Linking Scientific Instruments and HPC: Patterns, Technologies, Experiences

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Abstract—Powerful detectors at modern experimental facilities routinely collect data at multiple GB/s. Online analysis methods are needed to enable the collection of only interesting subsets of such massive data streams, such as by explicitly discarding some data elements or by directing instruments to relevant areas of experimental space. Such online analyses require methods for configuring and running high-performance distributed computing pipelines—what we call flows—linking instruments, HPC (e.g., for analysis, simulation, AI model training), edge computing (for analysis), data stores, metadata catalogs, and high-speed networks. In this article, we review common patterns associated with such flows and describe methods for instantiating those patterns. We also present experiences with the application of these methods to the processing of data from five different scientific instruments, each of which engages HPC resources for data inversion, machine learning model training, or other purposes. We also discuss implications of these new methods for operators and users of scientific facilities.

I. INTRODUCTION

Humphry Davy observed that “[n]othing tends so much to the advancement of knowledge as the application of a new instrument” [1]. Today, powerful new instruments such as upgraded synchrotron light sources [2–4], free-electron lasers [5], microscopes [6,7], telescopes [8], and robotic laboratories [9–11] provide exciting new means to study phenomena in a broad range of scientific disciplines.

The power of these new instruments derives from their ability to probe reality rapidly and at fine spatial and temporal scales. In so doing, they can generate data at rates (multi-GB/s) and volumes (100+ TB/day) that demand online computing, both to extract interesting information from data streams and to enable rapid configuration and steering of instruments to maximize information gained during scarce experimental time. Tight coupling with high-performance computing (HPC) resources is often needed both to process this fire hose of data and to enable real-time feedback to experiments.

Such coupling requires flexible methods for coordinating actions and resources across diverse experimental and computing environments. We describe here tools that enable convenient specification of high-level flows linking diverse actions and the flexible mapping of such flows onto diverse physical resources to meet reliability, scalability, timeliness, and security goals as an experiment runs. Specifically, we (i) consider the nature of the flows that scientists need to develop and run online data processing; (ii) present methods that can be used to implement such flows, and experiences with these methods; and (iii) examine the implications of such flows for both computing and experimental facilities.

II. NEW PATTERNS FOR NEW INSTRUMENTS

Exponential growth in the rate at which instruments can perform measurements requires corresponding exponential improvements in the speed at which the resulting data are processed. This means increasing use of automation and computation at every stage in the experimental process, including steps that were previously not rate-limiting and thus could be performed manually, such as recording and interpreting results and configuring the next experiment. New methods may be needed to capture data at high rates, extract interesting events in high rate streams, identify and filter out uninteresting phenomena, detect and/or correct errors, design further experiments, and perform simulations to choose between alternative experimental configurations—and to combine many such steps into automated experiment management flows.

As in other areas of design, the identification of recurring patterns [14,15] can contribute to cost reduction and performance improvement. A design pattern captures a solution to a problem or class of problems in a re-usable form, via documentation of its purpose/intent, applicability, solution structure, and sample implementations. In this section, we enumerate patterns we and others have observed when processing data from scientific instruments, and review the nature of the resources required to implement the patterns.

A. What: Actions that are frequently included in flows

**Data collection:** Capture data and associated metadata generated at high speeds, in unconventional formats, and on specialized devices, and make those data available to subsequent analyses.

**Data reduction:** Reduce the volume of data to be processed and/or stored in other steps by applying either general-purpose compression [16,17] or domain-specific feature detection (e.g., to find diffraction peaks in x-ray imaging [18,19]).

**Data inversion:** Sophisticated computations are often required to convert sensor data into useful forms: for example, to generate a 3D or 4D representation from multiple 2D images [20,21], or to generate a 2D image from diffraction...
patterns. This step may be performed incrementally while data are collected or after all data are available.

**Machine learning (ML) model training:** In this increasingly popular approach to data reduction, previously collected data (from current or prior experiments and/or simulations) are used to train ML models to recognize interesting phenomena for data reduction or rapid response [22][25].

**Experiment steering:** Even better than discarding uninteresting data is to collect only interesting data in the first place. Scientists may use analyses of results from current or prior experiments to determine what experiment or measurement to perform next. Steering can range from fine-grained control of apparatus, such as taking (more) data from one part of a sample, to coarse-grained (e.g., choosing the next sample). Experiment steering can use simple design of experiment methods or more sophisticated active learning [26], Gaussian processes [27], Bayesian optimization [28], reinforcement learning [29], or other methods.

