DIVA: A Declarative and Reactive Language for in situ Visualization

Qi Wu* University of California, Davis, United States

Konduri Aditya[§] Indian Institute of Science, India Tyson Neuroth[†] University of California, Davis, United States

Jacqueline H. Chen[¶] Sandia National Laboratories, United States Oleg Igouchkine[‡] University of California, Davis, United States

Kwan-Liu Ma^{II} University of California, Davis, United States

ABSTRACT

The use of adaptive workflow management for in situ visualization and analysis has been a growing trend in large-scale scientific simulations. However, coordinating adaptive workflows with traditional procedural programming languages can be difficult because system flow is determined by unpredictable scientific phenomena, which often appear in an unknown order and can evade event handling. This makes the implementation of adaptive workflows tedious and errorprone. Recently, reactive and declarative programming paradigms have been recognized as well-suited solutions to similar problems in other domains. However, there is a dearth of research on adapting these approaches to in situ visualization and analysis. With this paper, we present a language design and runtime system for developing adaptive systems through a declarative and reactive programming paradigm. We illustrate how an adaptive workflow programming system is implemented using our approach and demonstrate it with a use case from a combustion simulation.

1 INTRODUCTION

Scientific simulations running on petascale high-performance computing (HPC) platforms such as Summit [50] can easily produce datasets at scales beyond what can be efficiently processed. Therefore, scientists often have to compromise the allocation of strained resources, such as I/O bandwidth, to maximize the overall efficiency of simulations [8, 29]. An ideal solution is to manage the system workflow adaptively through trigger-action mechanisms (which are termed "in situ triggers" in some literature [11, 31]) because they can prioritize the allocation of these strained resources to the most interesting phenomena as they emerge [56]. However, adaptive workflows are usually more difficult and error-prone to program because they are *reactive* applications rather than *transformational* [48]. Control flows in adaptive workflows are often driven by evolving simulation outcomes and event sequences that cannot be predicted in advance. Therefore, domain scientists must anticipate all possible scenarios in advance and create sophisticated rules to dynamically trigger actions in response to the events [6]. Moreover, because the quality of adaptive workflows often relies heavily on the accuracy of trigger conditions, having an in situ infrastructure that simplifies the customization process is important [8,31].

A common approach to implementing reactive systems is through synchronous dataflow programming models [14, 15, 26]. In such models, programs are formed by wiring primitive processing elements and composition operators into a directed graph structure. The dataflow programming model provides a natural form of modularity for many applications. VTK [61] also partially adopted this approach, however, VTK is designed for programming unidirectional visualization pipelines, and provides limited support for highly dynamic dataflows. Moreover, the synchronous dataflow model is somewhat difficult to use and does not always lead to modular programs for large scale applications when control flows become complicated [19]. Functional reactive programming (FRP) [19,24,48,53] further improved this model by directly treating time-varying values as first-class primitives. This allowed programmers to write reactive programs using dataflows declaratively (as opposed to callback functions), hiding the mechanism that controls those flows under an abstraction. By enabling such a uniform and pervasive manner to handle complicated data flows, applications gain clarity and reliability.

Through our work, we demonstrate how FRP abstractions can be used to better assist adaptive *in situ* visualization and analysis workflow creation, using a domain-specific language (DSL) we created called DIVA. This language consists of two components: an FRPbased visualization specific language and a low-level C++-based dataflow API. Rather than replacing existing *in situ* infrastructures, it aims to work as a middle layer which can extend existing systems such as VTK [61]. Through the description of our design, we emphasize the key principles that ensure a correct implementation of the FPR abstractions in a parallel environment. These principles can also be applied to *in situ* systems that are aimed at enabling declarative and reactive programming, without adopting DIVA itself.

Our design provides four primary benefits:

Simple. Traditionally, in situ infrastructures employ callback functions to handle separated programming stages. Useful callback functions include initialization, per-timestep execution, finalization, and feedback loops [36]. As such, a single data dependency could be broken into multiple pieces that are controlled by interleaving control flows, making it hard to read and maintain. If an operation requires information from multiple timesteps, the handling of static storage will also be involved, making the implementation even more complex. Declarative programming simplifies these tedious and redundant low-level tasks by placing more of the burden on the tool developers. This allows the user to focus on specifying the results they desire. Meanwhile, reactive programming offers the ability to automatically coordinate data dependencies and propagate changes from inputs to outputs. This model is commonly used to greatly simplify the handling of time-varying signals, such as events triggered by human interaction. Since adaptive workflows similarly specify the reaction of a system to time-varying signals, we believe reactive programming is also a good solution for coordinating them.

Extensible. By providing a fully programmable interface and a low-level C++ API, DIVA allows flexible extension through the development of new custom modules.

Portable. The low-level API also makes the integration with existing visualization infrastructures easier, by only asking for a short binding implementation; this can typically be just one source file. Thus, DIVA can be used as a wrapper to enable declarative and reactive programming for these infrastructures. This also means that workflows written in DIVA for one infrastructure can be easily reused in a different infrastructure if the proper bindings are supplied

^{*}e-mail: qadwu@ucdavis.edu

[†]e-mail: taneuroth@ucdavis.edu

[‡]e-mail: oigouchkine@ucdavis.edu

[§]e-mail: konduri.adi@gmail.com ¶e-mail: ihchen@sandia.gov

^{*}e-man. jnenen@sandia.go

^Ie-mail: ma@cs.ucdavis.edu

for both of them.

Dynamic. DIVA's API resolves linking through dynamic loading; therefore, adding or updating linked libraries does not always require recompilation nor restarting. This feature can be useful for scientific simulations on HPC systems, because allocations for these simulations are usually limited; removing unnecessary restarts allows for more useful simulation work to be done and gives a higher chance for scientific discoveries.

In this paper, we first begin with a summary of related works. We then describe the principles and features of our language with a set of examples. We also provide a set of examples to demonstrate how our design meets the needs of *in situ* visualization and analysis, and how it supports our assertion that declarative and reactive models are good approaches for adaptive workflow management in this domain. Next, we discuss implementation details of our language. Finally, we showcase the use of DIVA to program an adaptive *in situ* workflow for a leading edge simulation code running on the Summit supercomputer.

2 BACKGROUND AND MOTIVATION

We begin with an overview of recent advances in reconfigurable *in situ* workflows, and a history of functional reactive programming. We then compare existing methods in our domain with the FRP model. Finally, we conclude with a discussion about how our approach is suitable for better assisting adaptive workflow design.

