runner** : Gets configured by the manager and started / checked by the Meta IOC. If running, processes a time sequence of setpoints for the lab devices, while also collecting measurement data and writing it into a file. Could do more since its just a python script loaded from the *archive*.
- **Manager** : Loads the runner sequences from the *archive*, stores the measurement data into *"archive"* (or also directly into the S3 storage with links for the *archive*. It can create preliminary analysis data.

In conclusion, the use of our EPICS infrastructure in the CaTLab as measurement and experiment control software gives us the following benefits:

- Flexible implementation of measurement protocols including newly conceived non-standard protocols, usable by the scientists without programming
- Provides open and robust interfaces so that these systems can also be programmed by scientists themselves for optimized use of experiments
- Retrieval and recording the time-stamped lab infrastructure status
- Automatic storage of FAIR-compliant data and rich metadata as a complete documentation of experiments allowing for detailed data evaluation and understanding as well as reproducibility of experiments

After the successful implementation of these systems in CatLAB we will extend this to further chemistry departments, enabling the use of machine learning and AI-driven multimodal analysis in chemistry in the future.

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