Projecting Performance Data Over Simulation Geometry Using SOSflow and Alpine

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ABSTRACT

The performance of HPC simulation codes is often tied to their simulated domains; e.g., properties of the input decks, boundaries of the underlying meshes, and parallel decomposition of the simulation space. A variety of research efforts have demonstrated the utility of projecting performance data onto the simulation geometry to enable analysis of these kinds of performance problems. However, current methods to do so are largely ad-hoc and limited in terms of extensibility and scalability. Furthermore, few methods enable this projection online, resulting in large storage and processing requirements for offline analysis. We present a general, extensible, and scalable solution for in-situ (online) visualization of performance data projected onto the underlying geometry of simulation codes. Our solution employs the scalable observation system SOSflow with the in-situ visualization framework Alpine to automatically extract simulation geometry and stream aggregated performance metrics to respective locations within the geometry at runtime. Our system decouples the resources and mechanisms to collect, aggregate, project, and visualize the resulting data, thus mitigating overhead and enabling online analysis at large scales. Furthermore, our method requires minimal user input and modification of existing code, enabling general and widespread adoption.

KEYWORDS

sos, sosflow, alpine, hpc, performance, visualization, in situ

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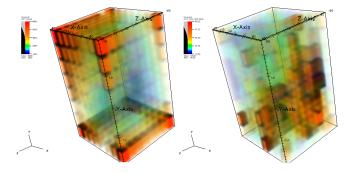


Figure 1: Loops (left) and maximum backlog (right) from one cycle of 512 KRIPKE ranks distributed to 32 nodes.

1 INTRODUCTION

Projecting application and performance data onto the scientific domain allows for the behavior of a code to be perceived in terms of the organization of the work it is doing, rather than the organization of its source code. This perspective can be especially helpful [14] for domain scientists developing aspects of a simulation primarily for its scientific utility, though it can also be useful for any HPC developer [13] engaged with the general maintenance requirements of a large and complicated codebase.

There have been practical challenges to providing these opportunities for insight. Extracting the spatial descriptions from an application traditionally has relied on hand-instrumenting codes to couple a simulation's geometry with some explicitly defined performance metrics. Performance tool wrappers and direct source-instrumentation need to be configurable so that users can disable their invasive presence during large production runs. Because it involves changes to the source code of an application, enabling or disabling the manual instrumentation of a code often involves full recompilation of a software stack. Insights gained by the domain projection are limited to what was selected a priori for contextualization with geometry.

Without an efficient runtime service providing an integrated context for multiple sources of performance information, it is difficult to combine performance observations across several components

during a run. Further limiting the value of the entire exercise, performance data collected outside of a runtime service must wait to be correlated and projected over a simulation's geometry during post-mortem analysis. Projections that are produced offline cannot be used for application steering, online parameter tuning, or other runtime interactions that include a human in the feedback loop. Scalability for offline projections also becomes a concern, as the potentially large amount of performance data and simulation geometry produced and operated over in a massively parallel cluster now must be integrated and rendered either from a single point or within an entirely different allocation.

The overhead of manually instrumenting large complex codes to extract meaningful geometries for use in performance analysis, combined with the limited value of offline coorelation of a fixed number of metrics, naturally limited the usage of scientific domain projections for gaining HPC workflow performance insights.

1.1 Research Contributions

This paper describes the use of SOSflow [15] and Alpine to overcome many prior limitations to projecting performance into the scientific domain. The methods used to produce our results can be implemented in other frameworks, though SOSflow and Alpine, discussed in detail in later sections, are generalized and intentionally engineered to deliver solutions of the type presented here. This research effort achieved the following:

- Eliminate the need to manually to capture geometry for projections of Alpine-enabled workflows
- Activate or deactivate the capture of performance and scientific domain data without requiring workflow recompilation
- Generalized filter to gather both static and dynamic spatial data from various simulations
- Provide online observation of performance projected over evolving geometries and metrics, along with automatic asynchronous storage of data for offline analysis and archival
- Facilitate interactive selection of one or many performance metrics and rendering parameters, adding dynamism to projections
- Enable simultaneous online projections from a common data source
- In situ architecture supporting both current and future-scale systems

2 RELATED WORK

Husain and Gimenez's work on Mitos [7] and MemAxes [6] is motivated similarly to ours. Mitos provides an integration API for combining information from multiple sources into a coherent memoized set for analysis and visualization, and MemAxes projects correlated information across domains to explore the origins of observed performance. SOSflow is being used in our research as an integration API, but takes a differnt optimization path by providing a general-purpose in situ (online) runtime.