**Coupled simulation:** Computational simulation can be used during experiment steering to eliminate (or prioritize) experimental configurations.

**Data storage and indexing:** A flow may include steps to organize and store data and associated metadata (e.g., concerning experimental sample, configuration of apparatus, data processing steps) so as to make it findable, accessible, interoperable, and reusable (FAIR) [30].

**B. Where: Alternative places to perform flow tasks**

Analysis methods such as those just described can easily overwhelm instrument computers. Indeed, some analyses can consume tens or even hundreds of thousands of cores [31][32], albeit typically in a bursty manner. Similarly, experiments can generate petabytes. The aggregate compute and storage demand across a research institution or multi-instrument research facility can be large, and shared (rather than per-instrument) computing facilities become attractive or even essential to exploit economies of scale in capital and operations costs.

Public cloud is a credible option for certain instrument workloads [33], but data center systems can be more cost effective [34], especially when high-capacity, low-latency networks can support high data rate instruments and experiment steering. Custom silicon may be required for certain data processing steps [35][36]. Specialized accelerators may be used for tasks such as ML model training and inference [37][38].

When demand outstrips supply, adaptive methods may be used to direct compute and storage requests to different resources, prioritize certain tasks, and substitute alternative computational methods. In effect, computation may occur across a computing continuum [39][41] that extends from data acquisition computers co-located with experiments to powerful HPC clusters in data centers. For a given flow, computation may occur at multiple points across this continuum. For example, rapid quality control may be executed near an instrument on a co-located device, machine learning training on specialized AI hardware, and large-scale reconstruction on an HPC cluster. The “best” location for a computation can be hard to determine and may change over time according to data location, resource availability, cost, and performance.

**C. Example realizations of patterns**

The three flows in Fig. 1 to be described in more detail in §V illustrate some of the elements just described. *Serial synchrotron crystallography* (SSX) experiments collect diffraction data from target crystals. Several flows combine to process batches of acquired images, identify ‘hits,’ refine crystal structures, and catalog results for later use. *Ptychography* is a diffraction imaging technique that can produce images with high resolution. The flow shown here first transfers raw and position data to specialized HPC resources before executing 2D reconstruction on GPUs. *High energy diffraction microscopy* (HEDM) is used to characterize polycrystalline microstructures. This flow uses acquired data to train a neural network model for detecting peak positions in raw data. After training on a suitable AI accelerator, the flow transfers the trained model to the instrument for online use.

**III. A Research Automation Fabric**

The ability to direct different compute and storage tasks to different resources requires that resources be, as much as possible, fungible. To that end we leverage services provided by the Globus platform [42] to provide a consistent view (from an API perspective) of diverse identity and access management (IAM) methods and data and compute resources, and to manage flows that engage with those resources. Specifically:

- **IAM services** (Auth, Groups) for single sign-on and management of identities and credentials, and delegation.
- **Data services** (Transfer, Share) for access to, and managed movement of, data.
• **Metadata management** (Search, Identifiers) for indexing and generating persistent references to data.
• **Compute services** (funcX, OAuthSSH) for invocation and management of computational tasks.
• **Automation services** (Flows, Triggers, Queues) for execution of flows.

These services together allow scientists to author flows that specify sequences of actions, where each action is dispatched to a suitable action provider for execution. Action providers can run programs (funcX [43], OAuthSSH [44]), transfer files (Globus Transfer [45, 46]), publish data to catalogs (Globus Search [47]), manage data permissions (Globus Share [48]), and generate persistent identifiers (Globus Identifiers [49]), among other tasks relevant to instrument data processing. Additional action providers may be deployed to support specific instruments, compute resources, or other customized needs by adhering to a well-defined interface.

The various Globus platform services are decoupled: they do not inherently depend on one another. Thus, different services and service calls can be substituted, added, or removed to suit specific scientific needs. This structure reduces the rigidity of the entire system. For example, Globus Search can be invoked to catalog a machine learning experiment or to provide a user search portal, or both, or can be absent entirely if not needed.

Each Globus platform service is implemented via a persistent cloud-hosted management service plus, in the case of Globus Transfer and funcX, local proxy agents for accessing specific storage and compute systems. The cloud services plus the proxy agents implement a universal compute and data fabric that encompasses any and all resources on which agents are deployed. The funcX agent uses Parsl [50] to provision resources dynamically on various compute platforms, from cloud providers to clusters and supercomputers that use a local resource manager to manage resource access. Globus Transfer and funcX agents can be deployed persistently at experimental and computational facilities, or can be deployed as needed by scientists to expand the fabric. Searchable registries support the discovery of agents that the user has permission to access. Web interfaces allow scientists to monitor flow progress and to browse results even while experiments are on-going—important for experiments that involve manual steering.