2.1 Reconfigurable in situ Workflows

We review recent research in reconfigurable in situ workflows from two categories that are particularly relevant to visualization: having a "human-in-the-loop" with a focus on improved interactivity, and automatically looking for regions of importance during the simulation. In the first category, many successful infrastructures for in situ visualization and analysis, such as Libsim [72] and Catalyst [4], support interactive exploration during the simulation. However, even with these infrastructures, tasks like searching for infrequent scientific phenomena can still be challenging, because scientists do not always know which aspects of the simulation to focus on. In the second category, many have attempted to automate the search for important regions for in-depth analysis, visualization, and storage [10, 46, 49]. Notably, recent works following in this direction usually involve defining indicator functions known as "in situ triggers" for characterizing features. These triggers can be domain-agnostic algorithms such as data reduction, aggregation, statistical analysis, and machine learning [7, 33, 40, 47, 77], or domain-specific routines that require special knowledge from domain-experts [11, 56, 67, 76]. Through this approach, a system could automatically focus resources on the most interesting phenomena from the simulation, but only if the triggers are well-designed. However, manually designing and implementing these triggers can be tedious (e.g., by directly working on an infrastructure's source code) or error-prone (e.g., misuse of algorithms). Tools to simplify the development and composition of in situ triggers into workflows are much needed. Recent work by Larson et al. demonstrates a flexible interface for creating in situ triggers in the ASCENT [31] infrastructure. Our work is inspired by this. However, with DIVA, we contribute a complete DSL for programming trigger-based dynamic workflows. In this language, fine-grained in situ triggers are automatically generated based on user-specified data dependencies and high-level constraints. This approach frees users from manually writing every trigger and allows them to create potentially better and more reliable workflows.

2.2 Functional Reactive Programming

Functional reactive programming (FRP) is a declarative programming paradigm for working with time-varying values. Particularly, FRP defines time-varying values as *signals*, which conceptually can be viewed as functions that include time as a parameter. In *in situ* workflow management, such *signals* can represent the outputs from a simulation [53]. Although there are many variations of FRP focusing on different applications, they all fall into two main branches: classical FRP [24] and arrowized FRP [48].

Classical FRP was first proposed for creating interactive animations. It introduced notations called *behaviors* (another name for signals) and *events*, to represent continuous time-varying values and sequences of time-stamped values respectively. Although initially focused on animation, it inspired many later works of broader scope due to its elegant semantics [20]. However, because it is a denotational model which does not restrict the length of a signal stream that can be operated on, classical FRP programs can have a high memory footprint and long computation times [20].

Arrowized FRP (AFRP) [48] aims to resolve the space and time leaks without losing the expressiveness of classical FRP. Instead of working with signals or similar notations directly, AFRP focuses on manipulating causal functions between signals, connecting to the outside world only at the top level [53]. However, programs written in AFRP can still suffer from issues like global delay or unnecessary updates, depending on their implementations [20].

Real-time FRP (RT-FRP) [70], event-driven FRP (E-FRP) [71] and asynchronous FRP (e.g., the original version of Elm) [21] are other variations developed to optimize classical FRP. RT-FRP introduced a two-tiered language design for reactive programming; It uses a closed, unrestricted language to give direct operational semantics, making it possible to measure computational expenses [70], along with a simpler and more limited reactive language for manipulating signals [70]. This separation makes it much easier to prove properties of RT-FRP, at the expense of expressiveness [20]. Similarly, E-FRP makes the assumption that signals are all discrete. This property makes it suitable for intensive event-driven applications, including interactive visualization [18, 43, 57-59]. Asynchronous FRP allows programmers to explicitly enable asynchronous event processing, and thus enables efficient concurrent execution of FRP programs. This ensures that the responsiveness of the user interface will not be affected by long-running computations [21]. Implementations of asynchronous FRP can also be found in many imperative languages through Reactive Extensions [1].

2.3 Dataflow Model for Visualization

There is a rich literature [9, 22, 23, 39, 42, 45, 51, 61, 65, 68] on using dataflow models to realize configurable visualization systems. In these frameworks, workflows are represented as simple pipelines or directed graphs, with nodes representing low-level visualization components (also called functions, filters, modules, or processors). Data is processed hierarchically as it flows through components to form a complete workflow [64]. Even though this method works very well for traditional post hoc scenarios, there is still room for improvements in terms of abstraction and efficiency when adaptive in situ workflows are considered. From the perspective of abstraction, these frameworks do not supply first-class representations for timevarying primitives. This makes the management of time-varying storage manual and tedious. From the perspective of efficiency, because in situ workflows are expected to be executed repeatedly for a large number of timesteps, lazy evaluation can help to avoid needless recomputation. However, many popular visualization frameworks lack system-wide support for lazy evaluation, leaving it to the developer to avoid unnecessary computation. This makes the quality of module implementations a more important factor for efficiency, and makes it difficult for novice programmers to implement efficient modules inside such frameworks.

2.4 Programmable Interfaces for Visualization

By directly incorporating low-level APIs (e.g., C++ or Fortran), users can always create visualizations and analyses using arbitrary algorithms, and fully utilize modern architectures for cutting-edge

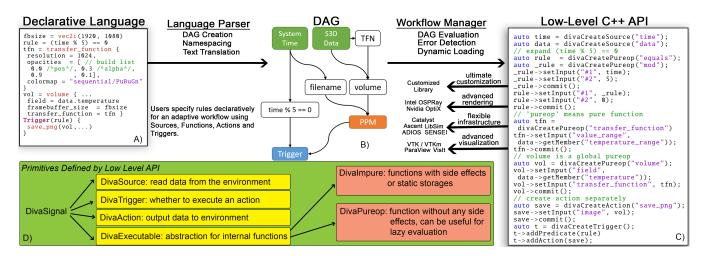


Figure 1: A DIVA program is processed through three layers. Users typically specify their program using the declarative interface (left); then the language parser will translate it into an internal DAG representation; this representation will then be interpreted into a low-level dataflow API for execution. A) A DIVA program computes a volume rendering for every 5 timesteps, and saves the rendering on disk. B) The same program in the DAG representation. C) The same program in the low-level API. Because the C++ API is not declarative, in part C), statements have to be executed in order. Moreover, because C++ does not track data dependencies automatically, all variables declared in C) should be wrapped by lifting operators (e.g., divaCreateSource). D) The hierarchy of primitives defined by the low-level dataflow API: All values in DIVA are signals; values depending on external inputs are sources; values returning to the environment are actions (e.g., a saved image file); triggers are special primitives that decide which actions to compute based on predicates; rest values are internal to the workflow and are represented by either pure (i.e., DivaPureOp) or impure functions (i.e., DivaImpure).