Boehme's Caliper [3] extracts performance data during execution in ways that serve a variety of uses, in much the same way our efforts here are oriented. Caliper's flexible data aggregation [4] model can be used to filter metrics in situ, allowing for tractible volumes of performance data to be made available for projections.

Both ALPINE and Caliper provide direct services to users, also serving as integration points for user-configurable services at run time. Caliper is capable of deep introspection on the behavior of a program in execution, yet is able to be easily disabled for production runs that require no introspection and want to minimize instrumentation overhead. ALPINE allows for visualization filters to be compiled seperately from a user's application and then introduced into, or removed from, an HPC code's visualization pipeline with a simple edit to that workflow's ALPINE configuration file.

BoxFish [8] also demonstrated the value of visualizing projections when interpreting performance data, adding a useful hierarchical data model for combining visualizations and interacting with data

SOSflow's flexible model for multi-source online data collection and analysis provides performance exploration opportunities using both new and existing HPC tools.

3 SOSFLOW

To better understand the role played by SOSflow, it is useful to examine its architecture. SOSflow is composed of four major components:

sosd : Daemonslibsos : Client Librarypub/sql : Data

• sosa : Analytics & Feedback

These components work together to provide extensive runtime capabilities to developers, administrators, and application end-users. SOSflow runs within a user's allocation, and does not require elevated priveledges for any of its features.

3.1 SOSflow Daemons

Online functionality of SOSflow is enabled by the presence of a user-space daemon. This daemon operates completely independently from any applications, and does not connect into or utilize any application data channels for SOSflow communications. The SOSflow daemons are launched from within a job script, before the user's applications are initialized. These daemons discover and communicate amongst each other across node boundaries within a user's allocation. When crossing node boundaries, SOSflow uses the machine's high-speed communication fabric. Inter-node communication may use either MPI or EVPath as needed, allowing for flexibility when configuring its deployment to various HPC environments.

The traditional deployment of SOSflow will have a single daemon instance running in situ for each node that a user's applications will be executing on. This daemon is called the **listener**. Additional resources can be allocated in support of the SOSflow runtime as-needed to support scaling and to minimize perturbation of application performance. One or more nodes are usually added to the user's allocation to host SOSflow **aggregator** daemons that combine the information that is being collected from the in situ daemons. These aggregator daemons are useful for providing holistic unified views at runtime, especially in service to online analytics modules. Because they have more work to do than the in situ listener daemons, and also are a useful place to host analytics

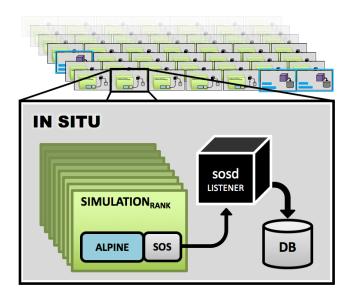


Figure 2: SOSflow's lightweight daemon runs on each node.

modules, it is advisable to place aggregation targets on their own dedicated node[s], co-located with online analytics codes.

3.1.1 In Situ. Data coming from SOSflow clients moves into the in situ daemon across a light-weight local socket connection. Any software that connects in to the SOSflow runtime can be thought of as a client. Clients connect only to the daemon that is running on their same node. No client connections are made across node boundaries, and no special permissions are required to use SOSflow, as the system considers the SOSflow runtime to be merely another part of a user's workflow.

The in situ listener daemon offers the complete functionality of the SOSflow runtime, including online query and delivery of results, feedback, or application steering messages. At startup, the daemon creates an in-memory data store with a file-based mirror in a user-defined location. Listeners asynchronously store all data that they receive into this store. The file-based mirror is ideal for offline analysis and archival. The local data store can be queried and updated via the SOSflow API, with all information moving over the daemon's socket, avoiding dependence on filesystem synchronization or centralized metadata services. Providing the full spectrum of data collected on node to clients and analytics modules on node allows for distributed online analytics processing. Analytics modules running in situ can observe a manageable data set, and then exchange small intermediate results amongst themselves in order to compute a final global view. SOSflow also supports running analytics at the aggregation points for direct query and analysis of global or enclave data, though it is potentially less scalable to perform centrally than in a distrubted fashion, depending on the amount of data being processed by the system.