All services build on the Globus Auth security fabric [51] that provides for the management of user identities and credentials, generation of the OAuth 2 access tokens needed for programmatic invocation of services, and generation of delegation tokens that allow services to act on a user’s behalf.

### IV. Flow Automation

The Globus automation services [52] allow a scientist to specify that the generation of new data at an instrument should trigger a user-supplied flow that engages a series of actions that may, for example, transfer data to a remote computer (via Globus Transfer), analyze data (funcX), update registries (Globus Search), and email results. In particular, the Globus Flows service manages flow execution and action invocation.

Each type of action engaged in a flow is handled by a persistent action provider service. All action providers implement a consistent, asynchronous REST API [53], facilitating the integration of new activities. The implementation of these services, like those of other Globus platform services, leverages cloud services (e.g., Amazon Lambda, Step Functions) for reliability and scalability. Cloud-based hosting enables delivery of research process automation capabilities to a wide user base, without requiring users to download and install software. It also provides economies of scale, thereby reducing the costs associated with distributing software.

To simplify and accelerate the development of flows for instrument science, we have developed a Python toolkit, Gladier [54], to assist in their authoring and management. This toolkit defines wrapper functions for registering funcX actions and flow definitions, invoking a new instance of a flow (a “run”) with specified inputs, and monitoring a specified directory for file events. These functions allow for concise definitions of instrument/HPC-specific flows, as shown in

```py
Listing 1 Client libraries deployed on remote sources (e.g., on a computer co-located with an experiment) enable the detection of events and invocation of flows.

Gladier allows scientists to organize their flows and actions by using Python. A Gladier “tool” definition, implemented as a Python object, provides the information needed to populate a flow action. The Gladier library provides implementations of common tools (e.g., transfer) as well as examples for experiment-specific tools (e.g., DIALS Stills processing); users may add other tools by implementing the Python class. To deploy and run a flow, users simply provide a list of tools to be used along with specific flow input arguments. Gladier uses this specification to register the necessary funcX functions and create and then register the flow definition.

To further simplify the development of flows for specific purposes, a GitHub repository [55] provides templates representing common experimental data processing patterns. These templates can be easily adapted to create new flows. Among other things, a template helps with the creation of new funcX functions and flows, and the various tasks associated with maintaining the structure of a flow. Flows can be shared, and scientists can adapt a shared flow specification by providing information for a specific deployment (e.g., compute and data endpoint identifiers and storage paths).

We observe that flows for different experiments tend to follow similar patterns, independent of the experiment modality; the major area of customization concerns application-specific functions used to operate on data. Thus, we find that users can adopt templates, modify the general structure of the flow by adding and deleting “tools” from the description, and writing and deploying to their agents new funcX functions.

### V. Application Experiences

We use five instrument+HPC applications to illustrate how the patterns and technologies described in preceding sections are realized and applied in practice. These applications link a number of scientific instruments and HPC facilities, including

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Listing 1: A simple SSX analysis flow, as defined with the Gladier library. The flow comprises two tasks, one for the Transfer from instrument to HPC, and one to run the DIALS Stills processing function on the transferred data. For brevity, we use U1–U3 and P1–P2 to represent UUIDs and paths, respectively.

```python
from gladier import GladierBaseClient

gladier_tools = ['gladier_tools.tools.Transfer', 'gladier_sxx.tools.DialsStills']

flow_input = {
    'transfer_endpoint': U1,
    'transfer_source_endpoint_id': U2,
    'transfer_destination_endpoint_id': U3,
    'transfer_source_path': P1,
    'transfer_destination_path': P2,
}