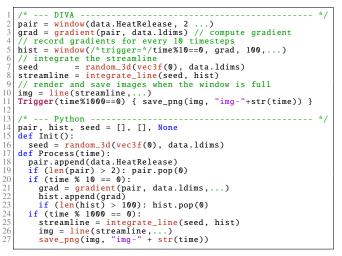
techniques such as ray-tracing [69], and heterogeneous parallelism. However, novice programmers are prevented from doing so due to the complexity and difficulty in low-level programming. End users often prefer to compose the low-level modules using high-level dynamic languages like Python; and in this field, almost all major in situ infrastructures provide this support, by employing one of two approaches [34-36]. In the first approach, the capabilities are exposed through wrapped objects or functions that can be configured using Python [3, 4, 16, 30, 44, 72]. In the other, the infrastructure embeds user-supplied high-level codes directly into its pipeline, providing users with direct access to the simulation data and the ability to analyze natively in the high-level language [5, 36]. However, Python has a major drawback when it comes to supporting FRP features. Because Python is designed for a much wider range of tasks than just programming adaptive in situ workflows, it makes fewer assumptions about data abstraction and data dependencies; the implementation of features like lazy evaluation and dependency tracking often rely on wrapper functions and special inheritance patterns, which can be complicated to use and increase the verbosity of the program.

DSLs use specialized grammars that are tailored for particular domains. Several DSLs have been designed for visualization and analysis over the years, including Data Explorer [38], Scout [41], Diderot [17, 28], ViSlang [54], Mathematica [74], MATLAB [66] etc. Such DSLs enable users to express programs in domain-specific semantics that they are familiar with, and hide more complicated implementation details [64]. A well-designed DSL can greatly simplify the learning process. A declarative design can further improve a DSL by introducing only declarative grammars for system configurations. It also improves usability by not only providing a large number of domain-specific built-in functions, but also introducing new language abstractions to hide underlying execution models [59]. Because FRP itself is a variant of declarative language (for handling time-varying data), implementing FRP abstractions using a declarative DSL approach is straightforward. Several information visualization toolkits have already adopted declarative [12, 13, 73] and reactive [57,58] grammars for specifying visual encodings. Some of these have become very popular due to their ease of use and flexibility. These works have inspired further work to improve usability in other areas, including high-performance information visualization systems [32], and for the configuration of complex GPU shader

pipelines for advanced volume rendering of scientific data [64]. Our work is inspired by these existing designs; however, we focus on using a declarative and reactive programming model to correctly handle parallel *in situ* visualization and analysis workflows.

2.5 Motivation for a New Language

Since it takes time to learn a new programming language, embedding our system within an existing language would have some advantages. However, we believe that, for programming complicated adaptive in situ workflows, DIVA is favorable, for the following reasons: First, data abstractions introduced by FRP enable not only declarative programming, but also systematic tracking of time-varying data dependencies. They also create a new way for users to think of the data (in terms of time-sequences rather than iteratively updated values). Implementing this abstraction in C++ or Python is possible, but that would require a new set of data wrappers to be provided. When programming using this API, they would also need to manually lift all the native types provided by the host language using these wrappers. This process alone might significantly steepen the learning curve. Second, workflows programmed in DIVA might be more flexible, better to optimize, and easier to debug, as the language compiler knows exactly what users write. For example, in a well-defined DSL environment, users only need to write down essential information about the algorithm; technical details such as updating the DAG and building the dependency diagram can be computed automatically. Thirdly, code written in an actively developed DSL can be more portable across platforms, because DSLs are usually simpler and easier to port (due to their limitations and simplicity). For example, it is fairly easy to rewrite our DIVA system in JavaScript and enable web-based visualization. However, porting Python or C++ to browsers can be challenging compared to rewriting the workflow entirely. Finally, we do observe that it might be difficult to fully understand DIVA's methods, but we believe that these difficulties are coming from the new abstractions and concepts being introduced, rather than the syntax of the language itself. DIVA's syntax shares many features from popular high-level languages including Python and Lua. Thus, understanding DIVA's syntax should not be a challenging task.



Listing 1: Code comparison between DIVA and Python. Both programs render streamlines that are computed by integrating the gradient of an input volume. By introducing the signal abstraction, DIVA can automatically remember the dependencies between variables. As it is optimized using lazy evaluation, it only updates variables that are changing. Therefore, users do not have to explicitly compute the "seed" in the initialization function. The signal abstraction also automatically create static storage, such as "pair" and "hist", nor to manipulate them iteratively. Note that, syntactically DIVA can use either "{}" or "()" to declare nodes with parameters.

3 THE DIVA LANGUAGE DESIGN

We implemented DIVA through three components (as shown in Fig. 1): the language parser for translating DIVA workflow specifications into DAG representations; the workflow manager, which is in charge of managing system resources, detecting logical errors, and making decisions about how to execute the DAG; and the C++ dataflow API for executing low-level components. In this section, we illustrate our design decisions using examples and discuss the advantages of these choices through comparison with code written in other models.

3.1 Signal Abstraction

DIVA adopts the abstraction of signals from classical functional reactive programming (FRP) to represent time-varying values. Specifically, a signal of type α in DIVA, denoted as $\hat{\alpha}$, can be considered as a function from time to typed values:

$$\widehat{\alpha}$$
: Time $\rightarrow \alpha$

In this formulation, time refers to the simulation timesteps, and can be represented as a non-negative integer. For the sake of simplicity, DIVA assumes that all variables are treated as signals implicitly and they cannot be deleted or modified upon construction. DIVA also assumes that new signals can only be created using pure functions, where the "pureness" is defined conventionally through referential transparency [55]. However, there are two exceptions, which are discussed in Sect. 3.3. These simplifications make it possible for our system to systematically resolve the evaluation schedule for signals and correctly update their values when necessary. It also allows users to process time-sequences directly using array-like operations rather than using iterative algorithms. The effects of the signal abstraction in DIVA can be found in Listing 1, where a code comparison between DIVA and Python is demonstrated. In this example, both programs compute and render streamlines from volume gradients. Because the computation of gradients and streamlines requires data from multiple timesteps, developers need to explicitly manipulate multiple static storages; to avoid unnecessary recomputations, they should also seed streamlines in the initialization function (e.g., Init). In DIVA, these steps are not needed. Users of DIVA can therefore focus less

on program execution (e.g., when to generate the initial seedings for streamlines) and more on the specification of desired results (e.g., seedings are the initial condition for the line integral).

3.2 Language Structure

Similar to RT-FRP, DIVA uses a two-tier language design to provide tractable notions of computational costs. In particular, there is a restricted reactive language for declaratively manipulating signals, and an unrestricted low-level imperative API for implementing details of the reactive abstraction.

