HydroCompute: An Open-Source Web-Based Computational Library for Hydrology and Environmental Sciences

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Abstract

We present HydroCompute, a high-performance client-side computational library specifically designed for web-based hydrological and environmental science applications. Leveraging state-of-the-art technologies in web-based scientific computing, the library facilitates both sequential and parallel simulations, optimizing computational efficiency. Employing multithreading via web workers, HydroCompute enables the porting and utilization of various engines, including WebGPU, Web Assembly, and native JavaScript code. Furthermore, the library supports local data transfers through peer-to-peer communication using WebRTC. The flexible architecture and open-source nature of HydroCompute provide effective data management and decision-making capabilities, allowing users to seamlessly integrate their own code into the framework. To demonstrate the capabilities of the library, we conducted two case studies: a benchmarking study assessing the performance of different engines, and a real-time data processing and analysis application for the state of Iowa. The results exemplify HydroCompute's potential to enhance computational efficiency and contribute to the interoperability and advancement of hydrological and environmental sciences.

Software Availability

Name	HydroCompute
Developer	Carlos Erazo Ramirez
Contact information	300 S. Riverside Dr., Iowa City, IA 52246 USA
Software required	Web Browser
Program language	JavaScript, HTML, CSS, C, WGSL, AS
Availability and cost	The code is open-source and free to use, and can be accessed on GitHub.
Code repository	https://github.com/uihilab/HydroCompute

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1. Introduction

Hydrology and environmental sciences deal with complex systems influenced by various factors. Mathematical models are crucial for analyzing and predicting these systems (Wagener & Kollat, 2007) (Maloszewski & Zuber, 1993). Researchers use large data sets to develop advanced models that capture environmental variables (Demir et al., 2015). However, these models require significant computational resources, resulting in extensive processing times and resources. To address this, optimized algorithms and data formats are developed to speed up simulations while maintaining accuracy (Demir & Szczepanek, 2017). The challenge lies in understanding the dependencies between different simulation tasks. By abstracting these dependencies, researchers can determine whether tasks can run in parallel or sequentially. This approach improves the efficiency of hydrological and environmental simulations and will continue to be important in the future.

The implementation of parallel computing applications in the fields of hydrology and environmental sciences has been extensively studied in the literature. (Asgari et al., 2022) reviewed the increasing applicability of computational challenges in the field of calibration of hydrologic models with the purpose of understanding parallelizing techniques and identifying knowledge gaps, with their results showing the potential and needs of developing evaluation metrics for parallelizing approaches and integration of other techniques as required. In terms of peer-to-peer communication, (Wu et al., 2013) studied the usage of parallel programming technology using MPI (Tennessee, 2021), to fully parallelize hydrological models. Another example is the multi-objective optimization of calibrating watershed hydrologic models using parallel computing (Reed et al., 2010).

Large-scale parallelization of hydrological models has been studied using standards such as OpenMP and Open ACC for graphical processing unit (GPU) simulations in HPC systems to create sequential and parallel executions that can potentially optimize the runtime, speedup, efficiency, and balance of different hydrologic models (Freitas & Mendes, 2018). Moreover, uncertainty and parameter stipulation through CPU/GPU hybrid performance clusters has been done to create a GLUE method with applications running on CUDA devices and multi-core computer clusters (Zuo et al., 2021). Applications leveraging GPU engines using different approaches in hydrological sciences have also been the focus of various studies, specifically with the release of low-level applications for C based code for flow routing algorithms (Rueda et al., 2016).

Web technologies have been an increasing field of interest for porting domain-specific applications, especially in the usage of cloud computing and client-side applications (Li et al., 2022). Cloud computing has been a field of continuous interest, mainly because of the number of services that are available for running intensive computations (Li & Demir, 2023). Platforms like HydroShare (Horsburgh et al., 2016), Tethys Platform (Swain, 2015), and others have been developed for cloud environments to create an easier pipeline for users to interface with ready-set models. Moreover, NOAA's next generation National Water Model integrates web application interfaces to create a seamless allocation of decision-making processes with spatiotemporal data resolutions and allows users to interactively change their specific processes through both plug-and-play and user-specified implementations (Cunha et al., 2021).

Client-side web applications have become increasingly popular in environmental science and hydrology (Demir & Beck, 2009; Xu et al., 2019) with advancements in both browser and computing technologies. Some examples for hydrological sciences include real-time flood mapping for running hydrologic models (Hu & Demir, 2021; Li and Demir, 2022), interactive hydrological models for educational case studies, highlighting the extensibility and scalability of client-side resources (Ewing et al., 2022), and environmental frameworks tailored towards connection with environmental data sources (Demir et al., 2009) to execute functions within a web browser with limited manipulation required as input from the user (Erazo et al., 2022a; 2022b). The use of web technologies has also been explored to expand the capabilities of running environmental applications from the perspective of standardizing modeling connections through OpenMI (OpenGIS, 2014) and Basic Model Interface (BMI) (Goodall, 2016). An example of this is the use of the BMI standard for the connection of resources that contain similar lexical connections (Ewing et al., 2022). A library that has been implementing cutting-edge technologies to create machine learning models is TensorFlow, a general-purpose library that contains methods and scaffoldings for running machine learning and artificial intelligence algorithms (Sit & Demir, 2023). Specifically, its web-based environment, TensorFlow.js, employs many of the technologies that will be described in this manuscript (Gerard, 2021).

The literature highlights the potential and increasing demand for leveraging the current technological power in modern-day computational architecture for web environments to create pathways for running faster computations on the client side (Demir & Galelli, 2022). For this purpose, we present HydroCompute, a computational library tailored towards hydrological and environmental sciences that leverages technologies found in the common web browser. This paper encompasses the technological background of next-generation hydrological information systems, a detailed description of HydroCompute's architecture, and benchmarked applications related to hydrology. A case study is presented to demonstrate the library's engines in action while constructing a dashboard for retrieving and analyzing long-term streamflow data across various stations in Iowa, illustrating the integration of routines from multiple programming interfaces.

The remainder of this paper is organized as follows: Section 2 delves into the methods and system architecture of HydroCompute, detailing the engines, connections, and parallel frameworks that make up the core functionalities of the library. In Section 3, this is followed by the presentation of case studies that demonstrate the library's performance capabilities, focusing on benchmarking matrix multiplication and streamflow analysis in the state of Iowa. Finally, Section 4 discusses the feedback obtained from workshops and surveys conducted among potential users to assess the library's usability and applicability in real-world scenarios.

2. Methods

2.1. Scope and Objectives

HydroCompute aims to address the computational challenges in hydrology and environmental sciences by providing a high-performance client-side computational library. The motivation behind HydroCompute is to leverage cutting-edge web technologies, such as Web Workers, WebGPU, Web Assembly, and WebRTC, to enable both sequential and parallel simulations, efficient data management, and decision-making capabilities. By offering an open-source and flexible architecture, HydroCompute allows users to seamlessly integrate their own code into the framework, enhancing the adaptability and applicability of the library across various hydrological and environmental applications.

HydroCompute targets researchers, practitioners, and educators in the fields of hydrology and environmental sciences who require efficient and scalable computational tools for their work. The library is designed to be accessible and user-friendly, enabling users with varying levels of expertise to benefit from its capabilities. Applications of HydroCompute include, but are not limited to, hydrological modeling, flood risk assessment, water resources management, environmental monitoring, and educational purposes. By providing a comprehensive and versatile computational library, HydroCompute aims to contribute to the advancement of hydrological and environmental sciences through improved data processing, analysis, and decision-making.

2.2. Technological Background

This study explores algorithmic optimizations for improving application performance, with a focus on parallel and sequential execution of dependent functions. Techniques based on graph theory, memory allocation, and tradeoffs between correctness and speedup were employed to identify and eliminate bottlenecks (Gerasoulis & Yang, 1992). Graph-based algorithms analyzed function dependencies, while dynamic memory allocation strategies optimized resource utilization. Both parallel and sequential execution were evaluated, with parallel execution involving simultaneous processing of independent tasks and sequential execution ensuring task order dependency (Rönngren & Ayani, 1997). These computational techniques find applications in fields like hydrology, where parallel execution processes large datasets and complex models while sequential execution handles interconnected phenomena modeling, such as assessing flooding risks or hydrological routing (Zhou et al., 1998; Vivoni et al., 2011). Emerging technologies like Web Assembly, WebGPU, Web Workers, and WebRTC enable multi-threaded execution and peer-to-peer data transfers, enhancing web browser capabilities beyond traditional single-threaded CPU architectures.

