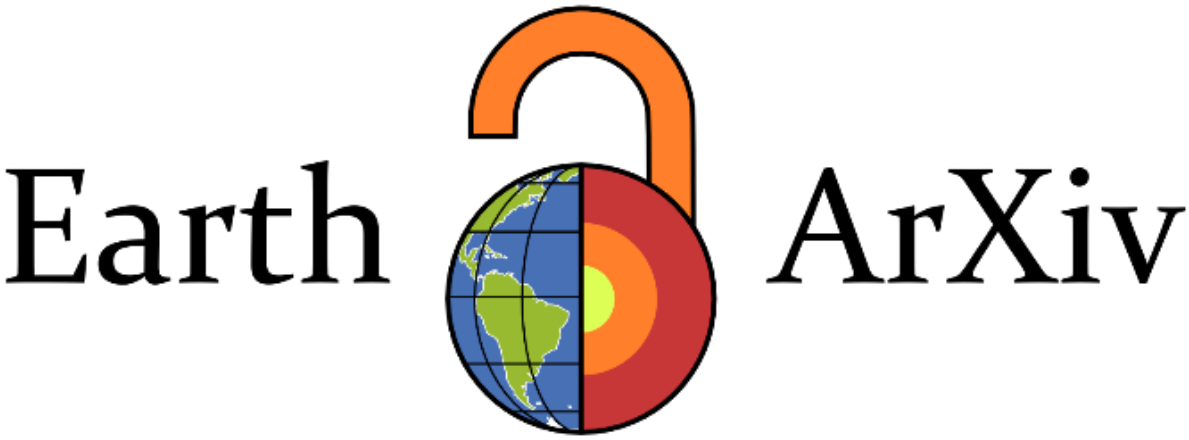


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Highlights

UpStream: A Modular, Metadata-First Architecture for Environmental Sensing During Intensive Observation Periods

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- UpStream is an API-first, metadata-supported architecture for campaign sensor data.
- Treats environmental sensing campaigns as first-class, explicitly governed entities.
- Embeds metadata capture at ingestion instead of end-of-lifecycle documentation.
- Evaluated via mobile PTR-MS, stationary flux-tower, and remote Alaska deployments.
- Yields transferable architectural principles for campaign-scale sensing systems.

UpStream: A Modular, Metadata-First Architecture for Environmental Sensing During Intensive Observation Periods

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ABSTRACT

Campaign-scale environmental sensing produces heterogeneous, high-frequency datasets that strain file- and portal-centric workflows and impede decision support. This paper presents UpStream, an API-first, metadata-supported, modular prototype for campaign-scale environmental sensor data. Co-designed with the SNIFFER air-quality laboratory, UpStream treats campaigns as first-class entities with explicit identity, scope, and governance, embeds metadata capture at ingestion, and provides selective, query-mediated access to high-resolution observations under concurrent use. We evaluate the architecture through three field deployments, a mobile PTR-MS laboratory and a stationary eddy-covariance flux tower, plus a remote, pull-based deployment in Alaska, showing that heterogeneous, evolving instrument outputs are absorbed without schema redesign while campaign boundaries, selective access, and metadata persist throughout the data lifecycle. We distill these results into transferable architectural principles for campaign-scale environmental sensing systems supporting decision support: modular service separation, flexible schema design, metadata-at-ingestion, query-mediated access, and federation designed in from the start.

1. Introduction

Environmental measurement campaigns are periods of focused, direct study of environmental processes within a defined region of interest, typically involving the coordinated deployment of sensing instruments to quantitatively characterize system behavior. In the context of air quality research, such campaigns form the backbone of observational data collection, supporting assessments of population exposure, intake fractions, and other public health–relevant metrics (Marshall, Riley, McKone and Nazaroff, 2003; Fantke, Jolliet, Apte, Hodas, Evans, Weschler, Stylianou, Jantunen and McKone, 2017). Critically, environmental campaigns provide calibrated, quality-controlled observations that serve as the ground truth against which environmental and atmospheric models are evaluated and refined, and in turn inform policy and stakeholder decision-making (Cros, Durand, Cachier, Drobinski, Fréjafon, Kottmeier, Perros, Peuch, Ponche, Robin, Saïd, Toupance and Wortham, 2004; Park, Oak, Emmons, Kim, Pfister, Carmichael, Saide, Cho, Kim, Woo, Crawford, Gaubert, Lee, Park, Jo, Gao, Tang, Stanier, Shin, Park, Bae and Kim, 2021). Because these outcomes depend directly on the data collected during campaigns, the planning and execution of measurement campaigns are central to the credibility and utility of downstream analyses. Intensive Observation Period (IOP) campaigns represent a particularly important class of these efforts (Revercomb, Turner, Tobin, Knuteson, Feltz, Barnard, Bösenberg, Clough, Cook, Ferrare, Goldsmith, Gutman, Halthore, Lesht, Liljegren, Linné, Michalsky, Morris, Porch, Richardson, Schmid, Splitt, Van Hove, Westwater and Whiteman, 2003; Cros et al., 2004). Although

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spatially and temporally limited, IOPs deliver high-value, place-based observations that capture key environmental processes and provide the validation data required to calibrate and constrain environmental models. By combining networks of stationary and mobile instruments, IOPs target specific phenomena with a level of detail that cannot be achieved through routine monitoring alone (Choi, Lamsal, Follette-Cook, Joiner, Krotkov, Swartz, Pickering, Loughner, Appel, Pfister, Saide, Cohen, Weinheimer and Herman, 2020; Park et al., 2021).

A particularly powerful form of these efforts is the Joint IOP, in which multiple institutions and agencies collaborate within a shared temporal window and geographic region. In a Joint IOP, participating groups deploy complementary instrumentation and personnel to a common site, coordinate measurement schedules, and establish shared operational protocols. This collaborative structure expands observational coverage across spatial and temporal scales while incorporating diverse measurement modalities. Some teams focus on gas-phase chemistry, others on particulate composition; some instruments provide rapid temporal feedback, while others deliver detailed chemical resolution at lower sampling frequencies. No single instrument captures the full complexity of atmospheric processes, but deploying complementary systems together widens coverage and lets each instrument check the others (Choi et al., 2020).

The complementary nature of Joint IOP instrumentation introduces additional data complexity. For example, instruments with high temporal resolution deployed on mobile laboratories may identify transient hotspots of elevated volatile organic compounds. These observations can then guide the repositioning of instruments that offer greater mass resolution but lower temporal frequency, allowing for sustained characterization of identified regions of interest. Replicated measurements from instruments with overlapping capabilities further enhance confidence in observed patterns. While this strategy strengthens scientific inference, it also produces heterogeneous, high-resolution datasets that must be integrated, compared, and queried across instruments, platforms, and deployment phases (Zeeman, Christen, Grimmond, Fenner, Morrison, Feigel, Sulzer and Chrysoulakis, 2024; Horsburgh, Lippold and Slaugh, 2024).