The reactive language is a combination of classical FRP abstractions and the dataflow model used by VTK for constructing visualization pipelines. However it enriches the use of directed acyclic graphs (DAGs) and expression of the data flow through sourcefilter-mapping, by replacing variables with signals. This enrichment makes DIVA's reactive programming interface more suitable for writing components that require inputs from multiple timesteps, because users are freed from the manual handling of global or static storage. Moreover, in this language, signals and their dependencies are conceptually represented as parameterized nodes and directed links. Based on the location of a node in the DAG, nodes are classified as a source, function, or action. Sources are root nodes in the graph for representing predefined signals (e.g., simulation outputs) that initiate data flows. Functions are internal nodes requiring both inputs and outputs for computing intermediate values within the workflow. Because all values in DIVA's declarative interface are signals, *functions* are essentially constructors for signals. As a result, most functions cannot produce side effects. Actions are terminating nodes in the graph, defining how the workflow interacts with the external environment. They are generalizations of VTK's mappers, because they can not only map visualizations to display devices, but also conduct tasks like data storage and *in situ* steering¹. They do not return values back to the workflow, and their implementations are expected to have side effects. In addition to the three categories mentioned above, DIVA also introduces a special type of node — triggers, which are higher-order² functions for signals of the following type:

Trigger
$$A$$
: (bool, A) \rightarrow Maybe A

where A refers to an *action* and Maybe A represents a type that can return either A or nothing. They are responsible for dynamically controlling the execution of *actions* based on a Boolean signal: when the signal evaluates to true, the corresponding *action* is returned and executed; signal evaluates to false, the execution is skipped. Fig. 1 A, shows an example where the "temperature" field is rendered once every 5 timesteps.

The low-level interface for DIVA is implemented in C++ following a traditional dataflow model. This API is intended for implementing all the reusable modules that can be called from DIVA, rather than implementing the workflow itself. Therefore, users of DIVA do not have to directly use this API. Because the low-level API is not declarative, code translated into this API is much more verbose (Fig. 1C) compared to code written declaratively (Fig. 1A). However, with this API, DIVA can be extended easily and flexibly, by taking advantages of three features. First, the low-level runtime provides a simple but generic command pattern API. Although simple, this API fully implements the reactive language's abstractions. For example, generic classes for signals, actions, and *pure* and *impure functions* are provided for programming different features as shown in Fig. 1D; within those classes, developers can manipulate parameters and return outputs using functions like

¹A feedback mechanism that allows the modification of the simulation based on visualization/analysis outputs while the simulation is running.

²A function that takes one or more functions as arguments or returns a function as its result.

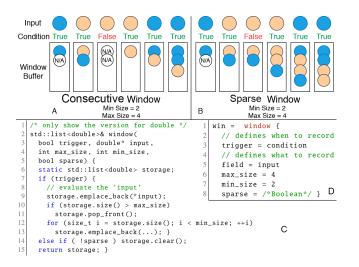


Figure 2: Window is a special *impure function* that collects a signal's historical values into an array at timesteps where the "condition" is true. A window can be constructed in sparse mode, or consecutive mode. In the sparse mode, up to "max_size" values are collected, even if they appeared sparsely in time. In the consecutive mode, values that appear within an interval of consecutive time steps are recorded, and when the condition becomes false, the window is cleared. As an example, a consecutive window can track history for a period time while a phenomena is active, then automatically reset when the phenomena subsides, and then begin tracking the phenomena again if it becomes active another time.

setInput, addAction, and setValue. Second, the API provides detailed indications about different stages of computation, such as initialize, and commit (which resolves types), and execute. This allows developers to better optimize their implementations when they are trying to extend DIVA with customized modules. However, this does not mean that all of the low-level development burdens are thrown to developers; instead, features such as lazy-evaluation (see Sect. 4) are implemented system wide in base classes, making them immediately available to all extensions. Third, through our low-level API, developers can register custom types, that can then be used directly in the reactive language layer. This helps make it easier to integrate existing, well-optimized libraries. Finally, integrating new packages into DIVA often does not require a full code recompilation. Instead, DIVA uses dynamic loading to look for registered function symbols during runtime. As long as the added packages are compiled with the core components and placed correctly, the DIVA back-end system can automatically link them, even while the simulation is running. This allows incremental development without restarting a simulation.

3.3 Impure Functions

As discussed previously, programs written in a classical FRP language have unrestricted access to a signal's history. Thus a correct classical FRP implementation will have to to track all signal values automatically. Although this method has been proven to be fast enough for many applications [70], holding extra copies of the simulation data might not be suitable for *in situ* workflows because of the high expense in terms of processing time and memory. To solve this issue, DIVA introduces dedicated *impure functions* for accessing values across time, while other *functions* are prohibited from doing so. Those *impure functions* are specialized constructors for creating stateful signals (i.e., signals with static storage). During the construction, a finite description of the computational cost must be presented explicitly, which effectively prevents users from accidentally writing programs that can produce large memory footprints unexpectedly.

Window is one of the *impure functions* provided by DIVA, which creates array-like signals by collecting values over a range of time. Its definition (shown in Fig. 2) takes a target signal (field)

as the value source, a Boolean condition (trigger) controlling when a value is saved, and a pair of integers (max_size and min_size) defining the shape of the output array. For example, window(true, isosurface, 10, 5) retains up to 10 isosurfaces at a time, where for *every* time step a new isosurface is pushed into the window; if the number of time steps computed falls between 5 and 10, then the size of this window is the same as the time step number; if the current time step is less than 5, then the size of the returned array will be 5 with the values in the empty space undefined. Such an operation offers support for time-sequence analysis, as well as backward feature tracking. For example, once a feature is detected, the data histories associated with the feature that are within a window can be retained. To provide the user with the ability to express complicated triggering conditions on events, DIVA also adopts operations from the field of temporal logic programming [25]. By abstracting commonly used Boolean operations on time sequences, they can simplify the expression of time-varying control logic. For example, until(x) creates a Boolean signal which will be true until the first true occurrence of x. Similarly, after(t>1700) defines a signal whose value is false until the first time where t is above 1700, and true thereafter. Other basic operators include first(x), firstN(x,n) and afterN(x,n). In addition to these basic temporal logic operations, developers can also implement other customized impure functions. However they must be inherited from a dedicated base class and evaluated once for each timestep to ensure correctness.