Web Workers: Web workers are a feature in web browsers that enable concurrent and background execution of JavaScript code, enhancing the responsiveness and performance of web applications (W3C, 2021). They provide a means to offload computationally intensive tasks from the main browser thread, preventing user interface blocking and enabling parallel processing. Web workers operate as separate threads, running in the background and communicating with the main thread through message passing. This allows for the execution of complex calculations, data processing, and other resource-intensive operations without impacting the user experience.

WebGPU: The development of GPUs as a powerful source of computational power has led to the creation of applications for general-purpose computing (Trompouki & Kosmidis, 2016; Huang et al., 2008). Standardizing the software controlling GPUs was a significant challenge, but the Vulkan group addressed this by implementing OpenGL (Segal & Akeley, 1999), which enabled vendors to create application programming interfaces (APIs) harnessing GPU power. While GPU APIs primarily focus on graphical computing, their underlying architecture also supports general-purpose computing. This capability has been utilized in web-based environments through libraries like Vulkan's WebGL (Angel & Shreiner, 2014) and the W3C WebGPU (W3C, 2023a). In 2022, the WebGPU API was implemented, providing developers with an alternative way to access GPUs. It simplifies working with graphics hardware, offers flexible APIs for different pipeline types, and automatically transforms the WebGPU shading language into a compatible format. The WebGPU standard has been added to the W3C and has been released and tested in popular web browsers, such as Google Chrome and Mozilla Firefox Nightly.

WebAssembly: WebAssembly is a technology that allows low-level programming languages like C, C++, AssemblyScript, FORTRAN, and Rust to be used in web applications (W3C, 2019). It converts code into a binary format that can be used in web apps, providing performance improvements for computationally intensive tasks. Running code in a stack-based virtual machine supported by major browsers, the technology offers faster, and more efficient execution compared to traditional web technologies. It also ensures security through its own memory management and execution context, enhancing stability and reliability. Furthermore, WebAssembly enables the utilization of legacy low-level applications, allowing developers to scale systems and applications by reusing existing code. This eliminates the need for complete application rewrites, leading to significant performance improvements and cost savings, particularly in industries with computationally demanding applications.

WebRTC: Peer-to-peer communication through WebRTC is a set of standards that allows intercommunication between peers through a semantic API that has been added to major web browsers (W3C, 2023b). It is continuously evolving and has been around for over 7 years at the time of writing, with technologies for video conferencing and communication leveraging the technology. Though not a directly intuitive API because of security constraints, it allows for large amounts of data to be shared among peers without the need for external servers to host and manage traffic for the data. Applications for water resources research and education are continuously researched, and promotion of research and application of flood modeling and simulation directly using the technology (Zhang et al., 2022).

2.3. System Architecture

HydroCompute is a web-based client-side JavaScript library for fast computations powered by the technologies commonly used for social media platforms, video and imagery manipulation, and data streaming that has been standardized to be available in most common web browsers. It is a library that allows users to run tasks sequentially or in parallel depending on: (1) data size and type; (2) task; (3) connection between tasks.

It has been designed using a modular architecture that registers, switches, and enables interfaces for different engines tailored to specific tasks. This is done through the interactions between library usage, optimization techniques, and the availability of technologies within the working environment. Using optimization techniques for writing algorithmic computations such as hoisting, data sharing, loop fusions, and others, the computational times required for running specific time-constrained calculations are significantly reduced.

The HydroCompute library contains three main computation engines focused on two different approaches, 3 for main computations (JavaScript, WebGPU, and Web Assembly) and one for peer-to-peer communication (WebRTC), depicted in Figure 1. Each engine is interfaced through a semantic API, which contains lexical declarations that assign the specific requirements set by the user in terms of data, steps, function connections, and results.

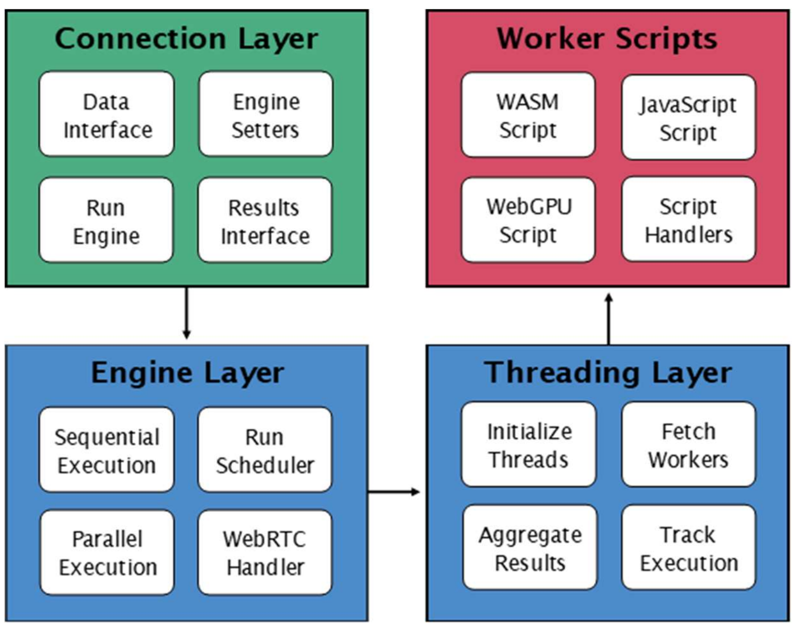


Figure 1. Architecture and components of the HydroCompute library.

2.3.1. Connection Layer Management

The connection layer keeps track of the number of engines available for usage, the times specific engines have been called, data management, the number of runs that have been created using specific engines, running a simulation, and the results from the simulation, as well as execution times, as shown in Figure 2. It is the main interface all the other engines interact with. The basic running requirements are saved and passed to the run function to set the requirements in the main engine. For initialization purposes, the JavaScript engine has been set as the default.

Upon library initialization, the main object interface, designated "engine," is called. The active engine used in an instance can be changed as needed by the user, allowing for the integration of the main computational engines or the peer-to-peer communication engine. These engines have been designed to deal mainly with multidimensional array structures that are fed into the connection layer. The connection layer calls helper functions that clone the data and transform it into typed buffers, which are stored globally within the library for further usage. In developing the connection layer, specific workflow assumptions were considered for effective data management:

(1) Data Sharing: The data must be shared between the contexts of the main thread (user interface, input/output commands) and the separate threads that run the heavy computations in the background.

(2) Data Availability: The running context must primarily access the data. To avoid further compiler optimization issues with memory management, the data is transferred, and not cloned, between the threading environment and the main engine. Transferring data makes better integration with the environment possible and saves space and computation time.

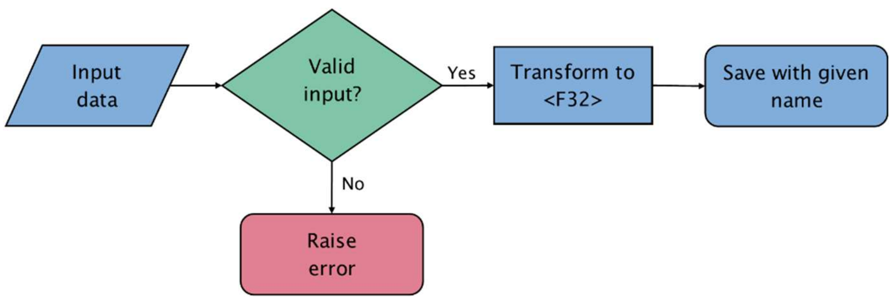


Figure 2. Setting data for a run.