SOSflow's internal data processing utilizes unbounded asynchrous queues for all messaging, aggregation, and data storage. Pervasive design around asynchronous data movement allows for the SOSflow runtime to efficiently handle requests from clients and

messaging between off-node daemons without incurring synchronization delays. Asynchronous in situ design allows the SOSflow runtime to scale out beyond the practical limits imposed by globally synchronous data movement patterns.

3.1.2 Aggregation Targets. A global perspective on application and system performance is often useful. SOSflow automatically migrates information it is given into one or more aggregation targets. This movement of information is transparent to user's of SOS, requiring no additional work on their part. Aggregation targets are fully-functional instances of the SOSflow daemon, except that their principle data sources are the distributed in situ daemons rather than local clients. The aggregated data contains identical information as the in situ data stores, it just has more of it, and it is assembled into one location. The aggregate daemons are useful for performing online analysis or information visualization that needs to include information from multiple nodes.

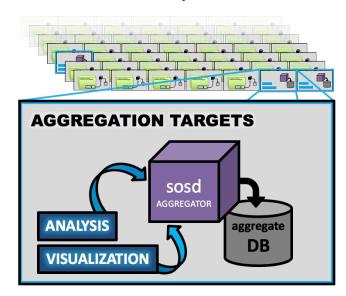


Figure 3: SOSflow supports one or more dedicated aggregation targets which serve as ideal places to co-locate analysis and visualization tasks, conserving in situ resources.

SOSflow is not a publish-subscribe system in the traditional sense, but uses a more scalable push and pull model. Everything sent into the system will automatically migrate to aggregation points unless it is explicitly tagged as being node-only. Requests for information from SOSflow are ad hoc and the scope of the request is constrained by the location where the request is targeted: in situ queries are resolved against the in situ database, aggregate queries are resolved against the aggregate database. If tagged node-only information is potentially useful for offline analysis or archival, the in situ data stores can be collected at the end of a job script, and their contents can be filtered for that node-only information, which can be simply concatenated together with the aggregate database[s] into a complete image of all data All information in SOSflow is tagged with a globally unique identifier (GUID). This allows SOSflow data to be mixed together while preserving its provenance and preventing data duplication or namespace collision.

3.2 SOSflow Client Library

Clients can directly interface with the SOSflow runtime system by calling a library of functions (libsos) through a standardized API. Applications can also transparently become clients of SOS by utilizing libraries and performance tools which interact with SOSflow on their behalf. All communication between the SOSflow library and daemon are transparent to users. Users do not need to write any socket code or introduce any state or additional complexity to their own code.

Information sent through the libsos API is copied into internal data structures, and can be freed or destroyed by the user after the SOSflow API function returns. Data provided to the API is published up to the in situ daemon with an explicit API call, allowing developers to control the frequency of interactions with the runtime environment. It also allows the user to register callback functions that can be triggered and provided data by user-defined analytics function, creating an end-to-end system for both monitoring as well as feedback and control.

To maximize compatibility with extant HPC applications, the SOSflow client library is currently implemented in C99. The use of C99 allows the library to be linked in with a wide variety of HPC application codes, performance tools, and operating environments. There are various custom object types employed by the SOSflow API, and these custom types can add a layer of complexity when binding the full API to a language other than C or C++. SOSflow provides a solution to this challenge by offering a "Simple SOS" (ssos) wrapper around the full client library, exposing an API that uses no custom types. The ssos wrapper was used to build a native Python module for SOSflow. Users can directly interact with the SOSflow runtime environment from within Python scripts, acting both as a source for data, but also a consumer of online query results.