3.4 Global Functions

Operations involving global synchronizations are very common for data-distributed simulations and visualizations. Although it is not completely obvious, it is important for lazily evaluated workflows to have them explicitly handled to ensure program efficiency and correctness. There are two reasons. Firstly, in a typical classical FRP language with lazy evaluation enabled, computations might be accumulated until they are needed. If computations are parallelized, there might be many synchronizations dispatched in a relatively short period of time, making the system less balanced and more difficult to be optimized toward overall throughput. Secondly, mainstream parallel programming interfaces typically implement global synchronization as matching calls (e.g., MPI_send, MPI_recv) that should be executed simultaneously on multiple ranks. However, in a lazily evaluated workflow, this requisite can easily be violated because the program control flows are data-driven; programs running on different ranks do not always yield the same data values and control flows.

DIVA resolves this problem by classifying *functions* as global or non-global. *Global functions* by definition are those whose execution

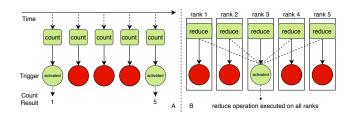


Figure 3: Special rules are used to control the evaluation of *impure functions* and global synchronizations. A) As a minimal example, the *impure function* "count" increments an internal counter automatically for each timestep. Because of that, the execution of this operation cannot be simply skipped, even if its output values are not immediately required. B) *Global function* "reduce" reduces values across multiple MPI ranks, and its result is then used by another operation. In this case, this operations is activated (by a triggered action on that rank), all instances of "reduce" shall be executed to ensure correctness.

involves global synchronizations. Thus reductions and distributed rendering are global functions. We refer to these as "intrinsic" global functions. Additionally, if a global function (g) is being used as an input to a normally *non-global function* (f), then the result $(f \circ g)$ is also a *global function*, because its evaluation would potentially invoke g. This behavior can also be understood as building dependencies across ranks as shown in Fig. 3B, where an activated function (A) is pulling data from an intrinsic global function (B). This makes A a dependent of all Bs (e.g. on each rank). Therefore, all the instances of B should be evaluated, even if only one instance of A needs to be evaluated. This is an example of the second type of global functions, which we refer to as inherited global functions. Different from impure functions, a global operation can sometimes still be evaluated lazily, because the entire program will be correct, as long as they are evaluated in unison on all ranks. Thus, both *pure* functions and impure functions can be global functions. Though being important for performance and correctness, in DIVA, the computation of "globalness" is totally transparent to users. Intrinsic global functions can be developed using DIVA's lower level API by calling parent constructors (e.g., DivaImpure or DivaPureop) with certain flags. If these flags are specified, parent classes will pass MPI handlers (initialized by the simulation) to their children. In contrast, inherited global functions can only be identified once the workflow has been composed. In this case, DIVA will traverse the DAG and propagate "globalness" at runtime by marking descendants of intrinsic global functions as global as well. Because the definition of a signal in DIVA cannot be changed after compilation, its "globalness" only needs to be checked once for each workflow.

4 IMPLEMENTATION DETAILS

4.1 Language Parser

The DIVA runtime translates a declarative and reactive DIVA code into an internal DAG representation using a parsing algorithm developed from scratch. In particular, the parser first scans through the program and constructs a namespace object for signals. If a signal value is defined using an inline expression, each operator used in the expression would create a separate namespace entry. This design makes it easy for the system to only re-evaluate signals whose values have been changed. Once the namespace has been built, a DAG representation can be easily constructed and validated. In particular, the parser checks for "cycles". A cycle means that two graph nodes are dependent on each other. Because DIVA does not allow variable rebinding at runtime, this structure can produce non-executable workflows. The parser also performs a topological sort on the DAG and computes a unique evaluation order for graph nodes. This effectively prevents the appearance of temporary inconsistencies in the DAG (i.e., "glitches"). Thus, a node can be evaluated if and only if all of its dependencies are up-to-date. After this, the DAG is sent to the workflow manager for execution. Listing 2 demonstrates how the DIVA parser should be used by the simulation in a nutshell.

4.2 Workflow Manager

The workflow manager is the component for evaluating the constructed DAG. For every timestep, it is invoked once by the simulation to execute an iteration of the workflow (see Listing 2). The workflow manager optimizes the execution following the lazy evaluation principle, by deferring the evaluations of computations until their results are absolutely needed. Additionally, it also implements a value caching mechanism, which avoids repeatedly executing the same computation [62]. (Details about how different signal types are cached can be found in Sect. 3.3.) Specifically, at each timestep, the workflow manager evaluates the DAG through the following four passes.

First, the workflow will try to reinitialize the execution environment and reload dynamic libraries if necessary. This step is intended to support programmers who wish to incrementally develop and

```
1 map<string,diva_source_t> sources; Language lang; ...
2 void Init(int tstep, double time, double* ...) {
3 sources["data"] = divaSourceCreate("data");
4 lang.parse("case-study.diva",...);
5 }
6 void Process(int tstep, double time) {
7 sources["data"]->addData("geom", GeomInput(...));
8 for (auto f : sim.fields())
9 sources["data"]->addData(f.name(), FieldInput(f));
10 sources["data"]->addData(f.name(), FieldInput(f));
11 /* code executed by the workflow manager */
12 lang.setSources(step, sources);
13 for (auto v : lang.getAllImpures()) v->evaluate();
14 for (auto v : lang.getAllTriggers()) v->evaluate();
15 }
```

Listing 2: Pseudocode demonstrating how DIVA is integrated into S3D. In particular, two C++ functions are introduced in S3D for initialization and *in situ* processing. Because we do not change workflow specifications while the simulation is running, the parsing process is written in the Init routine. Since *sources* are essentially inputs to the workflow, they are updated (with fields passed as pointers) for each timestep. After that, DIVA's workflow manager is invoked to evaluate *impure functions* and *triggers* respectively.

verify their ideas, without shutting down the simulation entirely. However, as shown in Sect. 3.3, if workflow specifications are never changed, repeated reinitialization is carefully avoid.

Then, it starts evaluating all of the *impure functions* that appear in the workflow. Even though they are internal computations, they need to be handled separately because they are allowed to produce sideeffects, such as mutations of static states. Processing them using lazy evaluation might lead to incorrect results. For instance, the count operation shown in Fig. 3A computes the number of timesteps that have gone by, by maintaining a counter locally; however, if the evaluation was skipped in a previous timestep, the value returned from the operation would be wrong when it is needed. Thus, to ensure the correctness of the program, these impure operations should be processed eagerly.

After having all impure internal components evaluated, DIVA will then move to impure external nodes — *actions*. Particularly, DIVA assumes that, in a DAG, only paths ending in *triggers* are meaningful, and all the other paths can be skipped. For example, the process of rendering can be skipped for some timesteps if the rendered image is not eventually saved in the current timestep. However, data storage processes should always be executed for each timestep, since they permanently save files to disks. Such a prioritized evaluation is correct because a workflow in DIVA can only produce side effects to the environment through *actions* and *impure functions* (but *impure functions* are already handled in the previous step).