The data is then registered using a naming convention specified by the user or a random assignment of letters and numbers. Given the domain of interest is in the fields of hydrology and environmental sciences, float 32-byte numbers were considered to be the maximum accuracy required and are used as typed arrays throughout the whole application lifecycle. The process for running a simulation is governed by specific criteria (Table 1). Once all default requirements have been established, the run commands trigger an instance of the engine class to execute the simulation, following the flow shown in Figure 3.

Table 1: Criteria for Running a Simulation

Criteria	Description
Stepwise Execution	Each step, including its dependencies, functions to be executed, and arguments, must be specified in an array.
Functions & Arguments	Appropriate arguments for each function must be specified.
Dependencies	Functional dependency within each step must be identified.
Step Linkage	A designation must be made to determine if results from a previous step should be passed to subsequent steps.

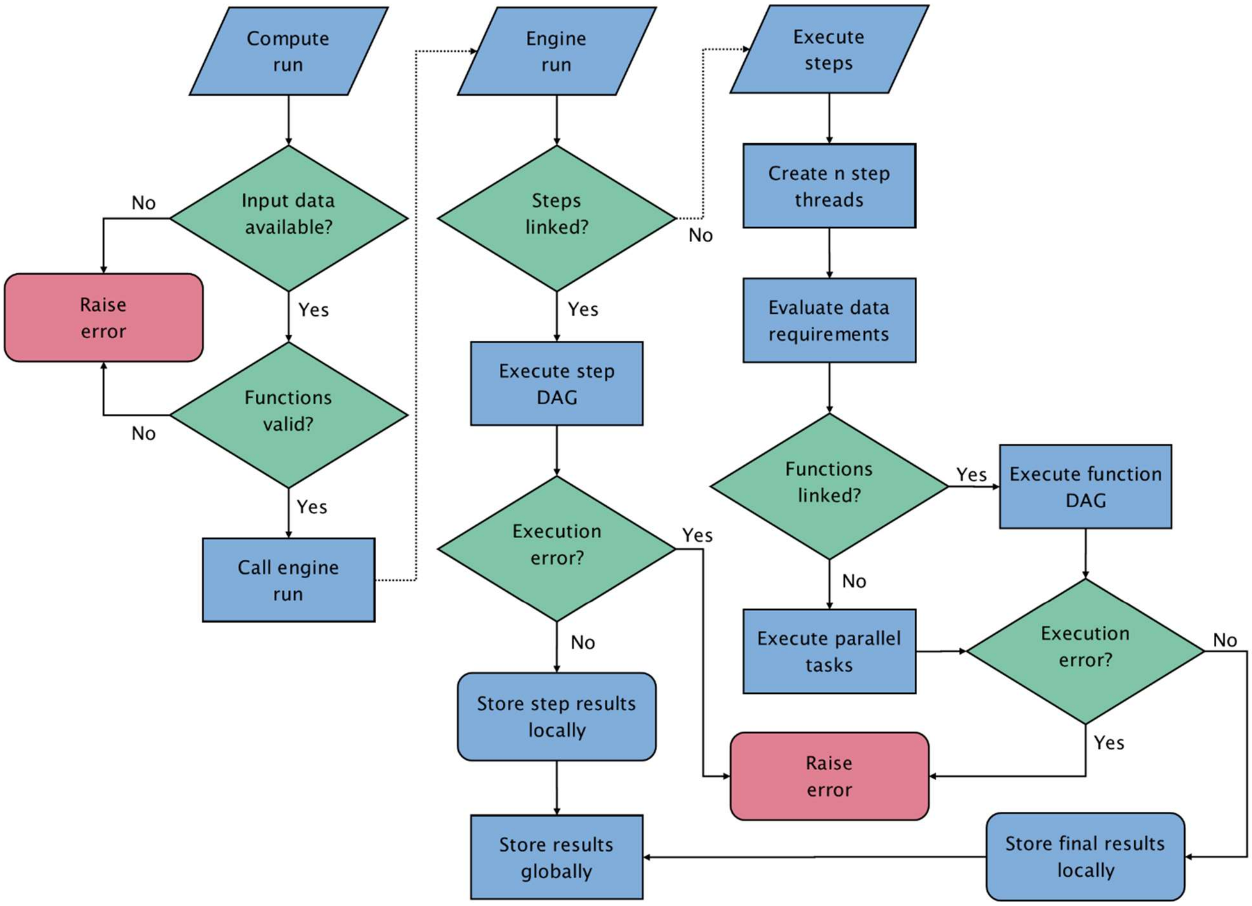


Figure 3. Flowchart of running a simulation.

2.3.2. *Engine Management*

The engine class serves as the fundamental driver for executing the available APIs within the HydroCompute framework (Figure 4). Its methods allow for the modification and analysis of arguments and data to initialize threads. The class provides specific implementations for running required functions sequentially or in parallel, based on the dependencies of arguments, data sizes, and user inputs.

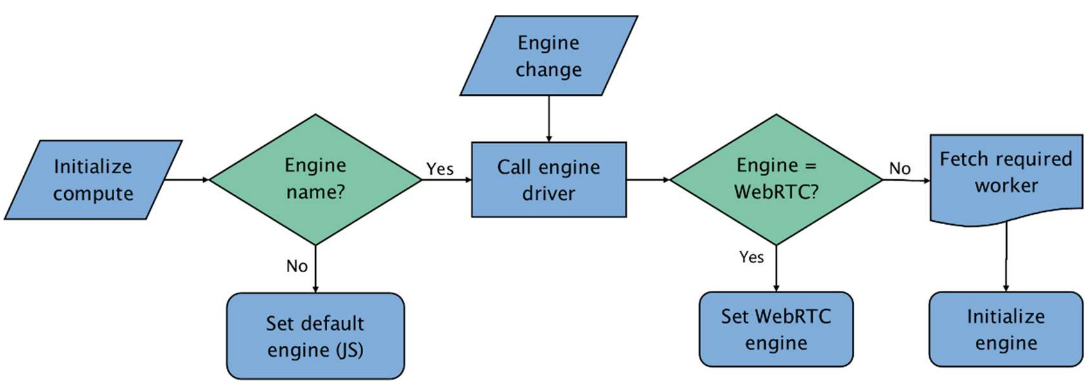


Figure 4. Flowchart of initializing the library or changing engines.

The scheduling of each thread is determined by the number of functions to run, their dependencies, and the data discretization. This is achieved either by partitioning the input data among the available engines or by assigning multiple functions to the same data. When multiple workers are required to process the same data, multithreading is achieved by dispatching several workers at the same time using parallel execution.

If dependencies exist, such as when different workers require the same chunk of data to complete or when execution contexts require different functions to finish, then a directed acyclic graph is implemented using promised-based executions to ensure efficient thread coordination. After each task is completed, the results are combined into a single result space, which is interfaced by the framework to return the final results.

2.3.3. Step Execution Management

The HydroCompute framework efficiently manages step execution by categorizing functions as sequential or parallel and implementing appropriate handling mechanisms. A step handling function determines the linkage between steps, the number of functions, and their dependencies, allowing for data partitioning, cloning, or direct passing based on the linkage. A task runner function determines the execution type, utilizing a directed acyclic graph implementation with promise-based executions for steps with dependencies and sequential execution for steps without dependencies. This approach ensures efficient function execution while satisfying specified dependencies and linkage requirements.

Parallel Execution: A promised-based approach has been implemented when the execution context requires n-number of threads to fire up at the same time, whether it is with the same data or with different data for each thread, as explained in Figure 5. The number of threads that are set to run is limited by the available threads available on the machine running the library. Batches of work are created to run an n-number of workers per batch and fired up to avoid race conditions on either the available data or the number of threads that the given web browser can run.

```
function PARALLELRUN(args, step)
    batches ← empty array
    results ← emtpy array
    last ← 0
    for i ← 0 and between threadCount and maxthreadCount do
        batch ← functions: empty array, funcArgs: emtpy array
        for j ← i to i + maxthreadCount and j less than threadCount do
            batch.functions.push(args.functions[j])
            batch.funcArgs.push(args.funcArgs[j])
        end for
        batches.push(batch)
    end for
    for batch in batches do
        batchTasks ← emtpy array
        for i ← 0 to batch.functions.length do
            j ← last + i
            d ← if data is split then get data[j].buffer, else get data.buffer
            workerArgs ← data: d, id: i, funcName: args.functions[i], fun-
cArgs: args.funcArgs[i], step: step
            threads.initializeWorkerThread(i)
            batchTasks.push(threads.workerThreads[i].worker(workerArgs))
        end for
        batchResults ← await Promise.all(batchTasks)
        results ← results.concat(batchResults)
        last ← last + batch.functions.length
    end for
    return results
end function
```

Figure 5. Parallel execution of a set of functions for a given step.