ssx_flow_client = SSXFlow()
run_id = ssx_flow_client.run(flow_input)
```

at Advanced Photon Source (APS) [56] and Stanford Synchrotron Radiation Lightsource (SSRL) [57] beamlines and the Argonne Leadership Computing Facility (ALCF) [58].

A. X-Ray Photon Correlation Spectroscopy (XPCS)

This experimental technique is used at synchrotron light sources to study materials dynamics at the mesoscale/nanoscale by identifying correlations in time series of area detector images [59–60]. Current detectors acquire megapixel frames at up to 2 kHz at 16-bit depth and 50 kHz at 2-bit depth (~4 GB/s); next-generation detectors are expected to generate 10s of GB/s or more [61,62]. Computing correlations at these rates requires HPC, both to process large quantities of data and to enable rapid response for experiment feedback.

We describe a flow developed to automate the collection, reduction, and publication of XPCS data at the APS 8-ID beamline. Each experiment can produce 100,000s of images, with precise rate and image size controlled by the scientist. During image acquisition, the instrument’s experiment management system typically creates a data file for every 20,000 images (~2.4 GB); to enable use of the automation services described in this paper, it is configured to trigger a flow each time such a file is created.

The flow, illustrated in Fig. 2 comprises 11 steps: 1) copy the experiment data file to an HPC facility (transfer); 2) extract metadata, such as data acquisition parameters and processing instructions, from the experiment data file (compute); 3) copy these metadata to persistent storage (transfer); 4) load metadata into a Globus Search catalog, providing visibility into the data that are being processed and the software version and input arguments to be used during subsequent processing steps (search); 5) pre-allocate nodes on the compute resource, to reduce the risk of the processing step waiting in the queue (compute); 6) run the XPCSBoost correlation analysis function, a matrix-heavy operation that is best run on a GPU (compute); 7) run a plotting function to create correlation plots and compact images for display in the portal (compute); 8) extract metadata from correlation plots (compute); 9) aggregate the correlation plots, new metadata, execution logs, and compact images for publication (compute); 10) transfer the aggregated data and metadata to persistent storage (transfer); and 11) add the aggregated metadata and associated data references to the catalog entry created in step 4, thus allowing the scientist to verify quality and also making data available for future uses (search).

Instances of this flow are initiated by the APS Data Management System [63], which copies each batch of new images, as they are acquired, from the instrument to storage accessible by Globus Transfer, and then invokes an instance of the flow. Many instances of the flow may be running concurrently.

We note that while all computational steps (2, 5-9) can run on general-purpose CPUs, step 6, XPCSBoost, benefits from use of GPUs and thus the flow is typically configured to access a funcX agent associated with a GPU resource. Using GPUs, the flow can process a dataset and provide feedback visualizations in ~50 seconds.

B. Serial Synchrotron Crystallography

Serial synchrotron crystallography (SSX) is a technique in which a bright synchrotron beam and specialized apparatus are used to collect diffraction data from many crystals, at rates of 10,000s of images per hour [64]. It can collect diffraction data from samples at room temperature and produce higher quality data than conventional crystallography due to reduced radiation damage [65].

We describe here methods used to process SSX data at APS Sector 19. A typical experiment generates around 40,000 1475×1255 16-bit pixel images per sample, with tens of samples processed during a beamtime. While the detector is capable of operating at 100Hz, for a data rate of 370 MB/s, the experiment is flux limited and is typically performed at roughly 10Hz, or 37 MB/s. As images are produced, they are processed (in batches) with the Diffraction Integration for Advanced Light Sources (DIALS) package [66] to identify at most one hit per image. As hits are accumulated, they are processed with the post-refinement and merging (PRIME) package [67] to solve the crystal structure. DIALS and PRIME outputs are published to an SSX repository and cataloged for subsequent use.

These activities are implemented by three distinct flows. The first, SSX-Stills, transfers a batch of acquired images to an HPC facility and uses the DIALS Stills package to perform quality analysis on each image and identify those that contain a good quality diffraction (a hit). It comprises 10 steps: 1) transfer image data from the beamline to an HPC facility (transfer); 2) confirm necessary input files are present (compute); 3) create configuration files for analysis (compute); 4) perform DIALS Stills processing on each raw image (compute); 5) extract metadata from files regarding hits (compute); 6) generate visualizations showing the sample and hit location (compute); 7) gather metadata and visualizations
for publication (compute); 8) transfer metadata and visualizations for publication (transfer); 9) ingest results, metadata, and visualizations to an SSX Globus Search catalog (search); and 10) transfer the results back to the beamline (transfer).

The **SSX-Prime** flow uses diffractions from SSX-Stills to solve the crystal structure. This flow is run first when at least 1000 hits have been identified, and then again to refine the structure as additional hits become available. It: 1) performs PRIME analysis to solve the structure (compute); and 2) copies the structure back to the beamline (transfer).