Finally, to avoid repeated evaluation of unused operations, DIVA also maintains a caching table to track pure *functions*' most recent input parameters and values. If none of the inputs are changed in the current timestep, then the evaluation of a pure *function* can be short-circuited. Notably, because users do not directly specify the execution order for all programs, DIVA also implements the same short-circuit mechanism internally for Boolean operations. This effectively allows Boolean expressions like "x and y" to terminate earlier without computing y when the result of x turns out to be false. This is a crucial feature for implementing multi-level triggers, because these triggers are typically designed by having expensive analyses guarded by some looser but cheaper constraints (e.g., y is being guarded by x in the expression mentioned above); computing the Boolean value after evaluating all input variables would defeat the purpose of multi-level triggers.

5 CASE STUDY: ANOMALY DETECTION IN S3D

In this section, we show a real visualization and analysis workflow for combustion simulations implemented using DIVA. Particularly, we begin with a review of the simulation and the anomaly detection algorithm. Then we explain the workflow with example codes and comparisons. Afterwards, we describe how we establish benchmarks on the Summit supercomputer. Finally, we conclude with benchmark results and discussion.

S3D is a scalable, reacting, compressible flow direct numerical simulation (DNS) solver, which is extensively used to simulate key combustion phenomena relevant to internal combustion and gas turbine engines [27]. The code solves the conservation equations for mass, momentum, energy, and chemical species at each grid point of a computational mesh, and over several hundreds of thousands of time steps. At extreme scale, the volumetric data (comprised of the velocity field, pressure, temperature, and mass fractions of about 10 to 110 chemical species) generated from each simulation runs into several terabytes, often overwhelming the I/O bandwidth and storage allowance. Therefore, the output is usually reduced by saving to disk at a significantly reduced temporal frequency. However, at this reduced frequency, the data often misses transient dynamics of exponential processes, such as auto-ignition that are essential for understanding the combustion phenomena. In many situations, events such as auto-ignition appear in highly localized regions of space and/or time. Hence, in situ algorithms and workflows that capture the events of interest are being developed to intelligently guide the saving of data and reduce the storage costs [2].

5.1 Case Overview

For the demonstration and evaluation of our system, we simulate a turbulent premixed auto-ignition problem that is relevant to homogeneous charge compression ignition (HCCI) and stationary gas turbine engines [60]. Some of the features of interest in analyzing such simulations are the conditions surrounding the ignition events and flame surfaces. Analyzing these conditions enables scientists to better understand the combustion phenomena, including the flame stabilization mechanisms, fuel consumption rates, and pollutant formation.

The inception and growth of ignition kernels in the premixed reactants occur rapidly and, are often missed in coarse check-pointing of the data. The anomaly detection algorithm mentioned earlier can be used to identify an ignition kernel at its inception, as it can be defined as an extreme event. The algorithm first computes feature moment metrics (FMM) for different sub-regions or MPI ranks of the computational domain. The FMMs are measures in state space that contain the signatures of the extreme events. They also quantify the contribution of different chemical components towards the ignition kernel formation. By comparing the FMM in the current MPI rank with the average FMM among all MPI ranks, we obtain a spatial anomaly metric (m_1); by comparing this FMM with its values from the previous timestep, we obtain a temporal anomaly metric (m_2). If any of these two metrics are large enough (e.g., $m_1 > 0.7$ or $m_2 > 0.7$), an anomaly (i.e., auto-ignition) can be pronounced.

However, this anomaly detection algorithm has two major drawbacks. Firstly, its complexity is bounded by $O(mn^4)$, where *n* is the number of chemical components and *m* is the number of grid points in the sub-domain. Thus, executing the algorithm can be quite expensive. Secondly, the algorithm can detect an auto-ignition event when it first occurs, but cannot be used to predict the event *a priori*. Hence, when an auto-ignition is detected, features leading to it, which need to be visualized, would already have disappeared. Other methods such as CEMA [37, 63] or noise-tolerant trigger detection [11] are also suitable for this problem and are interchangeable for anomaly detection in our study; but because they also suffer from the similar drawbacks, principles for designing workflows with them should remain the same.

5.1.1 Defining Pre-Filters for Auto-Ignition

Because the cost of running the anomaly detection is currently high, pre-filtering (i.e., ad-hoc conditions) can be introduced to identify candidate regions and timesteps in advance. There are two well established pre-conditions of auto-ignition. First, there is a delay time associated with the formation of ignition kernels, which can be estimated from simple *a priori* calculations. In our particular simulation setup, the delay time is about 200 timesteps. Second, an ignition is accompanied by "heat release" events, which can be computed *in situ*. In particular, the phenomena of auto-ignition can only happen when there is a big enough "heat release", which is characterized locally by the maximum value within an MPI rank. With this understanding, we formulated our pre-conditions:

1	/* a) DIVA*/
2	hr = max_array(data.HeatRelease)
	wait = (time > 200) && (time % 40 == 0)
4	adhoc, valid = $hr > 1E-3$, wait && adhoc
5	/* b) C++ Naive*/
6	<pre>double hr = max_array(data.data("HeatRelease"));</pre>
7	bool wait = (time_i > 200) && (time_i % 40 == 0);
8	bool adhoc = $hr < -1E-3;$
	<pre>bool valid = wait && adhoc;</pre>
10	<pre>/* c) C++ with Lazy Evaluation*/</pre>
11	<pre>bool flag = true; // define a callback function and a flag</pre>
	<pre>auto hr = [&]() { // to ensure the computation can only be</pre>
13	<pre>if (flag) { // done once per time step.</pre>
14	<pre>flag = false; return max_array(data.data("HeatRelease"));</pre>
15	} return 0.0;
16	
	<pre>bool wait = (time > 200) && (time % 40 == 0);</pre>
	<pre>bool adhoc = valid = false; // avoid re-evaluating</pre>
19	<pre>if (wait) { adhoc = hr() < -1E-3; if (adhoc) valid = true }</pre>

In this example, three code snapshots are displayed. Part a) is written using DIVA, part b) is a similar implementation in C++, and c) is an optimized version in C++ following the lazy evaluation principle. Clearly, program b) is very simple, but less efficient compared to the other programs, because in program b), the maximum "heat release" value will be calculated for every timestep. However, this value will be useful only when the Boolean variable "wait" becomes true. In part c), lazy evaluation is correctly implemented, at the expense of creating a callback function and using nested control flow.

Although we have only demonstrated one particular case here, the same principles apply to *in situ* analyses with multi-level filtering mechanisms in general. These types of workflows can be programmed in DIVA more concisely without compromising performance due to redundant computation.