By limiting the number of threads per batch to the total number of threads, the parallel execution function correctly leverages the engine's capabilities to expand on the required work. Once the data has finished running, it is returned as results to the main engine. The routine effectively utilizes multiple threads to perform a set of functions concurrently, thereby reducing the overall execution time.

Concurrent Execution: When there are dependencies between the functions of a single step, then the concurrent execution routine sets the required information for each function for each thread as an array of functions that will execute in the given order of the results required down the line (Figure 6). This workload is then submitted to run under dependency conditions.

```
function CONCURRENTRUN(args, step, dependencies)
    for i = 0 to this.threadCount do
        d ← if data is split then get data[j].buffer, else get data.buffer
        args ← data: d, id: i, funcName: args.functions[i], step: step, funcArgs: args.funcArgs[i]
        threads.initializeWorkerThread(i)
    end for
    res ← await DAG(functions: threads.workerThreads[key].worker), dag: dependencies, args: args, type: "functions")
    return res
end function
```

Figure 6. Concurrent execution of a set of functions for a given step.

```
function DAG(functions, dag, args, type)
    dag ← dag or set to empty array
    N ← length of functions
    if type = "steps" then
        dag ← create a linear DAG with N nodes
    end if
    counts ← an array of length N where each element is the number of incoming edges to the corresponding node in dag
    stopped ← false
    remaining ← N
    values ← []
    for i in 0 to N − 1 do
        if counts[i] > 0 then
            continue
        end if
        promise ← null
        if type = "steps" then
            promise ← execute function i in the collection of functions
        else
            promise ← execute function i with given arguments
        end if
        promise.then(value → handleResolution(promise, i, value), error → handleRejection(promise, i, error))
    end for
end function
```

Figure 7. Promise-based DAG implemented in the library.

Directed Acyclic Graph: A DAG algorithm was implemented to schedule the execution of multiple steps or functions in a specific order based on their dependencies (Figures 7 and 8). The algorithm is provided with an input object that includes the functions, a dependency DAG array, additional arguments, and the type of execution (stepwise or functionwise). Promises are used to execute the functions, resolving per dependent once all functions have completed execution. The values returned from each function are stored in an array and passed as arguments to subsequent functions as specified by the arguments. The precedence of each function is assumed within the algorithm, and parallel execution occurs when a function call has no dependencies. This implementation ensures efficient execution of the required functions while meeting the dependencies and linkage requirements specified in the step handling function.

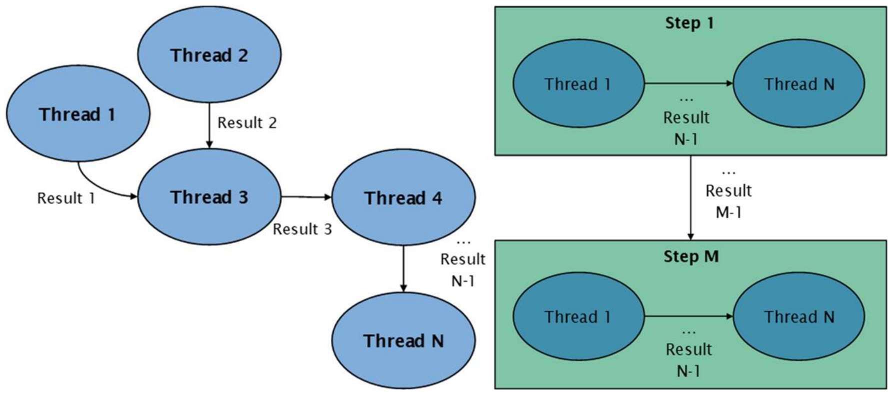


Figure 8. Execution for a single step DAG (a) and execution for a multiple steps DAG (b).

2.3.4. Thread Manager

The thread manager class creates a scaffold containing specific running implementations for each thread requirement (Figure 9). It contains setting variables that keep track of execution time, results, data, and additional arguments that run within each thread. The class provides methods for managing objects that keep track of the state of each worker, the results coming back from the worker, and the execution times.

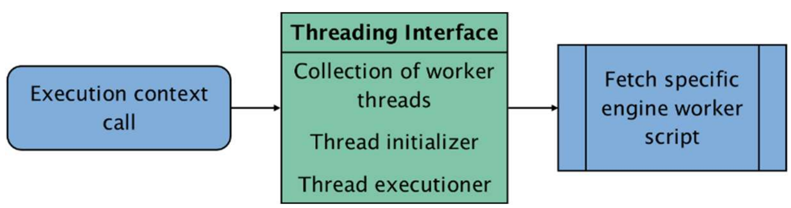


Figure 9. Thread initializer and executioner.

When an engine initializes the class, the location of where each worker is as well as the name of the engine are passed to keep track of the execution context required. The class provides variables that allow interfacing between the local class variables and the engine that instantiated them and are cleared once all the executions required are finished, with the results being lifted back into the connection layer. The thread manager is in charge of calling the worker scripts for all the available engines. These scripts contain specificities for the execution of the functions to be run. However, all the workers have commonalities in terms of data management, result management, and execution.

Once the engine has been instantiated, computations can be called by declaring the engine name in the constructor class. This enables all the methods from the HydroCompute core and the engine to be readily available for usage. Given the class declaration of ES6 modules, the architecture allows for multiple instances to be run simultaneously, allowing for separation of interests when possible. This also means that the engines can be changed according to the functions that are run by the framework. All engines are driven by worker scripts that contain ready-set methods for manipulating the input data, the engine method, and the results based on the specific requirements of the engine. The worker structure searches for the required function execution name in the collection of scripts available per engine, as shown in Figure 10.

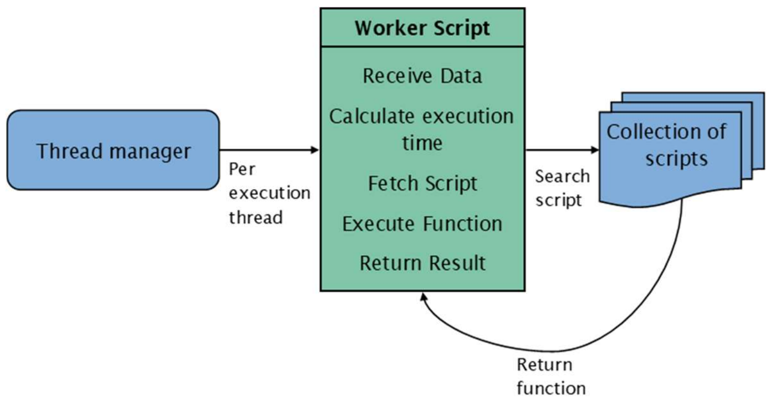


Figure 10. Worker script fetching a collection of functions.

JavaScript Worker: The JavaScript worker contains methods that call instructions directly written in the language optimized for typed arrays. Not having to parse, the execution performance is considerably faster for small-sized data and relatively complex computations. All instructions are added to a folder that contains the different types of scripts available to use. To enable easier data manipulation and the addition of new tools, each script that has been added or will be added in the future must have the same structure through an object-defined definition.

WebGPU Worker: The WebGPU worker hosts specific methods for calling the adapter and device available on the machine running the browser. The adapter is specific to the web browser engine and allows for memory growth and allocation. The engine is best suited for analyzing large memory chunks instead of smaller ones since the inert architecture of GPU chips allows for native parallelization for broader analysis. As with the other engines, the host code is kept as objects containing the GSLS shading language to be called using a name definition within the object. Buffers and shaders are created as modules that are dispatched to the chip to be copied from the CPU to the GPU and back. With the device finished, the memory is cleared up.