The **SSX-Publish** flow publishes results obtained to date, plus derived data such as histograms, to a repository and catalog. Its six steps: 1) gather results, metadata, and visualizations (compute); 2) create an archive file containing processed data (compute); 3) create histograms of the analysis (compute); 4) transfer metadata and results for publication (transfer); 5) publish results to the SSX repository and catalog (search); and 6) transfer results back to the beamline (transfer).

These three flows are initiated by a local agent deployed at the instrument that monitors the creation of files. In the experiments reported here, an SSX-Stills flow is triggered for each 512 images and an SSX-Publish flow for each 4096 images; an SSX-Prime flow is triggered initially when at least 1000 hits have been identified, and then again after each SSX-Still flow completion. This flexibility allows each activity to proceed at an appropriate pace, and permits new flows to be triggered given the result of previous flows, further advancing the automation of the scientific process.

The result is an indexed, searchable collection of processed images and associated statistics that is updated continuously while an experiment is running. Scientists use this catalog to determine whether sufficient data have been collected for a sample, a second sample is needed to produce suitable statistics, or a sample is not producing sufficient data to warrant continued processing [68].

### C. Ptychography

This coherent diffraction imaging technique can image samples with sub-20 nm resolutions [69]. A sample is scanned
with overlapping beam positions while corresponding far-field diffraction patterns, 2D small-angle scattering patterns containing frequency information about the object, are collected with a pixelated photon counting detector. Current detectors routinely generate $1030 \times 514$ 12-bit pixel frames at 3 kHz, for $\sim 20$ Gbps and TBs per experiment. Next-generation detectors will have readout speeds of more than 100 kHz and increased pixel counts, resulting in multi-PB datasets.

Phase retrieval is applied to ptychography data to recover phase information in reciprocal space. Typical phase retrieval algorithms are iterative and hence computationally expensive. ML-based methods that perform phase retrieval in a non-iterative manner can achieve $10$s to $1000$s times speedups, opening the door to real-time imaging and thus automated steering of experiments. However, phase retrieval is highly sensitive to material properties, and hence the ML model must be retrained for each new material.

The Ptycho flow performs 2D inversion and phase retrieval on diffraction patterns. It comprises three steps: 1) transfer data from experimental facility to HPC facility; 2) process each diffraction pattern to obtain a full image; and 3) transfer intermediate results back to experimental facility. During a ptychography experiment, hundreds of instances of this flow can be initiated concurrently. Further, this flow can be extended with 3D reconstruction steps and science-specific AI/ML methods: for example, feature segmentation and event or phenomena detection to enable feedback loops for experimental steering.

**D. High Energy Diffraction Microscopy**

This non-destructive technique combines imaging and crystallography algorithms to characterize polycrystalline material microstructure in three dimensions (3D) and under various in-situ thermo-mechanical conditions. The technique uses a synchrotron beam to map grains in a polycrystalline aggregate by considering diffraction patterns as a function of rotation angle. It thus requires identification of diffraction “spots” for each grain. Far-field ($\sim 10$ $\mu$m) HEDM, near-field ($\sim 1$ $\mu$m) HEDM, and tomography may be combined when studying a material, with for example far-field data used to guide near-field measurements.

We present two distinct HEDM applications that implement different approaches to HEDM data analysis. The first, HEDM, involves flows for collection, analysis, and storage of far-field and near-field data, and for coordination of those activities. We show in Fig. 2 the first of these flows, which involves eight steps: 1) transfer data from experimental facility to an HPC facility; 2) process each raw image by using MIDAS (compute); 3) extract metadata from files regarding hits (identified crystal diffractions) and generate visualizations showing the sample and hit locations (compute); 4) process each set of processed images (from step 2) to refine structure (compute); 5) gather metadata (compute); 6) transfer metadata to storage facility (transfer); 7) publish raw data, metadata, and visualizations (search); and 8) transfer the results back to the experimental facility (transfer). A single flow typically moves $\sim 11.5$ GB and consumes $\sim 400$ sec of compute time in steps 2 and 4.

The MIDAS package used by the HEDM application determines peak positions and shapes by fitting the observed intensities in area detector data to a theoretical peak shape such as pseudo-Voigt. While the HEDM flow just presented allows scientists to harness HPC for these computations, the higher data rates at new experimental facilities greatly increase overall computational costs. A promising alternative, explored in our second HEDM application, BraggNN, is to train and deploy a neural network approximator to the conventional curve fitting function. The neural network training can be performed on a powerful data center computer (e.g., conventional HPC or AI accelerator), after which the trained network can be deployed on a lightweight “edge” device at the instrument for real-time diffraction peak analysis to power applications such as experiment steering and anomaly detection.