3.3 SOSflow Data

The primary concept around which SOSflow organizes information is the "publication handle" (pub). Pubs provide a private namespace where many types and quantities of information can be stored as a key/value pair. SOSflow automatically annotates values with a variety of metadata, including a GUID, timestamps, origin application, node id, etc. This metadata is available in the persistent data store for online query and analysis. SOSflow's metadata is useful for a variety of purposes:

- Performance analysis
- Provenance of captured values for detection of source-specific patterns of behavior, failing hardware, etc.
- Interpolating values contributed from multiple source applications or nodes
- Re-examining data after it has been gathered, but organizing the data by metrics other than those originally used when it was gathered

The full history of a value, including updates to that value, is maintained in the daemon's persistent data store. When a key is re-used to store some new information that has not yet been transmitted to the in situ daemon, the client library enqueues it up as a snapshot of that value, preserving all associated metadata alongside the historical value. The next time the client publishes

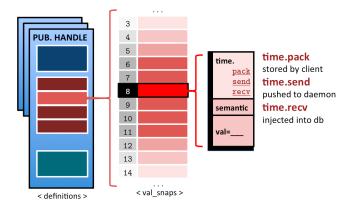


Figure 4: SOSflow retains the full history of every value.

to the daemon, the current and all enqueued historical values are transmitted.

SOSflow is built on a model of a global information space. Aggregate data stores are guaranteed to provide eventual consistency with the data stores of the in situ daemons that are targeting them. SOSflow's use of continuous but asynchronous movement of information through the runtime system does not allow for strict quality-of-service guarantees about the timeliness of information being available for analysis. This design constraint reflects the reality of future-scale HPC architectures and the need to elminate dependence on synchronous behavior to correlate context. SOSflow conserves contextual metadata when values are added inside the client library. This metadata is used during aggregation and query resolution to compose the asynchronously-transported data according to its original synchronous creation. The vissictitudes of asynchronous data migration strategies at scale become entirely transparent to the user.

SOSflow does not require the use of a domain-specific language when pushing values into its API. Pubs are self-defining through use: When a new key is used to pack a value into a pub, the schema is automatically updated to reflect the name and the type of that value. When the schema of a pub changes, the changes are automatically announced to the in situ daemon the next time the client publishes data to it. Once processed and injected into SOSflow's data store, values and their metadata are accessible via standardized SQL queries. SOSflow's online resolution of SQL queries provides a high-degree of programmability and online adaptivity to users. SQL views are built into the data store that mask off the internal schemas and provide results organized intuitively for grouping by application rank, node, time series, etc.

SOSflow uses the Alpine in situ visualization infrastructure described below to collect simulation geometry that it correlates with performance data.

4 ALPINE

ALPINE is a project that aims to build an in situ visualization infrastructure and analysis targeting leading edge supercomputers. ALPINE is part of the U.S. Department of Energy's Exascale Computing Project (ECP) [12], and the ALPINE effort is supported by

multiple institutions. The goal of ALPINE is two fold. First, create a hybrid-parallel library (i.e., both distributed-memory and shared-memory parallel) that can be included in other visualization tools such as ParaView [2] and VisIt [5] thus creating an ecosystem where new hybrid-parallel algorithms are easily deployed into downstream tools. Second, create a flyweight in situ infrastructure that directly leverages the hybrid-parallel library. In this work, we directly interface with the ALPINE in situ infrastructure.

The ALPINE in situ infrastructure is the descendant of Strawman [11], and ALPINE it tightly-coupled with simulations, i.e. it shares the same node resources as the simulation. Strawman is an in situ visualization mini-app meant to serve as an place to perform rapid prototyping of in situ visualization algorithms, and to that end, Strawman, and ALPINE, include three physics proxy-applications out of the box to allow immediately provide the infrastructure and algorithms with mesh data to consume. While Strawman's goal was to bootstrap in situ visualization research, the ALPINE in situ infrastructure is intended for production.

The design of the ALPINE in situ infrastructure is meant to be flexible and provides a means to have interoperability with software outside the ALPINE project. ALPINE uses the Conduit [10] data exchange library to marshal mesh data from simulations into ALPINE. Conduit provides an intuitive hierarchical model for describing mesh data, and Conduit provides a simple set of conventions for describing structured meshes to meshes that contain higher order elements. Once the simulation describes the mesh data, it publishes the data into ALPINE's in situ infrastructure along with a set of actions to perform (e.g., visualization and analysis) which can be chained together. Conceptually, the sum of these actions form a directed acyclic graph (DAG), and to support this execution model, ALPINE includes the Flow library. Flow is a simple dataflow library based on the Python dataflow library within VisIt.