As sensors become more refined and calibrated, they expand their ability to capture data. These cutting-edge environmental sensors are capturing very-high-resolution temporal and heterogeneous sensor datasets that strain file-based workflows and inhibit reuse (Zeeman et al., 2024; Horsburgh et al., 2024). The expansion of a sensor's capability occurs in numerous ways: how frequently it can capture data, the breadth of information it can capture, and the degree to which it can collect data while mobile. Storage for these instruments can occur in different ways. Often, an initially convenient method is a flat file structure. Whether this consists of multiple comma-separated values (CSV) files holding instrument datasets or alternative file types, this approach puts the onus on the user to know where the data of interest are located. File-based sharing systems also provide limited support for collaborative data capture, description, visualization, annotation, and reuse (Horsburgh, Morsy, Castronova, Goodall, Gan, Yi, Stealey and Tarboton, 2016). Alternatively, many data repositories and platforms have been created to give researchers the ability to query sensor data; however, these portals are often domain specific, such as HydroShare for hydrologic data and models (Horsburgh et al., 2016), standards-based but still requiring implementation decisions and technical expertise, such as SensorThings API and HydroServer (Horsburgh et al., 2024), or difficult to connect directly into computational analysis environments (Huber, D'Onofrio, Devaraju, Klump, Loescher, Kindermann, Guru, Grant, Morris, Wyborn, Evans, Goldfarb, Genazzio, Ren, Magagna, Thiemann and Stocker, 2021). Each of these approaches provides varying support for data discoverability, accessibility, interoperability, and reuse (Wilkinson, Dumontier, Aalbersberg, Appleton, Axton, Baak, Blomberg, Boiten, da Silva Santos, Bourne, Bouwman, Brookes, Clark, Crosas, Dillo, Dumon, Edmunds, Evelo, Finkers, Gonzalez-Beltran, Gray, Groth, Goble, Grethe, Heringa, 't Hoen, Hooft, Kuhn, Kok, Kok, Lusher, Martone, Mons, Packer, Persson, Rocca-Serra, Roos, van Schaik, Sansone, Schultes, Sengstag, Slater, Strawn, Swertz, Thompson, van der Lei, van Mulligen, Velterop, Waagmeester, Wittenburg, Wolstencroft, Zhao and Mons, 2016).

Decision-support workflows depend on readily accessible observational data; without timely access to heterogeneous sensor streams, pattern detection, model validation, and evaluation of interventions cannot proceed efficiently (Huber et al., 2021; Zeeman et al., 2024). Sensor data support three decision-support mechanisms: (1) identifying problems by patterns and trends observed over time and space; (2) ground-truthing models and informing the exploration of interventions; and (3) providing a measuring stick to evaluate how interventions have affected the system. However, these processes require distinct workflows within the system to deliver the right information to the right user. Consequently, these workflow designs can slow the analysis and visualization aspects across these mechanisms. To prevent bottlenecks, robust, query-first, metadata-supported infrastructure is essential to keep upstream data access from constraining downstream problem formulation and analysis (Wilkinson et al., 2016; Huber et al., 2021; Zeeman et al., 2024).

In this article, we describe UpStream, a modular environmental sensor repository that seeks to provide a scalable solution to support IOP campaigns. This article examines the architectural requirements and design patterns necessary to support campaign-scale environmental sensor data in decision-support contexts. We focus on infrastructure that spans the full data lifecycle, serves observations by subset query with their metadata attached, supports visualization for analysis, and integrates with scalable computing environments (Horsburgh et al., 2024; Zeeman et al., 2024). Rather than presenting a system in isolation, this work uses a modular prototype as an instantiation to evaluate how these architectural choices address the structural challenges identified in field-based sensing campaigns. The contribution of this paper lies in articulating generalizable infrastructure patterns that support heterogeneous environmental observations and reduce barriers to analysis and decision-support readiness.

Specifically, this paper makes four contributions. First, we derive campaign-scale requirements from sustained co-design with an operating measurement laboratory, showing that heterogeneity, campaign identity, selective access, and metadata capture are structural constraints of campaign-scale sensing rather than isolated workflow inconveniences (Section 4.1). Second, we treat campaigns as first-class architectural entities, with explicit identity, scope, and governance, so that campaigns can be kept apart or compared without reconstructing campaign semantics after the fact (Sections 4.1.2 and 4.3.4). Third, we present and evaluate an API-first prototype, in which the API is the primary path to data, metadata is written at ingestion rather than reconstructed later, and users retrieve subsets of high-resolution observations by time, place, sensor, or campaign under concurrent use, demonstrated through mobile, stationary, and remote field deployments (Sections 4.2–4.4). Fourth, we distill these results into five transferable architectural principles that generalize beyond any single instrument, laboratory, or platform: modular service separation, flexible schema design, metadata capture at ingestion, query-mediated access, and federation designed in from the beginning (Section 5). Throughout, we argue that decision-support readiness is an upstream infrastructure requirement: timeliness, provenance, and selective access are properties that must be designed into the sensing data layer rather than added downstream, consistent with science gateway approaches to decision support (Pierce, Pearson, Osorio, Tijerina, Trueheart, Faust and Mobley, 2026) and intelligent-systems research agendas for the geosciences (Gil, Pierce, Babaie, Banerjee, Borne, Bust, Cheatham, Ebert-Uphoff, Gomes, Hill, Horel, Hsu, Kinter, Knoblock, Krum, Kumar, Lermusiaux, Liu, North, Pankratius, Peters, Plale, Pope, Ravela, Restrepo, Ridley, Samet, Shekhar, Skinner, Smyth, Tikoff, Yarmey and Zhang, 2018).

2. Background: Existing Architectures and Their Limits

As environmental sensors become more robust, with higher temporal and spatial resolution, the volume and heterogeneity of observational data continue to increase. A wide variety of repositories exist for managing environmental sensing data. The growth of Internet of Things (IoT) devices has enabled proprietary architectures for commercial products that provide gateway-based dashboards for accessing stored data (Monios, Peladarinos, Cheimaras, Papageorgas and Piromalis, 2024). In parallel, research communities have developed open-source systems that allow users to capture and retain ownership of their data streams (Cleveland, Jamthe, Padhy, Powell, Stubbs, Daniels, Pierce and Jacobs, 2019). These systems emphasize real time ingestion and visualization, but often collapse ingestion, storage, and access into portal centric designs. As a result, campaigns are not consistently modeled as first class entities, and selective query mediated access across heterogeneous and evolving datasets is limited.

The expansion of high frequency sensing has further driven the development of cloud hosted, Application Programming Interface (API) mediated streaming platforms (Kerkez, Daniels, Graves, Chandrasekar, Keiser, Martin, Dye, Maskey and Vernon, 2016). Research systems such as CHORDS expose REST endpoints for accessing sites, sensors, and measurements (Cleveland et al., 2019; Powell, Stubbs, Cleveland, Pierce and Daniels, 2019), while newer portal architectures integrate FAIR aligned publication and dissemination capabilities (Quille, de Almeida, Ohara, Corrêa, de Freitas, Alves-Souza, de Almeida, Davis and Prakash, 2023). These architectures substantially reduce barriers to ingestion and operational monitoring. However, their primary orientation toward streaming and visibility does not inherently provide an explicit structural model for organizing observational data across multiple IOP campaigns. In campaign scale sensing contexts, where deployments evolve, instruments change, and comparisons across field efforts are required, architectural support for multi campaign governance, lifecycle consistent metadata persistence, and selective cross campaign querying becomes essential.