The BraggNN flow, as shown in Fig. 2 explores the feasibility of this approach and in particular the relative costs of data transfer, network training, and network deployment. It comprises just three steps: 1) copy data from beamline to an HPC facility; 2) train the BraggNN model; and 3) copy the trained model back to the beamline. In the experiments described below, data are collected at SSRL and transferred to ALCF for training on AI accelerators such as the Cerebras wafer-scale engine. The ease with which Gladier permits retargetting of compute tasks proves invaluable when selecting an appropriate platform for different neural network architectures.

**VI. Application Usage**

Scientists have employed the methods and tools described above at APS and ALCF since early 2020 at a cadence that has varied with instrument availability and research priorities, but is generally increasing. Usage across the five experiments described in this paper, summarized in Fig. 3, encompass 49,367 distinct flow runs that consumed over 11,700 node hours of compute and transferred roughly 108 TB. The variation in usage across experiments and over time is primarily due to the sporadic nature of experiments at large-scale facilities. There are periods of downtime in which few, or no, experiments are run. We see a general increase over time in the number of flows run and the amount of data transferred. The decrease in compute time in Q4 2021 is due to the fact that the compute-intensive ptychography experiment was not running during this period. Several experiments are deploying more ambitious and expensive computational methods now that the feasibility of on-demand HPC has been established.

We explore in Fig. 4 the ability for flows to keep pace with data acquisition rates. Specifically, we show a twelve hour period in which XPCS flows are executed during an experiment session. During a preparatory period of roughly four hours, the scientists run occasional bursts of flows to calibrate equipment and ensure that the analysis pipeline is operational. Here we see up to 39 instances of the XPCS flow executing concurrently, each with the eleven steps shown in Fig. 2. The
subsequent eight hours of the experiment, represents steady-state processing in which flows are executed as the result of data acquisition. We see here that approximately 10 flows are executing concurrently throughout the experiment. This shows the flows are meeting the required rate of data acquisition (one file per minute). The additional flows represent out-of-band reprocessing tasks executed by the scientists.

We compare the runtime of each flow in Fig 5. Here we see mean and quartiles for the more than 2600 flow runs. We see that the Ptycho flow has significantly longer execution times and also higher variance in execution time (25th to 75th percentile is approximately 2000s) than other flows. This variance is primarily due to unpredictable HPC queue delays.

We show in Fig 6 a breakdown of action execution time for a single instance of each flow. We select the instance of that flow with median total runtime, and show the time spent executing each action as measured by the respective action provider. We illustrate overhead as the difference between the time measured by the action provider to perform the task and the time recorded by the Globus Flows service to complete a step. Overheads include costs incurred as Globus Flows transitions between steps, invokes action providers to submit a task, and, most significantly, polls for action status. Globus Flows employs a back-off polling strategy that starts with a 1 second delay between polls and doubles to a maximum of 10 minutes. Flow durations rang from a mean of 31s for XPCS to 3527s for Ptycho. All except SSX-Prime are compute bound. In all cases, overheads represent only a small fraction of total flow execution time; see Table I.

Fig 7 drills down on the runtime and overhead of individual steps within the XPCS flow. The histograms in the top row are of runtimes for each of the flow’s 11 steps, over 2197 flow executions; those in the bottom row are the associated per-step overheads. The runtime graphs show varied performance for transfer and compute actions and consistent performance (within 20s) for the Globus Search action, which is to be expected as this action simply invokes the Globus Search API.

| Experiment | Runtime | Transfer | Compute | Search | OH | %OH |
|------------|---------|----------|---------|--------|----|-----|
| BraggNN    | 259.5   | 64       | 162.1   | 0      | 33.4 | 12.9 |
| HEDM       | 498.2   | 16       | 405.9   | 1      | 75.3 | 15.1 |
| Ptycho     | 2283.3  | 11       | 2259.4  | 0      | 13.0 | 6.6  |
| Psycho     | 335.2   | 3        | 306.2   | 1      | 44.9 | 12.7 |
| SSX-Publish| 332.6   | 152      | 53.7    | 0      | 126.9| 38.2 |
| SSX-Prime  | 1041.4  | 97       | 860.0   | 1      | 83.4 | 8.0  |
| SSX-Stills | 240.0   | 12       | 177.9   | 2      | 48.1 | 20.0 |

Fig. 3: Total flows, data transferred, and compute time used (on 64-core ALCF Theta nodes), per quarter, for the five experiments described in §V.

Fig. 4: The number of concurrent XPCS flows over 12 hours in March 2022. The initial peaks are burst tests before beginning the experiment; by 00:00, a constant stream of data from the beamline is processed.

Fig. 5: Distribution of runtimes for flows discussed in the text. Box plots show upper and lower quartiles, with whiskers to 1.5× the interquartile range.

TABLE I: For the instance of each flow with median runtime, the times taken by its individual actions and aggregate overhead (OH), in seconds, plus aggregate overhead as a percentage of total runtime (%OH).
external actions with the platform. This API and IAM model such that others can implement and integrate common asynchronous REST API and flexible OAuth-based offer a broad range of flows, it does not (and cannot) apply monolithic software stacks. Different ways to meet different needs, without the need to architecture also makes it easy for users to compose flows in different modalities, such as AI and digital twins [80].