Web Assembly Worker: The WASM worker contains methods for appropriately executing code directly from binary code compiled from different web assembly compliant programming languages. With the availability of running code in a secluded context with its own dynamic memory privately allocated, the compute engine is able to allow for the execution of different types of implementations under the same umbrella. As the starting point of this project, two assembly-compliant languages have been added: C and AssemblyScript. Being legacy code with extensive usage in the fields of hydrology, data science, and computing environments, C-implemented web assembly code has been added given the easier implementation through the EMSCRIPTEN compiler that allows fast and small-sized bundles. AssemblyScript, on the other hand, is a TypeScript-like subset for Web Assembly implementations that enables web developers to easily transition to writing code from a JS or TS ideology.

WebRTC Implementation: The WebRTC engine interface incorporates various implementation features for efficient data transfer, like results from a simulation on another machine or transfers from a peer's local machine. It provides ready-set methods to save large data sizes directly into the available sources object, leveraging the shared structure within the library. The implemented class plays a crucial role in managing connections between compute instances. During initialization, it sets up connection parameters, such as the maximum message size (65 kB), and required partitions, and connection type. The run method determines the connection type and establishes a data channel, enabling the transmission and reception of data. The received data is saved in the connection layer and readily accessible for use as input in simulations.

3. Results

This section presents a comprehensive evaluation of HydroCompute's performance in various scenarios, including benchmarking tests and a real-world case study. The purpose of this analysis is to assess the library's capabilities, execution times, and performance optimizations in handling large-scale computations related to hydrology and environmental sciences. The findings provide insights into the effectiveness of the library's engines and their potential impact on various applications within the field. Furthermore, we discuss feedback obtained from workshops and surveys conducted among potential users, offering valuable perspectives on the library's usability and applicability in real-world scenarios.

3.1. HydroCompute Performance Evaluation

Two case studies have been implemented to evaluate the performance of data-driven heavy computation: a classic benchmarking case and a time series analysis with real data. The implementation was executed on a machine equipped with an Intel Core i7-4790 CPU @ 3.60 GHz, 32 GB of RAM, and an integrated Intel HD Graphics 4600 with 2176 MB of shared memory and a 64-bit architecture. The development and testing environments were Chrome Canary v.106.0.5207.0 and Microsoft Edge v.110.0.1587.56. The Chrome browser was used for WebGPU executions, and both browsers were used for WASM and JS executions. Notably, testing was not conducted in any Firefox browsers, as discussed in the conclusions and limitations section.

3.1.1. Benchmarking: Results for Sequential and Parallel Simulations

The evaluation of engine performance was conducted using the matrix multiplication approach, a fundamental tool in environmental and hydrological sciences with broad scope and applicability across various disciplines, including numerical simulations, image and data manipulation, and solving equations (Volkov & Demmel, 2008). Moreover, the case study allowed for the setting of thresholds on the usage of specific engines based on the number of operations required.

To test the engines, square matrices of varying sizes (ranging from 16^2 to 2401^2) were generated and filled with random numbers between 0 and 1000. Two scenarios were analyzed to assess engine performance. The first involved running a single worker for increasing matrix sizes, as shown in Figure 11, while the second entailed using multiple workers for smaller matrices (Figures 12 and 13). The latter scenario was classified as running in parallel for an n-number of threads, each representing the maximum number of data allocated within the running environment.

To accurately evaluate worst-case scenarios and observe performance trends across all engines in the specified environment, the matrix algorithm implemented had an $O(n^3)$ time complexity and number of FLOPs. Regarding the number of transactions, it is worth noting that the WASM and JS implementations run directly using CPU resources, while WebGPU leverages GPU multicore architecture, resulting in different transactional operations. For very large square matrices, the number of multiplications using JS or WASM modules is proportional to $n^3 - n^2$, assuming a naive implementation. In contrast, for WebGPU, each transaction is divided into workgroups of size 8x8, corresponding to single row-column pairs within the result matrix. Since the implementation leverages parallel, same-size dispatch workgroups, the total number of transactions performed is proportional to $\frac{2n^3}{64}$. It's important to note that the estimates for the number of transactions provided above are based on scenarios without considering factors like memory caching and access, CPU speed, and other hardware and software specifications, which can significantly impact the actual number of transactions performed by each engine.

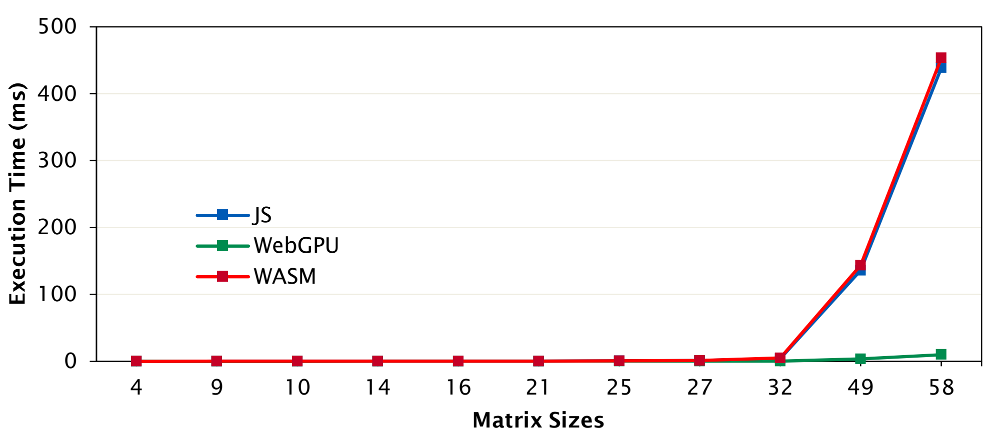


Figure 11. Results from using a single worker on multiple matrix sizes ranging from 4^2 to 60^2.

The evaluation of the engines' performance revealed that significant differences exist in terms of running time across the different implementations of the operation. While the WASM and JS code demonstrated faster performance for smaller-sized matrices, WebGPU proved to be more efficient for larger matrices. This disparity can be attributed to the optimization of CPU and GPU code for serial execution and parallelism, respectively. However, for smaller matrices, the number of parallel threads that can be dispatched is limited, leading to underutilization of GPU resources and higher overheads due to synchronization and coordination. Furthermore, suboptimal memory access patterns for small-sized operations result in higher memory access latencies and lower performance. Based on these findings, we conclude that the implemented WebGPU codes become increasingly important and accessible when dealing with large data chunks that require managing the massive parallelism of the GPU and leveraging its memory bandwidth and caching capabilities.