Providing FAIR data has become an important expectation within environmental research infrastructures (Wilkinson et al., 2016). FAIR principles emphasize machine actionable metadata that supports discovery, accessibility, interoperability, and reuse beyond initial study contexts. Best-practice guidance for geoscience publication likewise

treats provenance documentation as integral to reusable research products (Gil, David, Demir, Essawy, Fulweiler, Goodall, Karlstrom, Lee, Mills, Oh, Pierce, Pope, Tzeng, Villamizar and Yu, 2016). Datasets can be federated across systems only when their metadata are good enough to match on, yet writing consistent, complete metadata remains burdensome. Metadata is frequently registered at the end of the data lifecycle (Quille et al., 2023; Crystal-Ornelas, Varadharajan, O'Ryan, Beilsmith, Bond-Lamberty, Boye, Burrus, Cholia, Christianson, Crow, Damerow, Ely, Goldman, Heinz, Hendrix, Kakalia, Mathes, O'Brien, Pennington, Robles, Rogers, Simmonds, Velliquette, Weisenhorn, Welch, Whitenack and Agarwal, 2022), and empirical studies indicate that while researchers value data sharing, they often provide only minimal descriptive metadata when publishing their own datasets (Tenopir, Allard, Douglass, Aydinoglu, Wu, Read, Manoff and Frame, 2011; Tenopir, Rice, Allard, Baird, Borycz, Christian, Grant, Olendorf and Sandusky, 2020). Sparse or inconsistent metadata reduces the practical effectiveness of FAIR principles, particularly in high frequency sensing environments where contextual information is critical for interpretation.

Support for the full data lifecycle, from equipment inventory and deployment events to observation, processing, and publication, is necessary for environmental sensor networks (Jones, Horsburgh, Reeder, Ramírez and Caraballo, 2015). Such lifecycle awareness is frequently implemented through modular cyberinfrastructure components that separate storage, metadata registries, computational services, and dissemination interfaces (Wright and Wang, 2011). Comparable modular architectures are found in other data intensive domains, where systems explicitly distinguish between repositories, metadata layers, analysis pipelines, and sharing mechanisms (Bonacchi, Chapuis, Churchland, DeWitt, Faulkner, Harris, Huntenburg, Hunter, Laranjeira, Rossant, Sasaki, Schartner, Shen, Steinmetz, Walker, West, Winter and Wells, 2023). Separating these concerns lets each part grow or be replaced as instruments and analytical needs change.

Environmental decision support systems ultimately depend on structured and reproducible observational data infrastructures. Decisions rely on both real time and historical observations to frame problems, evaluate alternatives, and validate model outputs. Predictive models leverage curated observational records for training and calibration (Rodrigues and de la Riva, 2014), and automated calibration workflows assume stable and reproducible data pipelines (Baracchini, Hummel, Verlaan, Cimatoribus, Wüest and Bouffard, 2020). Intelligent geoscience systems further presume integrated and interoperable data infrastructures (Gil et al., 2018). AI-assisted modeling of complex systems similarly depends on curated, interoperable observational inputs to tame expert-model complexity (Gil, Garijo, Khider, Knoblock, Ratnakar, Osorio, Vargas, Pham, Pujara, Shbita, Vu, Chiang, Felman, Lin, Song, Kumar, Khandelwal, Steinbach, Tayal, Xu, Pierce, Pearson, Hardesty-Lewis, Deelman, Ferreira da Silva, Manaya, Kemanian, Shi, Leonard, Peckham, Stoica, Cobourn, Zhang, Duffy and Shu, 2021). Decision support credibility therefore requires selective access to large observational collections, persistent metadata linkage across deployments, and query-mediated retrieval so campaigns can be compared rather than inspected one dataset at a time.

3. Methods

Architectural design and evaluation were conducted through a structured, iterative process grounded in campaign-scale environmental sensing practice, rather than through speculative or purely theoretical system design. The UpStream architecture was co-designed through sustained engagement between the developers and researchers from the mobile SNIFFER laboratory. This process involved identifying recurring operational constraints observed during measurement campaigns, synthesizing architectural responses to those constraints, instantiating the resulting architecture as a functional prototype, and evaluating the prototype with respect to its ability to satisfy the identified constraints (Figure 1).

Co-design activities consisted of sustained technical engagement between developers and researchers, including workflow walkthroughs, shared examination of data products, and collaborative review of prototype behavior under representative campaign conditions. These interactions focused on understanding how campaign data are generated, accessed, interpreted, and reused over time, rather than on eliciting feature requests or interface preferences. Feedback from researchers was incorporated iteratively during prototype development, ensuring that architectural requirements reflected operational realities observed during IOP campaigns.

Initial technical engagement with the SNIFFER laboratory, centered on IOP workflows and resulting data products, revealed recurring structural limitations in existing data handling practices. Rather than treating these limitations as isolated workflow inefficiencies, they were interpreted as infrastructural constraints that must be addressed architecturally. These constraints emerged from common bottlenecks in data collection, management, and analysis, particularly those related to heterogeneous instrument outputs, scaling data-intensive workflows, selective data access,

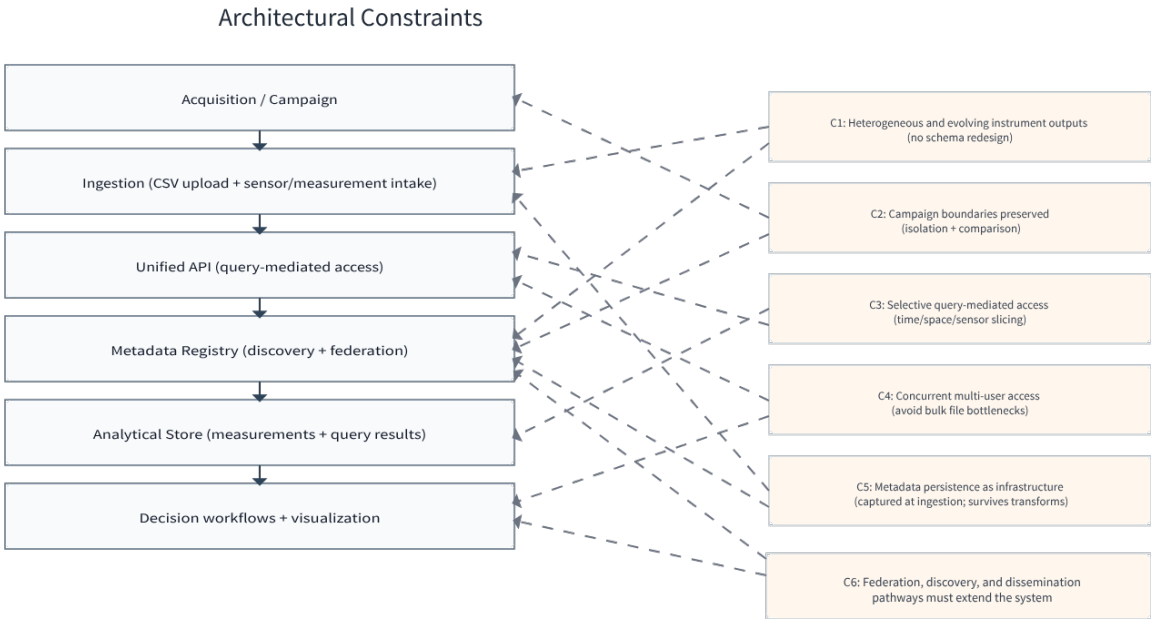


Figure 1: Architectural constraints identified through co-design with the SNIFFER laboratory, and the iterative design–instantiate–evaluate process used to address them.

and reliable data discovery. Only constraints that recurred across campaigns and persisted beyond individual tools or scripts were retained as architectural requirements.