Everything within Flow is a filter that can have multiple inputs and a single output of generic types. Filters have a simple interface to declare their inputs and output, and filters become available when they are registered with Flow. ALPINE includes built-in filters for all of the visualization and analysis algorithms in the hybrid parallel library. The flexibility of Flow allows for user defined filters, compiled outside of ALPINE, to be easily inserted into the dataflow, and when the dataflow network executes, custom filters have access to all of the simulation mesh data published to ALPINE.

5 EXPERIMENTS

5.1 Evaluation Platform

All results were obtained by running online queries (Figure 3) against the SOSflow runtime's aggregation targets using SOSflow's built-in Python API. The results of these queries were used to create input files for the VisIt visualization tool, which was invoked from within the allocation.

5.2 Experiment Setup

The experiments performed had the following purposes:

• Validation : Demonstrate the coupling of SOSflow with Alpine and its ability to extracy geometry from simulations transparently.

Introspection: Examine the overhead incurred by including the SOSflow geometry extraction filter in an Alpine visualization pipeline.

Alpine libraries were used to build a visualization module for online geometry extraction. Alpine's JSON configuration file describing the connectivity of the in situ visualization pipeline was modified to insert the geometry extraction module. The SOSflow implemen-

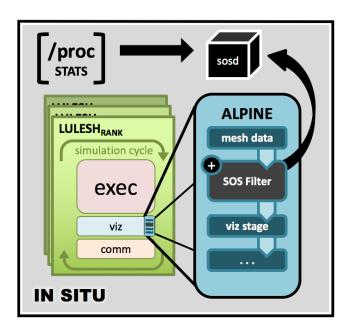


Figure 5: SOSflow collects runtime information to project over the simulation geometry.

tation used to conduct these experiments is general-purpose and was not tailored to the specific deployment environment or the simulations observed. The study was conducted on two machines, the details of which are included here -

- Quartz: A 2,634-node Penguin supercomputer at Lawrence Livermore National Laboratory (LLNL). Intel Xeon E5-2695 processors provide 36 cores/node. Each node offers 128 GB of memory and nodes are connected via Intel OmniPath.
- (2) Catalyst: A Cray CS300 supercomputer at LLNL. Each of the 324 nodes is outfitted with 128 GB of memory and 2x Intel Xeon E5-2695v2 2.40 GHz 12-core CPUs. Catalyst nodes transport data to each other using a QLogic InfiniBand QDR interconnect.

The following simulated workflows were used —

(1) **KRIPKE** [9]: A 3D deterministic neutron transport proxy application that implements a distributed-memory parallel sweep solver over a rectilinear mesh. At any given simulation cycle, there are simultaneous sweeps along a set of discrete directions to calculate angular fluxes. This results in a MPI communication pattern where ranks receive asynchronous requests from other ranks for each discrete direction.

(2) **LULESH** [1]: A 3D Lagrangian shock hydrodynamics proxy application that models Sedov blast test problem over a curvilinear mesh. As the simulation progresses, hexahedral elements deform to more accurately capture the problem state.

5.3 Overview of Processing Steps

The SOSflow runtime provided a modular filter for the Alpine in situ visualization framework. This filter was enabled for the simulation workflow at runtime to allow for the capture of evolving geometric details as the simulation progressed. The SOSflow runtime daemon automatically contextualized the geometry it received alongside the changing application performance metrics. SOSflow's API for Python was used to extract both geometry information and correlated performance metrics from the SOSflow runtime. This data set was used to generate sequences of input files to the VisIt scientific data visualization tool corresponding to the cycle of a the distributed simulation.

Each input file contained the geometric extents of every simulation rank, the portion of the simulated space that each part of the application was working within. Alongside that volumetric descriptions for that cycle, SOSflow integrated attribute dictionaries of all plottable numeric values it was provided during that cycle, grouped by simulation rank. Performance metrics could then be interactively selected and combined in VisIt with customizable plots, presenting an application rank's state and activity incident to its simulation effort, projected over the relevant spatial extent.

5.4 Evaluation of Geometry Extraction

The geometry extracted by Alpine's SOSflow filter was rendered and compared with existing visualizations of its simulation. Performance metrics can be coorelated in SQL queries to the correct geometric regions by various redundant means such as pub handle GUID, origin PID or MPI rank, simulation cycle, host node name, SOSflow publish frame, and creation timestamps.

Our experiments were validated by emperical analysis of projections rendered for the duration of their source simulation. Projections were required to reflect their simulation's expected deforming of geometry (LULESH) or algorithm-dependent workload imbalance (KRIPKE).