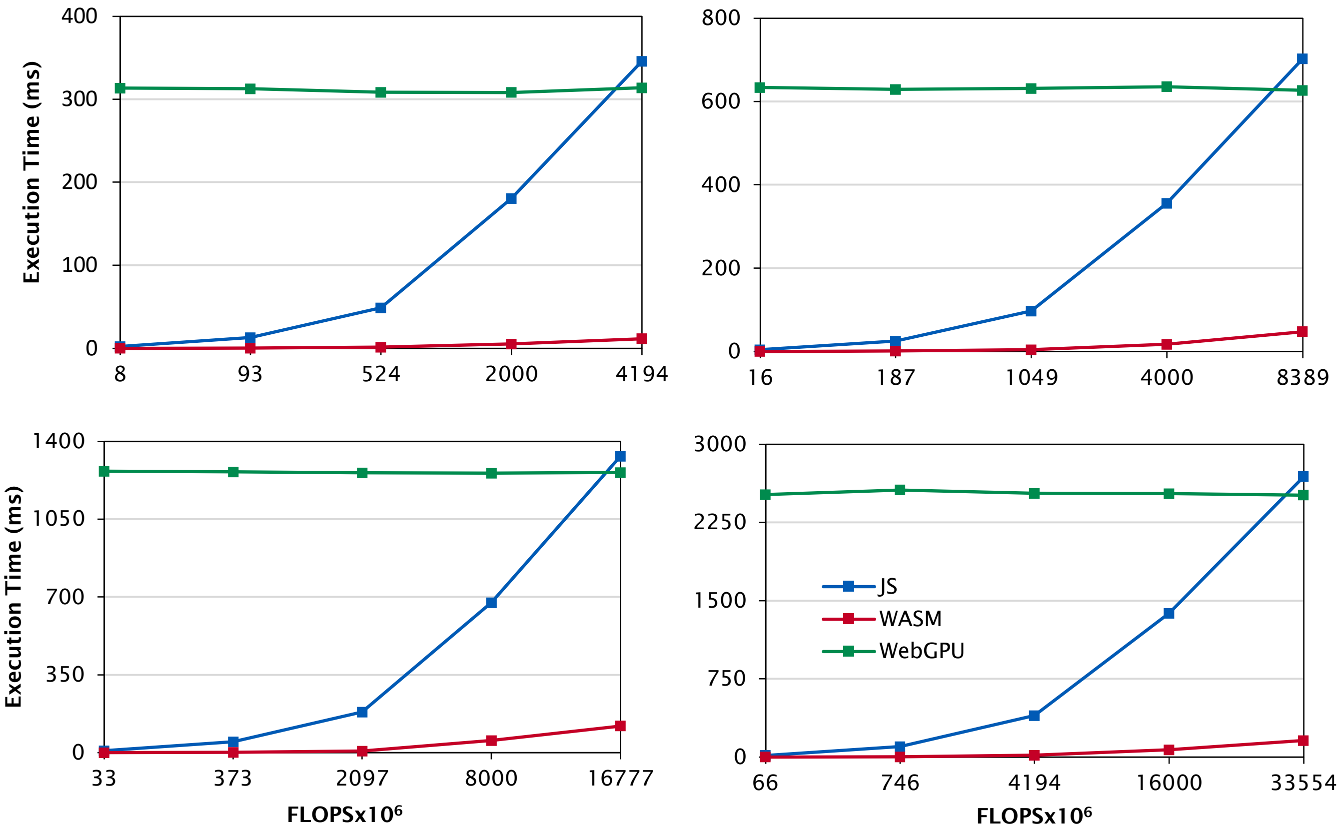


Figure 12. From top-left to bottom-right: FLOPx10^6 vs. execution time in seconds for 2,000, 4,000, 8,000, and 16,000 executions for matrices of sizes 16^2 through 128^2.

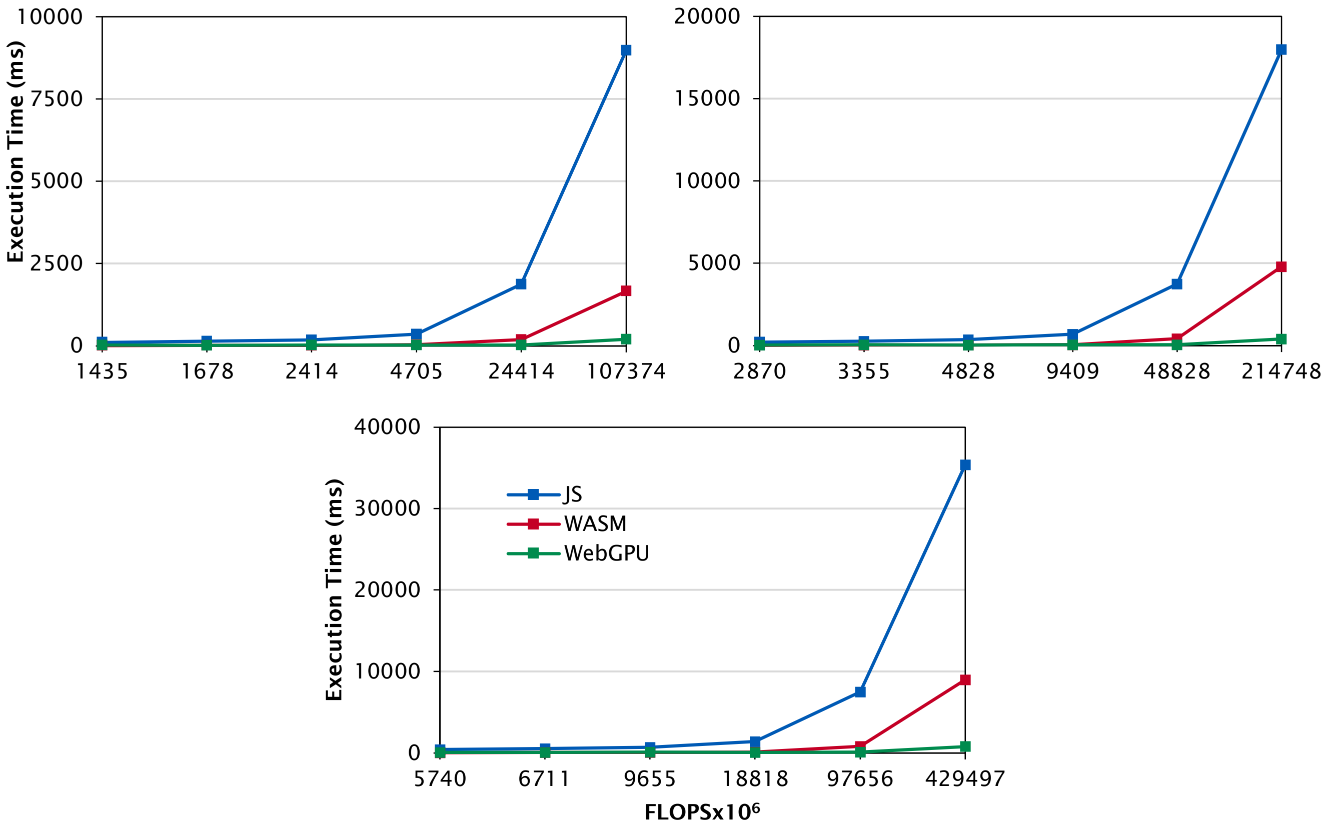
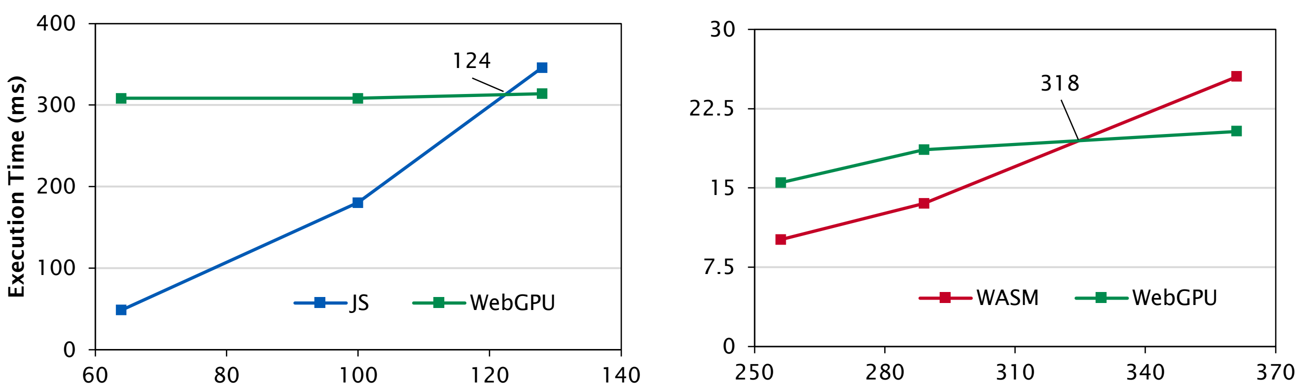


Figure 13. From top-left to bottom: FLOP x 10^6 vs. execution time in seconds for 100, 200, and 400 for matrices of sizes 240^2 through 1024^2.

Having shared GPU memory had a significant impact on the performance of the WebGPU, with rendering issues happening whenever there was an interaction between any other program and a submitted task. Breakpoints were found for both JS and WASM code vs. WebGPU to assess when a task should run on the GPU engine instead, as seen in Figure 14.