The architectural design was synthesized directly from the identified campaign-scale constraints. Rather than introducing features in response to individual workflow preferences, architectural principles were derived to structurally address recurring limitations observed across campaigns. Each architectural decision was evaluated based on its ability to satisfy one or more of the identified constraints, ensuring traceability between operational bottlenecks and system structure.

Although co-design was conducted with a single laboratory, architectural synthesis focused on constraints that extend beyond any specific instrument configuration or campaign workflow. Instrument-specific practices and lab-specific scripting patterns were intentionally abstracted into broader structural requirements, including heterogeneous data handling, campaign identity, metadata persistence, and selective access. Only constraints that remained stable across contexts were retained, resulting in a design intended to generalize to campaign-scale environmental sensing beyond the originating laboratory.

The architectural design was instantiated as a research prototype so it could be evaluated under real campaign conditions. Implementing the design as a working system allowed assessment of whether the identified constraints were structurally addressed in practice rather than only conceptually satisfied. The objective was to develop a prototype that was complete with respect to the identified architectural constraints, rather than feature-complete in a product sense.

The resulting prototype comprised the core infrastructural components required to evaluate campaign-scale requirements, including data ingestion with embedded metadata capture, a metadata registry supporting discovery and organization, an analytical data store designed for selective access to high-resolution datasets, and a unified API layer providing consistent access semantics.

Evaluation was structured around four architectural dimensions derived from the campaign-scale constraints identified during co-design. Rather than assessing usability or performance metrics in isolation, evaluation focused on whether core structural properties of the architecture held under realistic campaign conditions. Specifically, evaluation examined: (i) support for heterogeneous and evolving instrument outputs without schema redesign; (ii) preservation of explicit campaign boundaries during ingestion, access, and comparison; (iii) subset queries on high-resolution datasets under concurrent use; and (iv) persistence of metadata as an infrastructural property throughout the data lifecycle.

Evaluation of the architectural design and prototype was conducted empirically through deployment with laboratories engaged in campaign-scale environmental sensing. Treating infrastructure design as an empirical process allows

architectural claims to be assessed through operational use rather than asserted in abstraction. The following section presents the resulting architectural response, describing how the identified campaign-scale constraints were instantiated within the UpStream prototype.

4. Results

4.1. Requirements Derived from Campaign-Scale Operation

The goal of the UpStream system was to develop a flexible sensor data repository that allows research users access but also provides a way to share with decision makers. When developing the UpStream platform, we worked directly with a research lab to identify needs and constraints for a system they could upload, view, and share high resolution data within the team and stakeholders. Through multiple conversations with members of the research lab, we co-designed constraints and requirements for the UpStream system to support their sensor data life cycle. Through the rest of this section, we will highlight those constraints and requirements.

4.1.1. Data Capture Support

Through iterative co-design with the SNIFFER air quality laboratory, we identified heterogeneity as a defining characteristic of campaign-scale environmental sensing. In these campaigns, a single instrument may produce multiple measurement streams whose structure and semantics vary over time, and campaigns may further evolve to incorporate additional instruments operated by collaborating groups. This pattern is representative of many environmental sensing efforts, where observational diversity arises not only across instruments but also within a single deployment as sensing objectives change.

As a result, environmental sensor data infrastructure must support instrument-agnostic, entity-stable data models that accommodate heterogeneous measurements across campaigns without requiring schema redesign as instruments or campaigns evolve. Flexibility here means a small fixed core (campaign, station, sensor, and measurement) with extensible relationships attached to it, so the same tables hold a tilt meter and a mass spectrometer. Schema-less storage would discard the relationships that make comparison across campaigns possible.

In addition to measurement heterogeneity, campaign observations must retain time and location semantics. Temporal and spatial context are essential for interpreting observations, aligning measurements across instruments, and supporting downstream analysis. Treating time and location as integral components of observational data, rather than ancillary metadata, is therefore a fundamental requirement for campaign-scale sensing infrastructure.

4.1.2. Multi-Campaign Isolation and Comparison

Campaign-scale environmental sensing is organized around bounded operational units that define a shared temporal scope, spatial extent, and measurement context. In Joint IOPs, these boundaries are explicit: participating instruments and teams coordinate measurement plans within a defined campaign window, producing data that are meaningful only when interpreted in relation to campaign objectives, deployment configuration, and timing. As a result, campaigns function as first-class scientific and operational entities rather than incidental groupings of measurements. Infrastructure supporting campaign-scale sensing must therefore represent campaigns explicitly, with associated identity, scope, and governance, rather than treating campaign context as informal or external metadata. Treating campaign structure as ad hoc directory hierarchies or project-level documentation obscures these boundaries, making it difficult to enforce access controls, preserve provenance, or reliably compare results across campaigns once data move beyond their original acquisition environment.

Within these bounded campaign units, Joint IOPs intentionally deploy heterogeneous instruments with complementary capabilities rather than redundant coverage. Instruments differ in temporal resolution, chemical specificity, spatial mobility, and data latency, and are often used in coordinated ways: fast-response measurements may identify transient features or hotspots that inform the deployment or operation of slower, higher-fidelity instruments. This operational pattern depends on the ability to rapidly access, interpret, and relate subsets of data across instruments during the campaign, rather than relying on post hoc aggregation. Consequently, campaign-scale infrastructure must support selective, concurrent access to heterogeneous datasets while preserving cross-instrument context, a requirement that file-oriented workflows serve poorly because they isolate measurements by instrument, platform, or acquisition system.

Although Joint IOPs are collaborative by design, they remain distinct observational efforts with their own scientific objectives, configurations, and governance constraints. Infrastructure must therefore preserve clear campaign boundaries to avoid conflating data, metadata, or access policies across campaigns, while still allowing comparison

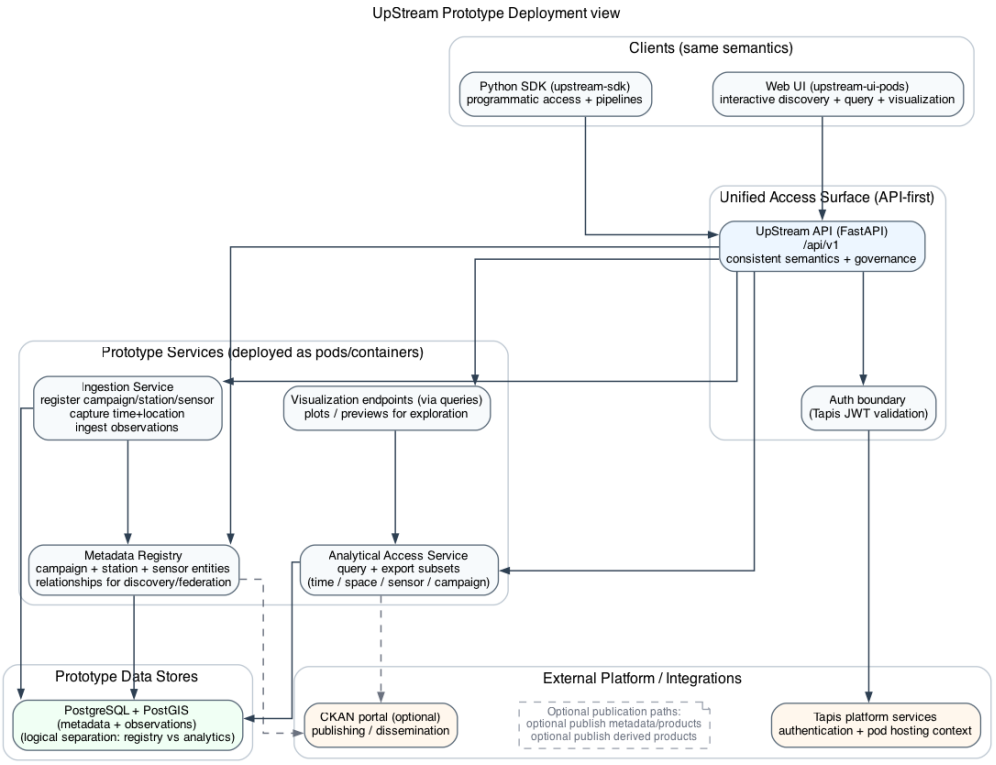


Figure 2: UpStream prototype architecture: ingestion, metadata registry, analytical store, and unified API access layer, with UI and SDK clients operating against the same governed semantics.