5.1.2 Automatic Synchronization

To correctly detect the anomalous events, we need to compare the feature moment metrics across time, and across the decomposed domain. To achieve that in a traditional language, static storage and standard MPI synchronizations can be used as shown in Listing 3B. Since metrics m1 and m2 are only used once in a while (when variable "valid" is true), we can further optimize the code by guarding anomaly_detection, MPI_Allreduce and the manipulation of "fmm_win" with an if-statement. However, part of this optimization is in fact wrong, as the value of the Boolean condition "valid" can be different on different MPI ranks. Clearly, if one of the program instance enters a different branch, the execution of the simulation will be blocked infinitely. To fix this issue, we have to synchronize the Boolean condition before entering the associated control flows (by calling the globalSync function in Listing 3B). As we can see in practice, correctly deciding which control flow conditions to synchronize can be tedious and error-prone. In DIVA, with the help of its built in dependency tracking, synchronizations are automatically handled, which results in a much simpler code (as shown in Listing 3A). These details are discussed in Sect. 3.4.

5.1.3 Establishing Short-Term Memory

The second drawback of the anomaly detection algorithm, is that it cannot predict anomalies in advance. Because this algorithm is also expensive, it is undesirable to execute the algorithm at every timestep. Therefore, it is very likely that when an auto-ignition event is found, the regions of interests for visualization have already been missed. One approach to solve the issue is to aggressively memorize all features of interests from candidate regions in a limited RAM space. Within these candidate regions, the anomaly detection

```
Code A
                                         -- DIVA ---
       features = [data.H2, ..., data.temperature]
/* feature moment metrics */
     /* feature moment metrics */
fmm = anomaly_detection(features);
fmm_hst = window(/*trigger=*/valid, fmm, 2, 2)
fmm_avg = reduce_avg(fmm)
/* determine anomaly */
m1 = anomaly_metrics(d1=fmm, d2=fmm_avg)
m2 = anomaly_metrics(data=fmm_hst)
anomaly = valid && (m1 > 0.7 || m2 > 0.7)
Trigger(valid) { print("m1=" + str(m1)) }
Trigger(valid) { print("m2=" + str(m2)) }

 6
                         Code B -
                                                 C++ with Lazy Evaluation
      /* ---- Code B -- C++ With Lazy Evaluation -------
inline bool globalSync(int ret,...) {
    MPI_Allreduce(&ret,&ret,/* MPI_BOR...*/); return ret;
16
      }
                                 es = vector<double*>{...};
= deque<vector<double>>();
       auto features
      auto fmm
      static auto fmm_avg = vector<double>(features.size());
static auto fmm_win = deque<vector<double>();
if (globalSync(valid,...)) {
fmm = anomaly_detection(features);
20
21
22
24
25
26
           // compute the average fmm per-feature across ranks
       if (valid) {
27
28
           fmm_win.push_back(fmm);
if (fmm_win.size() > 2) fmm_win.pop_front();
29
30
       // spatial metrics (m1) & temporal metrics (m2)
      // spattal metrics (may = 0;
double m1 = 0, m2 = 0;
if (globalSync(valid,...)) m1=anomaly_metrics(fmm,fmm
if (valid) m2=anomaly_metrics(fmm_win[1],fmm_win[0]);
31
                                                                                                                           fmm_avg);
```

Listing 3: Code comparison between DIVA and C++. Both codes compute the anomaly metrics by comparing the local FMM with the average FMM among all MPI ranks and with its values from the previous timestep. In the C++ version (B), because the MPI operation is guarded by a if-statement, the Boolean condition needs to be manually synchronized; however, because the manipulation of "fmm_win" is local to the MPI rank, its control flow condition should not be synchronized. This creates complexities for users. In the DIVA version (A), global synchronization steps for control flows are automatically handled, which not only makes coding easier, but also reduces the chances for mistakes.

algorithm can then be executed. If an auto-ignition is found in a region, recorded data in the short-term, within this region, can then be transferred to long term storage, or be used to trigger downstream visualization and analyses for causality studies. This approach is practical, because data stored in short term memory are limited, and local to a small number of regions. We also consider this solution superior to traditional fixed policy workflows, because it can capture pre-ignition events correctly with much less overhead. In DIVA we can implement this method using the window function:

```
1 stats_ftr_avg = avg_list(features) // pre-ignition
2 stats_ftr_min = min_list(features) // statistics
3 stats_ftr_max = max_list(features)
4 len = 40 /* record 40 steps */
5 recorded_avg = window(stats_ftr_avg, len)
6 recorded_min = window(stats_ftr_max, len)
7 recorded_max = window(stats_ftr_max, len)
8 Trigger(anomaly) { save_statistics(data=recorded_avg,...)
9 save_statistics(data=recorded_min,...)
10 save_statistics(data=recorded_max,...) }
```

5.1.4 Temporal Logic to Simplify Control Flow

One important objective for this workflow is to correctly visualize spatialtemporal regions near the ignition kernel. In particular, this means we should not only identify the period of time before the autoignition, but also start downstream visualizations after the ignition (as illustrated by Fig. 5). Formally, the pre-ignition period is defined as the time interval between the appearance of the first pre-filtering condition till the appearance of anomaly; while the post-ignition interval starts with the anomaly and lasts for a fixed period of time. However, because the pre-filtering condition is data-driven, it will naturally fluctuate as the data changes, making it unsuitable for defining continuous time intervals. In DIVA, these sort of problems are handled by built-in temporal logic functions (as discussed in Sect. 3.3). Particularly, DIVA provides functions like "switch"³ and

³The "switch" function is analogous to the behavior of a light switch, which can be turned on by the first "on" condition if it is currently off, and

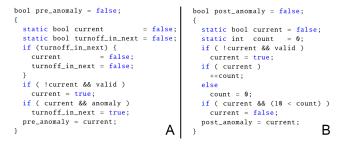


Figure 4: C++ implementations of the pre-anomaly condition and the post-anomaly condition. The pre-anomaly phase is defined as a continuous time interval from the moment that variable "valid" becomes true, to the moment that variable "anomaly" becomes true. The post-anomaly phase is defined as a fixed length interval since "anomaly" becomes true. As we can see, defining continuous time intervals from time-varying values can be tedious in traditional languages such as C++.