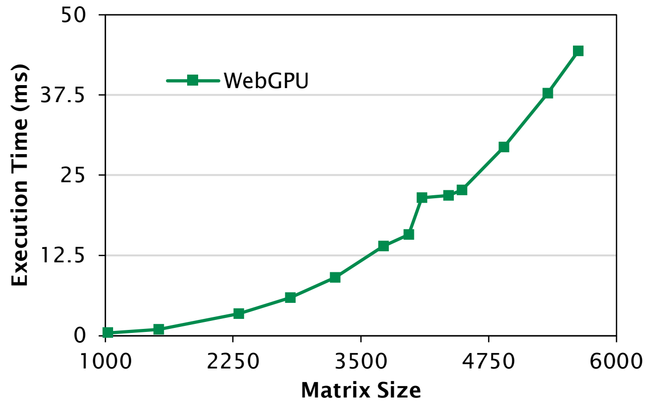


Figure 14. Cutoff for JS and WASM engines in comparison to the WebGPU, at sizes >124 and >318 respectively, and results from the execution of large matrices using the WebGPU on a single worker.

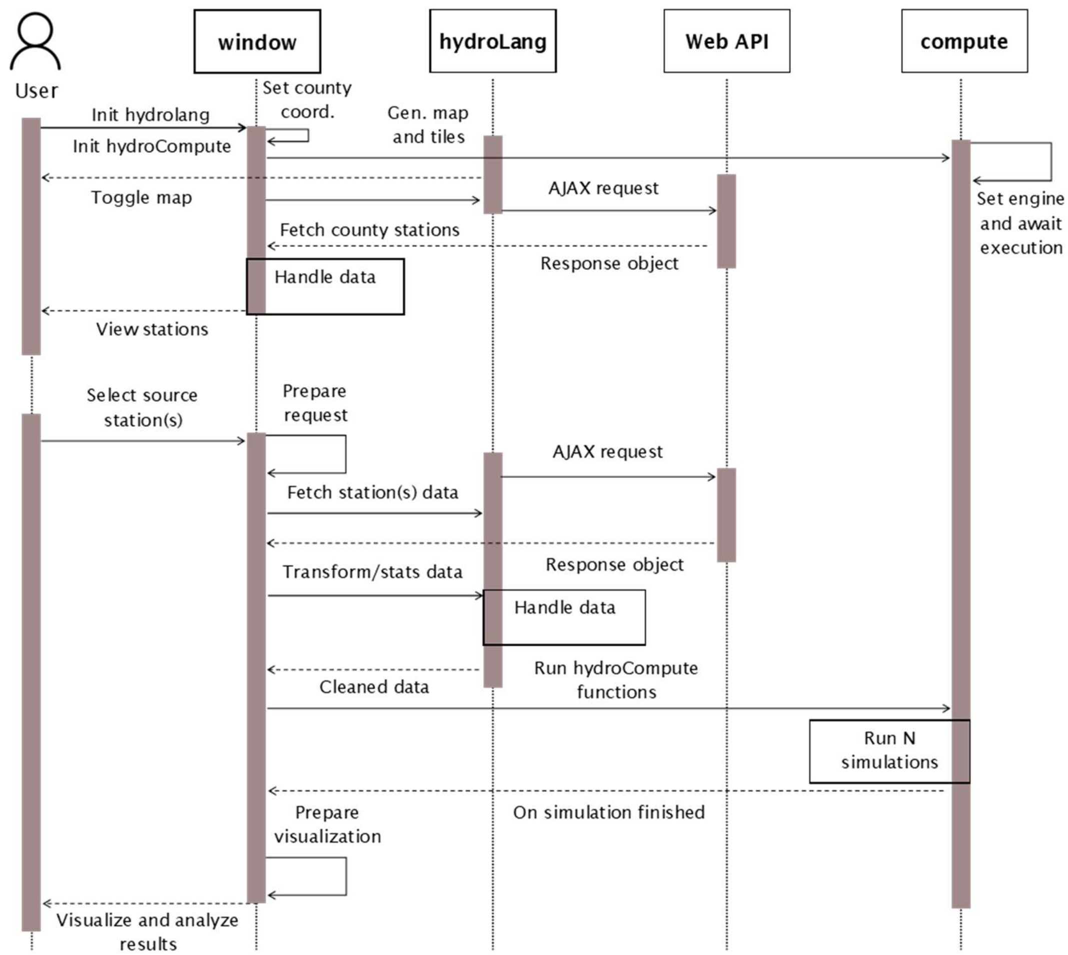


Figure 15. Sequence diagram for the case study.

To evaluate the limits of the WebGPU engine in terms of maximum floating-point operations available, testing was done with matrices of sizes $1{,}024^2$ through $5{,}625^2$. The calculation was done as a single instruction, and a log-linear tendency was observed for very large matrix sizes. The results highlight a logarithmic tendency, while increasing the matrix size, the execution time increases at a decreasing rate.

3.1.2. Case Study: Real-Time Data Processing and Analysis for Iowa

To highlight performance optimizations while using the framework, a case study was developed to present a visual dashboard that enables users to retrieve and analyze real-time streamflow data from different sources across the state of Iowa. The main purpose is to create a clear development pipeline that promotes easy usage of the framework, with the sequence diagram and user interface shown in Figures 15 and 16. The application connects through statewide rectangular coordinates per county or per selection on screen to CUAHSI WaterOneFlow services (CUAHSI, 2018) for daily values from USGS (USGS, 2023), MOPEX (Shaake et al., 2009), and NOAA GHCN (Peterson et al., 1997) to query all the available streamflow stations falling within the boundary within a daily scale from 1900 through the day of analysis. This is done using the hydrological framework HydroLang (Erazo et al., 2022b) to retrieve and clean streamflow data downloaded from different sources from CUAHSI data sources, with the HydroCompute library used to predict timebound streamflow using autocorrelation functions, ARMA process, and moving averages, following a similar pathway as (Vecchia, 1985).

The design of the dashboard is highly driven by tools found within the HydroLang framework, including data retrieval, cleaning, maps, and graphs. These are the less computationally extensive tasks, while all the heavy lifting for the analytical part is done by HydroCompute using both functions from HydroLang and additional functions for time series analysis. The user interface is kept organized for further data manipulation and cleaning while the compute framework handles the heavy workload on the backend.

The performance of the application was evaluated based on factors such as portability, code complexity, and execution times for the compute library when processing large amounts of data. However, the time required to acquire and clean data was not evaluated due to factors such as latency times, server traffic, and internet latency that would not highlight the library's usage. Regarding data manipulation tasks, HydroLang was used to clean and format the data as accurately as possible, considering outliers, faulty values (NaN or undefined), and other factors. The number of executions varied by station, as the implemented analysis functions depend on the number of executions per algorithm and the number of required transactions, which are heavily influenced by the time series data's size. Specifically, there were 33 algorithmic function calls per station done on the HydroCompute library, as described in Table 2.