While the Globus platform provides capabilities needed to implement a broad range of flows, it does not (and cannot) offer every capability desired by users. Another advantage of the platform model is that we are able to prescribe a common asynchronous REST API and flexible OAuth-based IAM model such that others can implement and integrate external actions with the platform. This API and IAM model could be used to integrate capabilities provided by other cloud-hosted research platforms, such as Tapis [23] and CILogon/Con-Manage [78].

The Globus platform’s use of web authentication and authorization standards (e.g., OAuth 2) provides a rich IAM ecosystem for managing the security of complex flows. This approach allows users and resource owners to manage what actions are performed and by whom, and also supports the complexities of real-world use cases. For example, Globus Auth allows for secure integration with external tools (e.g., facility data management systems) by using various OAuth 2 grant types (e.g., for public clients), group-based community accounts for shared computing access, and delegated authorizations for flows to securely invoke external services.

The ease with which the platform can be extended to edge resources by deploying compute and data agents is important for use cases that require edge computing. These agents, while lightweight and easy to install, offer crucial capabilities that allow execution of actions on remote and diverse resources. Further, local agents may be operated by resource owners to support any authorized users, or alternatively may be deployed by an individual user to process their own requests only.

B. Implications for HPC Facilities

Rapidly advancing and evolving experimental apparatus and associated computational methods result in growing demands for computing and storage. The appropriate combination of custom silicon, edge computing, and data center computing likely will evolve over the next decade and beyond; however, it remains natural to turn to HPC facilities for both capacity and hardware specialization (e.g., accelerators). Such facilities are natural rallying points for data storage and organization coupled with close access to compute resources. These needs are particularly important given the adoption of new computing modalities, such as AI and digital twins [80].

The experiences reported here show the benefits of a platform that permits easy redirection of tasks to different destinations, so that choices can be made based on user preferences and/or institutional policies. However, enabling such redirection relies on facilities exposing interfaces for remote access to data and computing; IAM infrastructure to enable seamless, yet secure, access to such resources; and methods for enabling access (e.g., to service accounts) without prior direct trust relationships.

Even simple mechanisms can drive innovation. For example, ScienceDMZs have enabled unobstructed data flows to/from HPC facilities; deployment of user-managed and Globus-accessible storage has allowed scientists to rapidly collaborate using shared data; and support for container technologies has reduced barriers for porting applications between...
systems [82]. These mechanisms should all be universally adopted by HPC facilities to enable instrument+HPC flows.

Our work has highlighted other capabilities that could reduce barriers for linking instruments and HPC [83]. Flexible, on-demand access to computing capacity is needed to support bursty online workloads. The modest HPC demands associated with our five experiments were satisfied by a backfill queue at ALCF, but that capability may no longer suffice as demands increase. Some sites operate both specialized queues and dedicated and on-demand clusters [84–86], but more flexible scheduling mechanisms are likely needed. In high-demand situations the ability either to transition automatically (through standardized and exposed IAM infrastructure) to other HPC facilities or to burst to the commercial cloud without direct intervention from experimental scientists could allow the scientists to stay focused on real-time needs. New facility evaluation metrics are needed that encompass not only utilization but also responsiveness for real-time workloads.

Planning for future HPC-enhanced experimental science suffers from inadequate knowledge of future demand and the cost-performance tradeoffs associated with meeting demand in different ways. It will be important to establish systematic tracking of resource demand and availability at both experimental and computing facilities.

A final area of need is for a cohort of staff with expertise in both experimental science and computing to assist with the development, deployment, and executing of flows such as those described here.

C. Implications for Experimental Facilities

Effective coupling of experiment and computational facilities requires both modern computing infrastructure at experiments and high-quality internal and external network connections; many facilities still have deficiencies in these areas. Adoption of the ScienceDMZ architecture [81,87] is essential so as to eliminate bottlenecks in network paths.

Experimental facilities must support deployment of the data and compute agents needed to integrate with the cloud-based compute and data fabric described here. This is both a social and technical challenge. Administrators must allow for policies that permit deployment and provide for external connectivity, both to computing facilities and to cloud-hosted platform services. Facilities must provision hardware near instruments so that agents can be deployed close to data sources. Work is also needed to integrate IAM ecosystems. Many facility users are locked within a single siloed IAM domain. Adoption of federated IAM, such as that provided by Globus Auth, and adopted by HPC facilities, can integrate diverse IAM domains. By adopting standard mechanisms, facilities can make their identities accessible to modern cloud platforms.