and reuse where scientifically appropriate. This dual requirement is central to longitudinal analysis, cross-campaign synthesis, and retrospective model evaluation, all of which depend on retaining campaign-specific context during analysis. Supporting both isolation and comparison requires treating campaigns as explicit organizational units within the infrastructure.

4.1.3. Selective, Concurrent Access to Large Datasets

High-resolution instruments such as those used by the SNIFFER laboratory produce observational datasets at a scale and dimensionality that exceed those typically encountered in many environmental sensing efforts. A single deployment may generate high-frequency measurements across hundreds of molecular species simultaneously, resulting in very large volumes of observational data over the duration of an IOP campaign. When campaigns extend over multiple weeks, file-based storage approaches become insufficient, as they require bulk data transfer and extensive parsing before analysts can identify the subsets of data relevant to a given analysis. In addition to data volume, these campaigns often involve multiple researchers accessing the same datasets concurrently, further exposing the limitations of bulk, file-oriented access patterns. Despite these constraints, researchers still require data to be organized and visualized early in the analysis process.

Constraints identified through co-design with the SNIFFER team therefore motivate the requirement for selective access to observational data. Analysts must be able to retrieve constrained subsets of campaign data, particularly along temporal and spatial dimensions, without processing entire datasets. Several researchers must be able to use it at once, and explore and prepare data for analysis without waiting on one another. At campaign scale, the ability to selectively access relevant observations is a prerequisite for analysis and visualization workflows, rather than an optional optimization.

4.1.4. Metadata Capture Embedded at Ingestion

As researchers accumulate data across multiple IOPs, discovering relevant datasets from prior campaigns becomes increasingly difficult. This challenge limits reuse of place-based observations that are critical for comparative analysis and decision support. The metadata that matters are the fields that let an analyst find an observation from a different campaign or instrument: which campaign, which station, which sensor, when, and where. However, reliable discoverability depends on the availability and quality of metadata describing observational context. Manual metadata completion is time-consuming and frequently results in incomplete or inaccurate records, particularly when metadata is reconstructed after data collection has concluded. These challenges are compounded by the diversity of domain-specific metadata schemas, which share overlapping but non-identical fields and are difficult to reconcile post hoc.

To support reliable discovery and reuse of campaign data, metadata capture must therefore be treated as an infrastructural concern rather than a downstream documentation task. Campaign-scale systems must support metadata capture synchronously with data ingestion, when contextual information about instruments, deployment conditions, and observational intent is most readily available. Embedding metadata capture at ingestion reduces data friction, preserves provenance across campaigns, and establishes the conditions necessary for downstream discoverability and reuse without requiring retrospective reconstruction.

This work does not attempt to present a single-project data portal, a streaming-only monitoring system, or a file-centric data repository intended for bulk data exchange (Table 1). While files may be used as internal implementation artifacts for ingestion or storage, they are not treated as primary interfaces for analysis or reuse. Likewise, real-time streaming and visualization capabilities alone are insufficient to support campaign-scale reuse, cross-campaign comparison, or decision-support workflows. Instead, the proposed architecture defines an IOP campaign-scale data repository, discovery, and access layer designed so that users request a slice of heterogeneous observational data by time, place, sensor, or campaign instead of downloading files.

4.2. Architectural Response: An API-First, Metadata-Supported Prototype

This section presents an architectural response to the requirements identified in Section 4.1. UpStream is a prototype built from loosely coupled microservices (Figure 2) for storing and querying campaign-scale sensor data, with discovery supported by metadata captured at ingestion. Rather than optimizing for a single instrument or workflow, the architecture is intended to reduce data access and analysis limitations by letting users query subsets of heterogeneous observational data across campaigns.

UpStream was designed to support querying and comparing subsets of IOP campaign data. This requirement motivates an API-first architectural stance, in which APIs serve as the primary interface for data ingestion, discovery, and access. By coupling API-mediated access with metadata captured at ingestion, campaigns and laboratories can be federated without sharing storage or workflows. API-mediated interaction further supports multiple concurrent users and analytical workflows without requiring coordination through shared files.

The UpStream architecture is organized as a set of loosely coupled services, each responsible for a distinct function in the sensor data lifecycle. Ingestion services handle the registration of campaign context and observational data, while an analytical data store supports selective access to high-frequency measurements for analysis. A separate metadata registry supports discovery and federation across campaigns without constraining how analytical data are stored or accessed. Interaction with these components is mediated through a single access layer, so ingestion, storage, discovery, and downstream use can change independently. This separation of concerns allows individual components to evolve independently while maintaining coherent support for campaign-scale sensing workflows.

Ingestion services are designed as the primary point at which both observational data and contextual metadata enter the system. At this stage, campaign- and instrument-level information, including campaign descriptions, sensor measurement types, instrument configuration, and the time and location of data collection, is captured alongside measurements. Treating ingestion as a metadata capture event reduces reliance on metadata reconstruction later, when data are prepared for discovery or publication. While some contextual information may be provided explicitly by users, the architecture supports automated propagation of metadata through ingestion workflows, reducing opportunities for omission and preserving observational context across the data lifecycle.

Tracking sensors and measurements across IOP campaigns, and letting other labs find them, is essential for scientific reuse and decision support. Within the UpStream architecture, this role is addressed through a metadata registry that supports federation and discovery across campaigns while remaining distinct from the analytical store's responsibility for selective querying and analysis. The registry provides search and linkage over campaign and instrument context, allowing researchers to identify relevant datasets and related observations across deployments and labs. Discovery runs

Table 1: Capabilities of representative environmental sensor data systems relative to the campaign-scale requirements identified in Section 4.1. Legend: *full* = core capability; *partial* = partial or implementation-dependent; *open* = not a design goal. (The Markdown draft used filled/half-filled/open circle glyphs; replaced here with words to avoid requiring extra symbol packages. Restore glyphs with `pifont` or similar if the journal's style prefers them.)