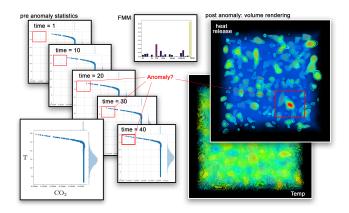


Figure 5: Visualizations generated by our case study workflow. The maximum heat release value and feature moment metrics are used to jointly detect the phenomena of auto-ignition. To study the cause of auto-ignition, we visualize the statistics of raw variables computed by the simulation (e.g., chemical mass fractions, temperature, pressure, etc.) using joint PDF plots (at time steps leading up to, and till the moment of ignition). We use volume renderings of important characteristic variables (e.g., the heat release and temperature), to visualize the geometry and scales of the phenomena. We also generate histograms of the feature moment metrics as guidance for statistical analysis.

"countN" to convert discrete events into intervals. Therefore, we can easily define our pre-ignition and post-ignition events as in the following example:

```
pre_anomaly = switch(on = valid, off = anomaly)
post_anomaly = countN(since = anomaly, n = 10)
/* render the heat release after anomaly for 10 steps */
vol = volume(field = data.HeatRelease,...)
Trigger(post_anomaly) { save_ppm(vol, "img-" + str(time)) }
```

Although these temporal functions look very simple in DIVA, they can be fairly hard to implement in traditional languages like C++ or Python (examples are shown in Fig. 4). This is not only because the manipulation of static storage can be complicated, but also because those functions should only be executed once globally for each timestep. In other words, these functions can only be implemented with separately maintained local storage (as DIVA does internally).

5.2 Benchmark

To effectively estimate the performance of our system, we compare our adaptive workflow implemented using DIVA with a reference implementation of the workflow written directly using C++. We optimized this reference implementation following almost the same principles we used to optimize DIVA, except we did not implement

```
turned off by the first "off" condition if it's currently on.
```

Table 1: Benchmark Results.

Grid Size	128^3	128 ³	256^{3}	256 ³	512^3	512 ³
Size per Rank	32^3	16 ³	32^{3}	16 ³	32^3	16 ³
Nodes	2	16	16	128	128	1024
Proc per Node	32	32	32	32	32	32
GPU per Node	1	1	1	1	1	1
Time _{Ref} (s)	1677	769	2321	980	2959	1444
Time _{DIVA} (s)	1639	779	2194	959	2607	1388
% Difference	-2.3%	1.3%	-5.5%	-2.1%	-12.0%	-3.9%

lazy evaluation for trivial computations, such as simple arithmetic. We believe our reference implementation is an efficient implementation of the workflow when no additional parallelism layers are involved. For modular operations, such as the computation of the feature moment metrics, identical implementations are used in both workflows.

To verify our assertions, we compiled both implementations with a CPU-based S3D using identical compiler settings (PGI compiler in the default "Release" mode configured by CMake), and benchmarked them across 6 different configurations on the Summit supercomputer. For each configuration, we ran both implementations once. For each configuration, we placed 32 MPI ranks on each compute node with 2 IBM POWER9 22-core CPUs, and requested 1 NVIDIA Volta V100 GPU for each compute node. The GPUs were used by the GPU-based volume rendering library integrated in DIVA. The number of compute nodes we requested for each configuration can be found in Table 1. To qualitatively assess our implementation, we measured the overall workflow processing time for each run by summing the workflow time of each timestep. In particular, we profiled each run for exactly 220 steps, starting from a middle timestep checkpoint, and we guaranteed that: first, runs of the same configuration shared the same checkpoint file; second, auto-ignition was happening by the end of each run; third, visualizations and statistics produced by runs from the same configurations agreed with each other.

Our results are summarized in Table 1 with all timings measured in seconds. We found that, for most of the configurations, the two implementations indeed have similar performance, with low percentage differences⁴ ($<\pm 6\%$). The 512³-32³ configuration was the only exception. For this configuration, we found that DIVA was able to compute FMM faster consistently (by about 10 seconds). However, we did not observe the same phenomenon with other configurations, which suggests that the discrepancy might not be due to DIVA.

6 **DISCUSSION**

There are other potential uses of DIVA beyond programming dynamic in situ workflows. For example, the current implementation of DIVA does not directly support in transit workflows. But we could implement a workaround by developing customized sources and actions using in transit libraries such as ADIOS [35] and having two workflows running alongside each-other either synchronously or asynchronously. In particular, this would require one workflow to be running in situ and writing data using an ADIOS action, and the other workflow to be running separately and receiving data using a connected ADIOS source. With a focus on expressiveness and code portability, DIVA can also be used as a thin layer to enable declarative and reactive programming on existing frameworks like ALPINE [30] and SENSEI [5]. This would also allow users to port codes across different platforms and frameworks. For example, one could use the native DIVA implementation and a GPU workstation to develop and debug a workflow, and then directly deploy the

⁴ Percentage Difference (%) = $\frac{\text{Time}_{\text{DIVA}} - \text{Time}_{\text{Ref}}}{\text{Time}_{\text{Ref}}} \times 100$

program to a supercomputer that features a CPU-based rendering infrastructure such as VisIt-OSPRay [75].

There are several limitations for DIVA. First, DIVA currently does not support programming loops and functions directly in its declarative interface. If these are needed, the low-level API needs to be used. Second, DIVA's current implementation has almost no restrictions for module implementations. Bugs in the extension (e.g., accessing MPI handlers from non-global functions) can be very hard to find and can lead to unpredictable results as workflows are highly dynamic. Third, DIVA currently allows global functions to communicate directly through MPI. While modules can also exploit heterogeneous parallelism internally (e.g., through VTKm worklets), there are remaining challenges towards optimizing data and resource management (e.g. through dynamic resource allocation). To solve this problem, a more generic low-level data parallel programming environment such as Legion [52] would be needed. Fourth, integrating DIVA into simulations currently requires changes to be made to the simulation code because the simulation would be in charge of creating DIVA sources. This could result in many different customized versions being maintained for only slightly different purposes. Thus a simpler and more generic way for the simulation side integration would be very helpful. Finally, DIVA's current design prohibits variable re-definition. Thus, data dependencies in a DIVA workflow can not be modified once compiled. This assumption greatly reduces the complexity of DIVA in design; however, it also prohibits the use of triggers on internal functions. Finding a way to achieve this could be an interesting direction for future work.

7 CONCLUSION

As we enter the age of extreme scale supercomputing and Big Data, the support of *in situ* data analysis and visualization becomes indispensable to application developers and domain scientists. The introduction of DIVA, a declarative and reactive programming environment, overall makes adaptive *in situ* workflow development a simpler process. We find the key benefits that it provides include: more autonomy between developers, modularity of workflow components, extensibility through the back-end runtime system, protection against logical programming errors by using implicit control flow execution, and a more results-oriented paradigm that better reflects end goals. As DIVA matures, it shall continue to be refined and extended to support a wide range of applications.

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