There are opportunities for yet more sophisticated integration. For example, direct integration of the methods described here with the software tools employed by scientists reduces barriers for use by providing familiar interfaces to automation capabilities. Another goal should be to enable use of flows to control experiments, a practice that will require implementation of common APIs, perhaps aligning with the action provider API, for instruments and other devices.

Full automation (without human intervention) will require that experiments generate meaningful events that can be used to trigger flow executions [88]. In the applications reported here, flows are triggered by mechanisms that monitor co-located file systems to integrate with beamline software. Other integrations are possible, such as connecting with instrument control systems like EPICS [89], Bluesky [90], LabView [91], and ROS [92] that allow for generation of events.

D. Implications for Scientists

Higher data acquisition rates, larger datasets, and more complex processing flows mean that scientists must increasingly embrace automation to remain competitive. The outsourcing of automation tasks to cloud-hosted platforms, as described here, can simplify this transition by avoiding the need for larger local hardware and software deployments. However, scientists must be willing to trust external providers to handle mission-critical functionality. The growing reliance on cloud-hosted services in our daily lives, coupled with their extreme availability and reliability, helps to expedite this transition.

Adopting the patterns and methods proposed here requires that scientists decouple traditionally monolithic workflows into series of discrete steps that may be executed separately. This approach can improve understandability and make it easier to substitute implementations for individual steps (e.g., to update an analysis routine) and to execute steps in more preferable locations (e.g., in terms of cost, availability, performance).
Experimental facilities use control systems such as EPICS [89] to drive instruments and monitor experiments. Bluesky [90] provides Python interfaces for experiment control and data collection [108]. Workflow systems are often used to coordinate activities and orchestrate computational campaigns [109–111] that may execute local programs, submit jobs to HPC systems, or invoke web services [112]. Streaming protocols can be used to expedite data movement [113] [114].

Bridging instruments and distributed HPC requires capabilities for reliable and secure remote task submission. This challenge motivated Grid computing [115] and the superfacility concept [116]. Facilities have developed specialized interfaces to enable remote job submission [117] and for managing computational workloads on and across systems [84] [118] [120]. Remote execution has also been integrated with Jupyter notebooks [121] [124]. The ability to compute anywhere enables users to leverage specialized computing resources designed for low-cost, distributed, and edge computing [35] [125]. Groups are deploying AI systems at experimental facilities for rapid data filtering at the edge [23] [25].

Domain-specific data repositories can play a pivotal role in fostering collaboration [126] [128]. Science gateways [111] [129] [130] address data and compute challenges by abstracting underlying resources and providing intuitive analysis interfaces. Globus Auth uses OAuth tokens [131] to delegate to third parties (e.g., a funX server) the right to perform certain tasks on a user’s behalf. Delegation methods have been developed previously [132] [134].

IX. Summary

Maximizing the value obtained from new instruments requires tight coupling with heterogeneous and large-scale computing facilities, and new online computing methods to automate data collection, processing, and dissemination. We have reported on our experiences working with five groups of instrument scientists, first to understand their current and future computing challenges and second to automate various of their research flows. We described an automation approach that leverages Globus platform services to enable construction of flows by composing modular components that execute programs, transfer files, publish data to catalogs, manage data permissions, and generate persistent identifiers, among other tasks. Importantly given dynamic resource availability, our approach achieves a separation of concerns between what actions are applied in each flow and where those actions are performed. We also described Gladier, a Python toolkit that abstracts registration of funX functions, flow authoring, and flow execution with specific input arguments, and simplifies the coupling of such flows to experiments.

The five experiments discussed here vary significantly in their data rates, flow and action runtimes, use of heterogeneous resources, and geographically distributed execution. We reported on quantitative evaluations in real-world settings that characterize these differences and demonstrate that our methods can in each case support the robust, scalable, and
performant overheads required for production use. We quantified overheads and determined that they are modest even for complex and long-running flows.

This work represents a first step towards identifying and capturing in reusable forms, a broad collection of patterns for processing data from scientific instruments—patterns that range from online data processing to machine learning training and data cataloging. We believe that understanding these patterns and the methods and resources required to support their execution will have important implications for a range of stakeholders, from individual scientists to HPC facilities, experimental facilities, and cloud-based research platforms.

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