Capability	CHORDS	SensorThings / HydroServer	HydroShare	ESS-DIVE	Ike Wai Gateway	UpStream
Campaign as first-class entity (identity, scope, governance)	open	partial: Thing/Datastream	partial: resource/collection	partial: dataset package	partial: project/site	full
Metadata capture embedded at ingestion (vs. end-of-lifecycle)	partial	partial	open: at publication	open: at publication	partial	full
API-first ingestion and access (REST for write and query)	full	full	partial: dataset API	partial: dataset API	full	full
Selective spatio-temporal subset query (no bulk transfer)	partial: time series	full: OData filters	open	open	full	full
Concurrent multi-user analytical access	partial	partial	partial	partial	partial	full
Heterogeneous instruments without schema redesign	partial	partial: impl. effort	full: file-based	full: file-based	partial	full
FAIR publication path (DOI/registry integration)	open	open	full: DOI	full: DOI	partial	partial: via CKAN
Programmatic SDK for pipelines and reproducibility	partial	partial: client libs	partial: hsclient	partial	partial	full
Browser-based discovery and visualization UI	full: dashboards	partial: impl.-dep.	full	full: search	full	full
Decision-support orientation (provenance, analysis-ready outputs)	open	open	partial	partial	partial	full

on the metadata and entity relationships captured at ingestion, not on copies of the measurement data restructured into new files solely for discovery or exchange.

Discovery finds the right dataset. Analysis then needs constrained subsets of much larger campaign-scale collections. The UpStream architecture addresses this need through an analytical data store designed to support selective access along temporal and spatial dimensions. Multiple users can work on overlapping datasets at the same time because reads and writes are isolated. In contrast, flat file-based storage approaches treat datasets as indivisible artifacts, limiting selective access and providing weak support for concurrent use. As a result, file-centric workflows become a bottleneck for campaign-scale analysis, particularly when multiple researchers require simultaneous access to shared observational data. Access to analytical data is provided through an API layer that serves as a unified interface between users, visualization tools, and downstream analysis systems. By decoupling data storage from data use, this access layer serves observations programmatically, enforces campaign boundaries, and handles concurrent analyses.

By separating ingestion, storage, discovery, and access into distinct services, the UpStream architecture supports extensibility without requiring redesign as instruments, campaigns, or analytical needs evolve. This modular organization allows labs to initiate data capture for their own sensing campaigns regardless of sensor type, measurement modality, and campaign structure. Because access and storage are decoupled, external computing environments can pull campaign data directly, so analysis is not confined to the repository. Reproducible cookbook environments developed for science gateways illustrate this pattern, packaging analyses that operate directly against gateway-managed data (Mobley, Pearson, Osorio, Tijerina, Trueheart, Faust and Pierce, 2024). The following sections describe how this architecture is realized in practice and evaluate its performance through representative field campaigns, providing evidence that the proposed design supports real-world sensing workflows.

4.3. Prototype Implementation

The implementation reflects the needs of collaborative research teams managing evolving, multi-sensor campaigns who require timely access to observational data for analysis and decision support. Central design principles are API-first access and metadata-supported workflows that support cross-campaign federation within strict campaign boundaries. The prototype implements four-layer services, ingestion/metadata capture, metadata registry for discovery, analytical store for querying, and a unified access surface for analytics and visualization.

UpStream's four service layers are supported by a single, authoritative access layer through its API, but provides access through a web UI and SDK that operate as clients against the same semantics and authorization. These three modalities provide bespoke access to the system that can be mixed and matched and tailored to the users' needs. The UI acts as a frontend client that supports interactive discovery, selective querying and visualization, while the SDK acts as a programmatic client to support data pipelines, reproducibility, and analysis integration.

4.3.1. Ingestion

The first service of UpStream is getting a user's data from their sensors into data storage. Ingestion is the architectural entry point where observations and their contextual metadata are captured together. Users register the campaign, station, and sensors and then upload and store their sensor measurements, allowing measurements to bind to stable identifiers rather than file conventions. Authorization follows a role-based protocol, where users can read, edit, or admin the system, supporting collaborative lab use while preserving security at the lab level. Ingested measurements persist within a relational, query-first data store, while contextual metadata and relationships are committed to a registry to support discovery and federation.

4.3.2. Data Storage and Query Design

High-resolution observations require storage from which several analysts can pull subsets at once, without bulk I/O. After ingestion, data are stored in a relational database, allowing users to query subsets of their IOP campaign data. Analysts and downstream systems retrieve subsets of observations by time, place, sensor, and campaign without touching the whole dataset. While observational measurements are stored in the relational database, metadata are maintained in a separate registry, preserving a clear separation between query-intensive analysis and discovery-oriented metadata services. Because metadata are captured throughout the data lifecycle and propagated across services, observations remain reliably interpretable and discoverable across campaigns.

4.3.3. API-first, Flexible Querying and Ingestion: Abstraction over Data Access

The UpStream prototype adopts an API-first architectural stance, in which APIs serve as the coordinating boundary that governs how campaign data are ingested, queried, and shared, regardless of how users interact with the system.

Interactive user interfaces and software development kits operate as clients and the primary way users will interact with the system. By routing access through APIs, every UpStream instance exposes the same semantics and governance rules, the precondition for federating instances. This abstraction allows interactive tools, automated pipelines, and external analysis environments to evolve independently while operating over the same governed data.

4.3.4. Multi-campaign Organization and Isolation: Governance, Reuse, and Federation at the Architectural Level

Within the UpStream API model, campaigns provide the primary organizational and governance boundaries that determine how data are isolated, shared, and reused. Campaign boundaries provide a logical organization for the system and provide a default for access control and coordination. Campaigns act as guide rails: each stays isolated, and teams still compare observations across deployments, seasons, or study areas. Campaigns can be managed independently while still supporting cross-campaign comparison and long-term reuse of observational records. Federation across campaigns is achieved through linked metadata within the metadata registry, rather than through manual file restructuring for observational data. This separation between orchestration, metadata services, and analytical storage keeps campaigns isolated at the governance level while leaving them discoverable and reusable across instances.

4.4. Prototype Evaluation Through Field Campaigns

We evaluated the prototype system using three field deployments: (1) registration and operation of a mobile IOP campaign from the SNIFFER laboratory, (2) ingestion and management of data from an eddy covariance (EC) flux tower sited at a coastal marsh in the J.D. Murphree Wildlife Management Area, Southeast Texas (SETx), and (3) a remote, pull-based deployment of tilt meters at a subarctic Alaska site. The evaluation focused on architectural performance under operational conditions and assessed system behavior across four dimensions: (i) support for heterogeneous and evolving instrument outputs without schema redesign; (ii) preservation of explicit campaign boundaries during ingestion, access, and comparison; (iii) subset queries on high-resolution datasets under concurrent use; and (iv) persistence of metadata as an infrastructural property throughout the data lifecycle.

4.4.1. PTR-MS Mobile Laboratory: Heterogeneity, Mobility, and Selective Access

The SETx region hosts a diverse range of biogenic and anthropogenic emission sources that affect air chemistry at local and regional scales. These include vegetation such as the marshes along the Gulf Coast and the mixed pine-hardwood thickets farther inland, and industrial point sources like petrochemical refineries and storage facilities. These sources affect the air quality in the region through both routine emissions and acute events (marsh fires, accidental releases, etc.), as well as the secondary reactions of their emissions in the atmosphere.

To elucidate the chemical composition of these sources and their contributions to the overall air quality in the region, a mobile laboratory was deployed periodically from 2023 to 2025 during the SETx-UIFL project timeframe. This consisted of an electric cargo van that housed a suite of air chemistry instrumentation, including the Vocus Proton Transfer Reaction Time of Flight Mass Spectrometer (PTR-ToF-MS) to detect volatile organic compounds (VOCs), LICOR LI-850 Analyzer to quantify moisture and carbon dioxide concentrations, and Thermo Fisher gas monitors to measure ozone and hydrogen sulfide/sulfur dioxide concentrations. These instruments spanned a range of time resolutions, from one datapoint per second on the Vocus, to one datapoint per minute on the gas monitors. Additionally, the mobile laboratory was equipped with GPS systems to log geospatial data every second, which was used to relate the measured concentrations to the corresponding location along the driven route.