5.5 Evaluation of Overhead

Millisecond-resolution timers were added to the per-cycle execution method of the SOSflow Alpine geometry extraction filter. Each rank tracked the amount of time it spent extracting its geometry, packing the geometry into an SOSflow pub handle, and transmitting it to the runtime daemon. Every cycle's individual time cost was computed and transmitted to SOSflow, as well as a running total of the time that Alpine had spent in the SOSflow filter. From a region outside the timers, the timer values were packed into the same SOSflow publication handle used for the geometric data. Timer values were transmitted at the end of the following cycle, alongside that cycle's geometry. The additional transmission cost of these two timer values once per simulation cycle had no perceivable impact on the performance they were measuring.

6 RESULTS

NOTE TO REVIEWERS: Additional and larger runs were not possible due to machine DATs and time constraints at the time of this draft, but larger scales may be available for a photo-ready draft. Further, the projections rendered in this draft will be re-rendered to increase their clarity.

6.1 Geometry Extraction and Performance Data Projection

Geometry was successfully extracted (Figures 1, 6, 7, and 8) with minimal overhead from simulations run at a variety of scales from 2 to 33 nodes. Along with the geometry, performance metrics were gathered and projected over their correlated domains.

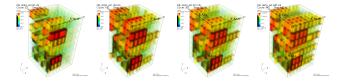


Figure 6: Cumulative user cpu ticks during 440 cycles of 512 KRIPKE ranks on 32 nodes.

6.2 Overhead

When gathering *only the simulation geometry*, execution never exceeded 2ms. Collecting 31 unique Alpine performance data and system metrics within the filter added additional overhead, but the filter time but did not exceed 4ms for any of the projections shown in this paper. The filter's execute time was logged as a metric alongside the other in situ performance data, and is visualized for LULESH in Figure 7.

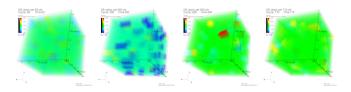


Figure 7: Filter execution (1-4ms) over 710 LULESH cycles.

7 CONCLUSION

Services from both SOSflow and ALPINE were successfully integrated to provide a scalable in situ (online) geometry extraction and performance data projection capability.

7.1 Future Work

Workflows that use the Alpine framework but have complex irregular meshes, feature overlapping "halo regions", or that operate over non-continuous regions of space within a single process, may require additional effort to extract geometry from, depending on the organization of spatial descriptions they employ. The addition of a general convex hull algorithm to VTK-m will simplify the task

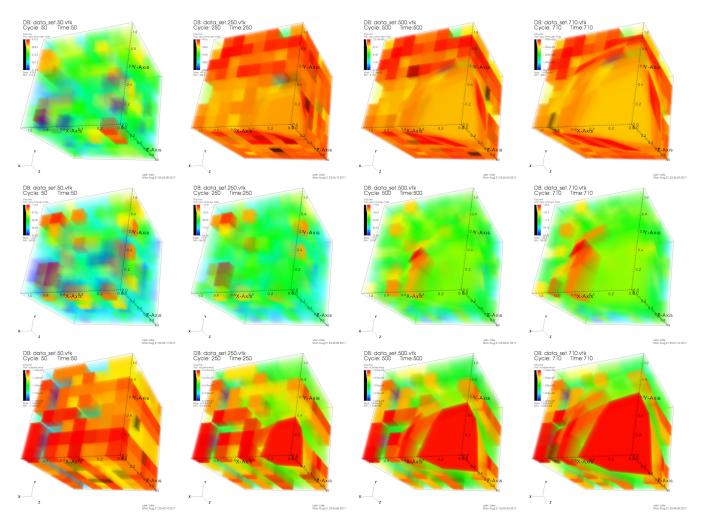


Figure 8: Many metrics can be projected from one run. Here we see (top to bottom) user cpu ticks, system cpu ticks, and bytes read during 710 cycles of 512 LULESH ranks distributed across 32 nodes.

of uniformly describing any spatial extent[s] being operated on by a process.

The VisIt UI can be extended to support interactivity with the SOSflow runtime. This will allow data exploration with VisIt to engage with HPC applications as they are running, interrogating the distributed data stores with custom SQL, and enable interactive code steering based on what is observed.

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