The mobile laboratory collected an expansive chemical dataset across multiple field campaigns in the SETx region. These data were sorted by campaign, and processed into 1-minute averages for public access. Vocus data processing procedures included calibration using VOC standards, assessment of instrument sensitivities, and the determination of concentration for each compound in relation to the detected signal. Each datapoint was associated with a location via its timestamp, so a user can query compound concentrations by place and time (by specifying the campaign date and location of interest).

The measurement team took precautions to preserve metadata during both the measurement phase and data analysis, first by ensuring that all instrument and GPS clocks were synchronized prior to starting measurements, and by applying a unified time and geolocation series on which the measured compounds could be mapped. Metadata describing instrument configurations, instrument health, engineering variables, and measurement context are linked to the measurement data, allowing users to distinguish between datapoints that overlap spatially and between campaigns

that have repeated routes. The metadata would accompany the chemical data queried by the user, ensuring that the time, location, and instrument parameters remain intact.

The resulting interface supports both temporal inspection of individual compounds and spatial interpretation of mobile measurements (Figure 3). The concentration view summarizes the selected compound and its distribution over the campaign period, while the map view displays the corresponding route measurements using the interval-based heat-map legend.

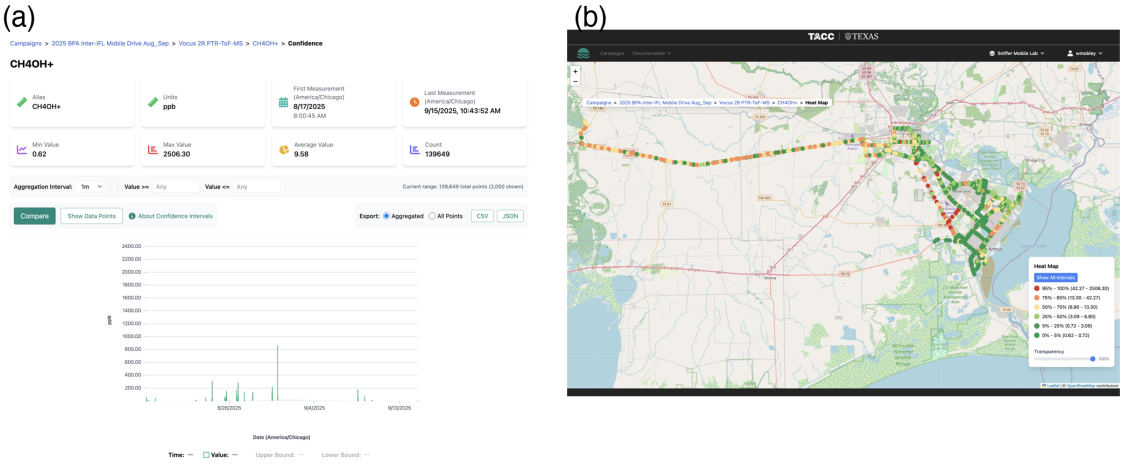


Figure 3: UpStream interface views for the PTR-MS mobile laboratory campaign. (a) Temporal concentration view for CH_4OH^+, including summary statistics and the aggregated measurement series. (b) Spatial heat map of the mobile route, with colors indicating percentile intervals of the selected measurement.

4.4.2. Flux Tower Campaign: Longevity, Accumulation, and Reuse

The SETx region faces frequent "acute-on-chronic" hazards, in which natural stressors (e.g., hurricanes) occur alongside long-term/chronic environmental stressors (e.g., sea-level rise, subsidence). Measuring ecosystem function and land-atmosphere fluxes in the critical period before, during, and after major storm events is important for understanding ecosystem responses to environmental disturbance. The EC flux tower campaign in SETx was used to evaluate the prototype system under continuous, long-term, and stationary sensing conditions. Unlike mobile deployments, the EC flux tower collected high-frequency measurements of carbon dioxide, methane, water, and energy fluxes, together with hydrometeorological variables data at a fixed location. Measurements were made at 10 Hz and processed into 30-minute flux data for public use. Data processing includes gap filling and partitioning of carbon dioxide, methane, and water fluxes into ecosystem productivity and respiration, which allows detailed interpretation of patterns in vegetation function and subsurface biogeochemistry.

The resulting data stream accumulated into a long-term dataset that tested query-mediated access to continuous observations. Users could selectively retrieve subsets of data based on variables, instruments, and time ranges without restructuring, duplicating, or manually separating the datasets. This was important because the same continuous tower record needed to support comparisons across seasons, disturbance events, and recovery periods while remaining organized as a single dataset. Metadata describing instruments, measured variables, deployment configurations, processing methods, and site characteristics, and campaign context remained linked to observations as data accumulated over time. These persistent relationships preserved the distinction between different campaign or analysis periods within the long-running record, supported reuse across campaigns through shared instrument and site metadata, and reduced the need to reconstruct contextual information.

4.4.3. Remote Tilt Meters, Alaska: Transferability Beyond SETx

Tilt meters at a remote subarctic Alaska site are connected to the same UpStream service through a pull-based Tapis Actor that retrieves telemetry over an intermittent satellite link, transforms it into the identical campaign–station–sensor–measurement schema, and ingests it with provenance captured at arrival (Mobley, Faust and Pierce, 2026). No schema or service modifications were required to accommodate this third instrument class, and the

Table 2
Evaluation evidence mapped to the four architectural dimensions defined in Section 3, by field campaign.

Evaluation dimension	PTR-MS mobile laboratory (SNIFFER IOP)	EC flux tower (SETx coastal marsh)	Remote tilt meters, Alaska
(i) Heterogeneous, evolving instrument outputs without schema redesign	Vocus PTR-ToF-MS (1 Hz), LICOR LI-850, Thermo Fisher gas monitors (1/min), GPS (1 Hz) ingested through the same campaign–station–sensor–measurement schema.	10 Hz raw fluxes processed to 30-min across 18 variables including CO_2, CH_4, H_2O, and energy fluxes plus hydrometeorological variables; stationary continuous stream added with no schema changes.	Tilt meter telemetry retrieved by pull-based Tapis Actor; new stations/sensors registered under the same schema, demonstrating transfer to a third instrument class.
(ii) Preservation of explicit campaign boundaries during ingestion, access, and comparison	Periodic deployments (2023–2025) registered as distinct campaigns; repeated routes distinguishable via campaign metadata; spatially overlapping datapoints separable by campaign.	Single long-running campaign retaining internal analysis periods (seasons, disturbance events, recovery) without splitting the record; remained isolated from concurrent mobile campaigns in the same instance.	Remote campaign operated in a project-specific deployment, isolated by Tapis Auth; governance boundary maintained across institutional collaborators.
(iii) Selective, query-mediated access to high-resolution data under concurrent use	Compound concentrations queryable by campaign date and location; 1-min averages served for public access without bulk file transfer.	Subset retrieval by variable, instrument, and time range without duplicating or restructuring the accumulated record.	Nightly pull-based ingestion tolerant of intermittent connectivity; data accessible via UI, API, and SDK on arrival.
(iv) Metadata persistence as an infrastructural property across the lifecycle	Synchronized instrument/GPS clocks; instrument configuration, health, and engineering variables linked to measurements at ingestion and returned with queried data.	Instruments, variables, deployment configurations, processing methods, and site characteristics remained linked as data accumulated; no retrospective reconstruction required.	Provenance and lineage captured at ingestion (campaigns, sensors, locations) supporting downstream decision provenance.

deployment's tolerance of intermittent connectivity demonstrates that the architecture's pull-based ingestion pattern transfers to operating conditions more remote and harsher than those tested in SETx.

4.4.4. Synthesis: Architectural Claims Under Operational Stress

The three field deployments provide complementary examples of mobile, stationary, and remote sensor campaigns: the PTR-MS Mobile Laboratory IOP, the flux tower campaign, and the remote Alaska tilt-meter deployment (Table 2). Through these three use cases we were able to show a flexible schema that allowed ingestion of all three instrument classes through the same API and schema. Through this evaluation all three deployments remained independent of each other and allowed users from separate campaigns to work in the same system at the same time while providing fidelity to the underlying data. Finally, the system auto-populated metadata that allowed users from the research groups to discover the datasets.

4.5. Alignment with Decision Support Workflows

The UpStream architecture supports decision workflows by serving campaign-scale sensor data in the subsets a decision actually needs. Decision support in environmental campaigns begins with problem formulation, during which analysts and stakeholders must determine which patterns, comparisons, or temporal windows are relevant before formal modeling is undertaken. Access to ground-truth observational data during this stage is therefore essential. This framing aligns with science gateway approaches that carry decision processes from problem formulation through evaluation (Pierce et al., 2026; Pierce, 2026), and with AI-enabled stakeholder modeling workflows that depend on structured knowledge capture during engagement (Pierce, Mobley, Faust and Stephens, 2024).

By adopting a query-first design, the architecture allows stakeholders to retrieve constrained subsets of heterogeneous campaign data along temporal, spatial, sensor, and campaign dimensions without requiring bulk file transfer or extensive preprocessing. This selective access supports exploratory analysis, comparative reasoning, and hypothesis refinement prior to model execution. Users query for the records they need instead of confronting an undifferentiated data volume, which matches how environmental decision support actually proceeds: iteratively.

Timeliness is itself a decision-support requirement. Observations that arrive after a decision window has closed cannot inform problem formulation, intervention, or evaluation, and urgent-computing perspectives increasingly treat timely, trustworthy access to observational data as a first-order property of decision-oriented cyberinfrastructure rather than a performance optimization (Parashar and Pierce, 2026). UpStream puts timeliness in the data layer. An observation is queryable as soon as it is ingested, with no export or reformatting step between collection and use.

Visualization within the UpStream architecture is a direct consequence of query-mediated access rather than a standalone presentation layer. Because observational data are accessible across temporal, spatial, sensor, and campaign dimensions through stable schema relationships, visual representations can be generated dynamically over heterogeneous datasets without manual file restructuring. Analysts can compare sensors, filter, and explore within a campaign's boundaries. In campaign-scale decision settings, visualization thus functions as a shared interpretive surface, supporting collaborative reasoning and preliminary understanding prior to formal modeling. This shared interpretive role echoes the participatory modeling literature, in which jointly examined representations anchor collaborative reasoning among stakeholders and analysts (Voinov, Kolagani, McCall, Glynn, Kragt, Ostermann, Pierce and Ramu, 2016).

5. Discussion: Generalizable Architectural Lessons

The UpStream prototype results provided an example of a modular system with distinct architectural layers. This allows systems to remain flexible and scalable across different research contexts without requiring a full redesign (Kaginalkar, Kumar, Gargava, Kharkar and Niyogi, 2022). This aligns with other modern architectural systems like Tapis, which separate core research functions into distinct APIs, allowing each component to be developed and scaled independently (Stubbs, Cardone, Packard, Jamthe, Padhy, Terry, Looney, Meiring, Black, Dahan, Cleveland and Jacobs, 2021). As the UpStream architecture becomes more mature, or as pieces become outdated, they can be swapped for more modern approaches.

The three use cases, PTR-MS mobile laboratory, the flux tower, and the remote Alaska tilt-meter deployment, produced different datasets and data structures, showing that campaign systems must support heterogeneous instruments and evolving measurement structures through a flexible schema. This aligns with the designs of other sensor repositories (Hertweck, Hellmund, van der Schaaf, Moßgraber and Blume, 2019; Porter, Hanson and Lin, 2012). For example, large-scale networks like iUTAH GAMUT must manage a wide variety of aquatic and climate sensors across different watersheds, necessitating a workflow that handles diverse variables (e.g., snow depth, water quality, and barometric pressure) within a consistent management framework (Jones et al., 2015).

The UpStream system highlights that capturing metadata during the ingestion process is critical for data quality, interpretability, and long-term reuse. Capturing metadata at the same time as the data avoids the errors that arise when metadata is reconstructed after the fact, where inconsistencies frequently lead to "redundant" or unreliable information (Manso-Callejo, Wachowicz and Bernabé-Poveda, 2010). In large-scale sensor networks, it is "imperative" to link equipment inventory, site visits, calibrations, and maintenance events directly to the observational data to ensure the quality of derived data products (Jones et al., 2015). Integrating the UpStream Prototype with a CKAN data registry provides FAIR human-readable metadata and discovery. The team's SETx data products published through ESS-DIVE (e.g., Buschow, Luo, Mobley and Pierce, 2024) illustrate the archival publication pathway this registry integration is designed to feed.

UpStream stores and serves observations. It does not yet prepare them for models. That is the gap that matters most now, because the intelligent geoscience systems and stakeholder modeling workflows that motivate this work (Gil et al., 2018; Pierce et al., 2024) need AI-ready data: observations with consistent structure, units, calibration, and location attached, retrievable as a defined subset rather than reassembled from files. Metadata written at ingestion and a stable core schema take UpStream most of the way there. The next step is to make a query result itself a versioned, citable dataset, carrying the metadata that produced it, so that a training set or an evaluation benchmark can be regenerated from the same query.

6. Conclusion

Campaign-scale environmental sensing increasingly produces heterogeneous, high-frequency, and spatially complex datasets that exceed the practical limits of file-based and portal-centric workflows. These workflows often obscure campaign context, separate observations from metadata, and make selective access difficult at the moment when data

are most needed for analysis, visualization, and decision support. UpStream demonstrates one architectural response to this problem: an API-first, modular repository that writes metadata when data arrive and holds campaigns, sensors, and measurements as linked records rather than files.

Through the PTR-MS mobile laboratory, flux tower, and Alaska tilt-meter use cases, the prototype shows that heterogeneous mobile, stationary, and remote sensing datasets can be ingested, organized, queried, and reused within a common architectural model while preserving campaign boundaries and observational context. The results suggest that the most transferable contribution of UpStream is not any single software platform, but a set of architectural principles: modular service separation, flexible schema design, metadata capture at ingestion, query-mediated access, and federation designed into the system from the beginning. For environmental decision support, these principles matter because downstream modeling, visualization, and stakeholder analysis depend on timely access to trusted, contextualized observational data. Campaign-scale sensing systems should therefore treat decision support as an infrastructure requirement fixed before the first instrument is deployed, not an analytical step added afterward.

Code availability

The version of UpStream used in this study is v1.2.0, available at the UpStream v1.2.0 GitHub release. This coordinated release identifies the source versions of the UpStream platform components used in the study.

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