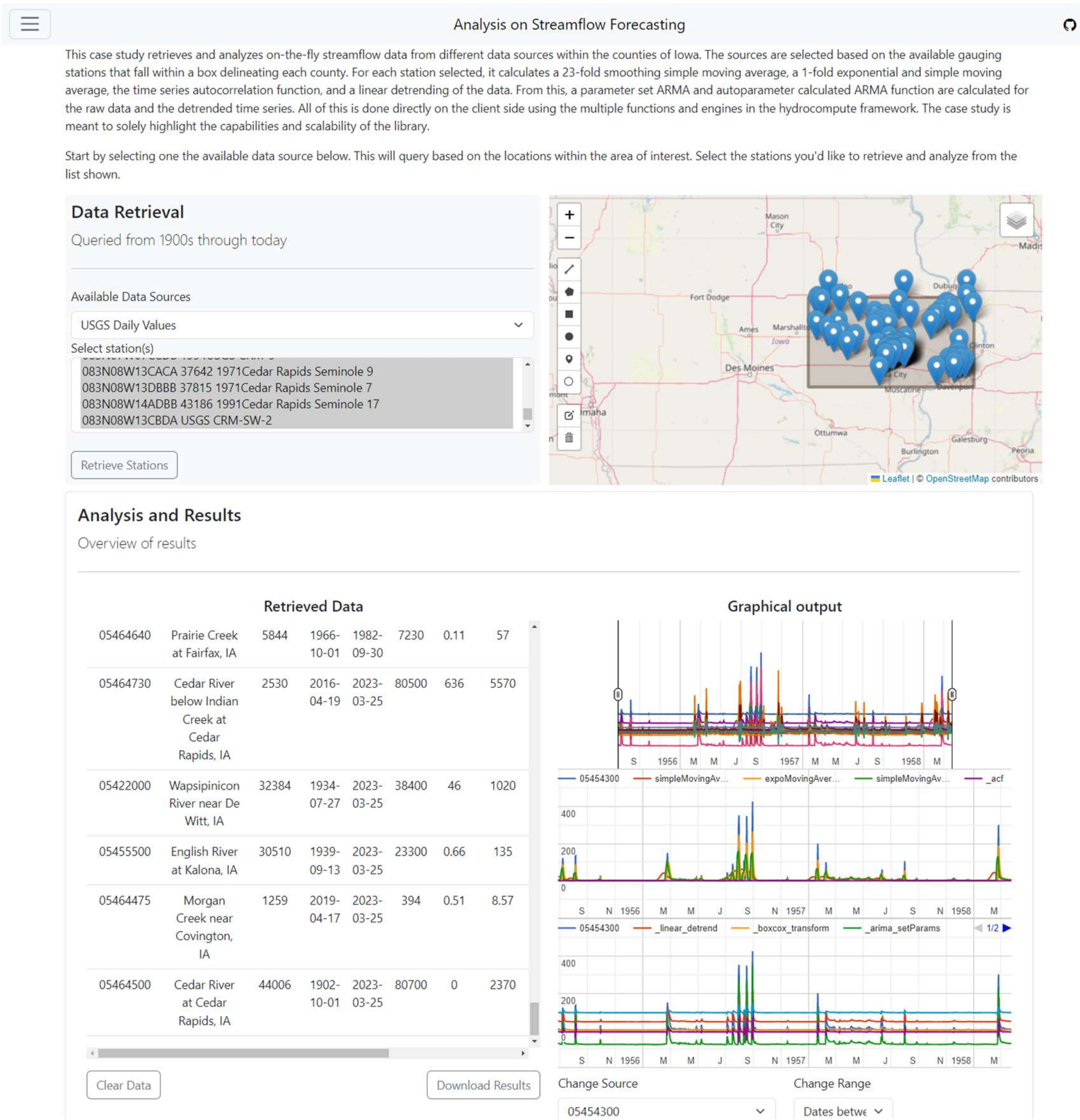


Figure 16. Screenshot of the web dashboard for streamflow time series analysis for real time USGS gauge stations in eastern Iowa.

Table 2: Simulation methods for the case study.

Simulation	Description
#1	Execute exponential moving averages and simple moving averages an arbitrary number of times and observe a gradual smoothing of results with each iteration.
#2	Compute simple moving averages and exponential moving averages in parallel.
#3	Compute the autocorrelation function, Box-Cox transformation, linear de-trended time series and ARMA with auto parameter update in parallel.
#4	Compute de-trended linear time series, and ARMA with auto parameter update using the previous results.
#5	Compute exponential moving average and ARMA with auto parameter update using the previous results.

To test the application, stations across different counties in the state were queried, and the provided map was used to search for new stations based on rectangular selections. The results indicated a linear trend that was overshadowed by the number of data points available at each station and the number of stations within the selected area. Figure 17 shows querying a quarter of the state (around 250 stations in the northwestern part of the state), retrieving and cleaning data, and running the 33 functions in both parallel and sequential modes, with the entire process taking approximately 9 minutes.

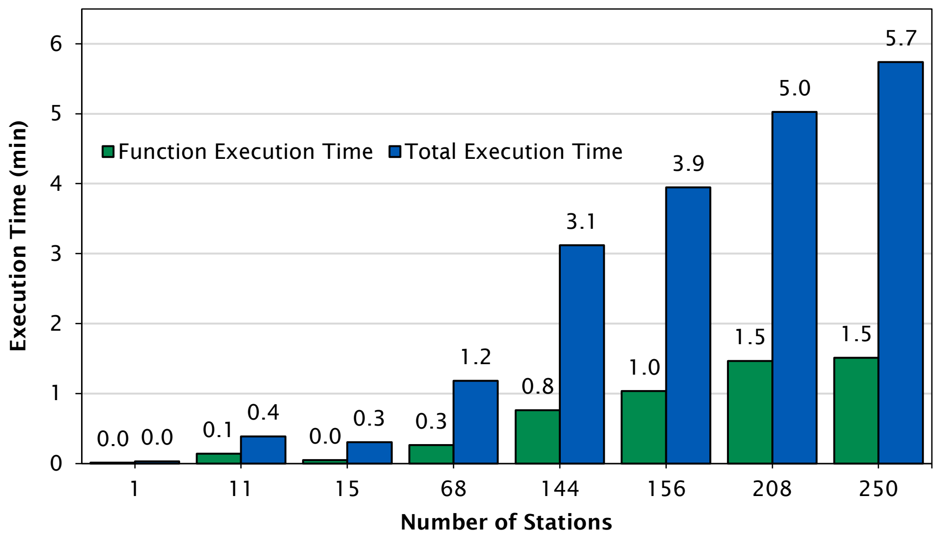


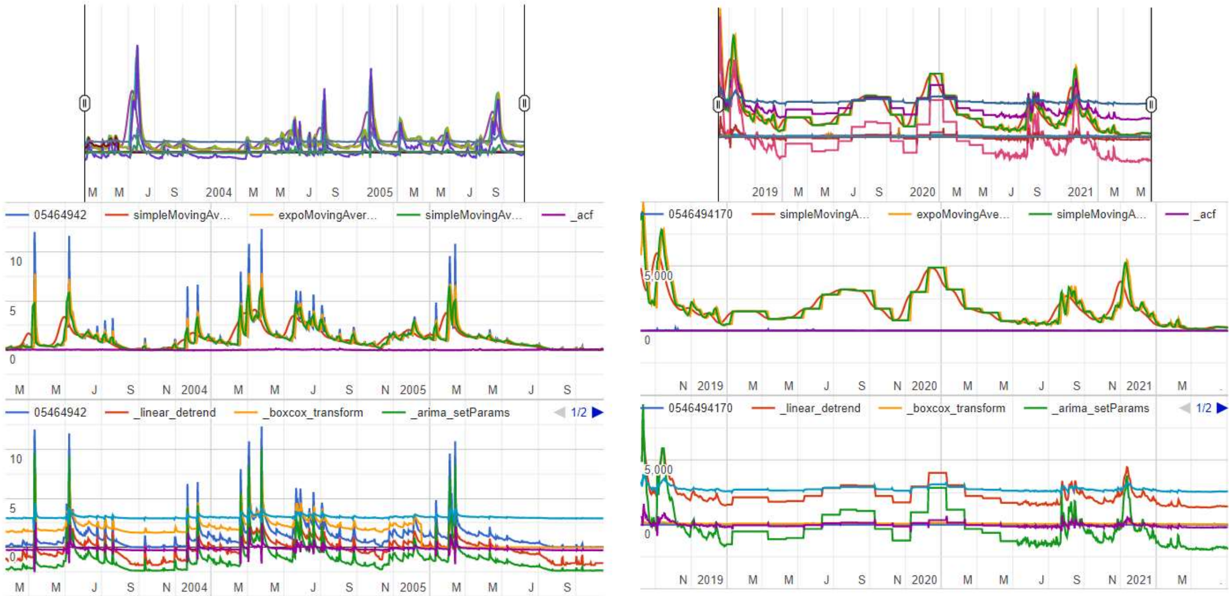
Figure 17. Elapsed time for executions at 250 stations in the case study.

The results of each of the simulations vary depending on the number of data points available within a specific station, temporal resolution, and errors that might be within the data itself. Figure 18 shows the different results obtained for different stations in the same area.

3.2. Workshop Feedback and User Experiences

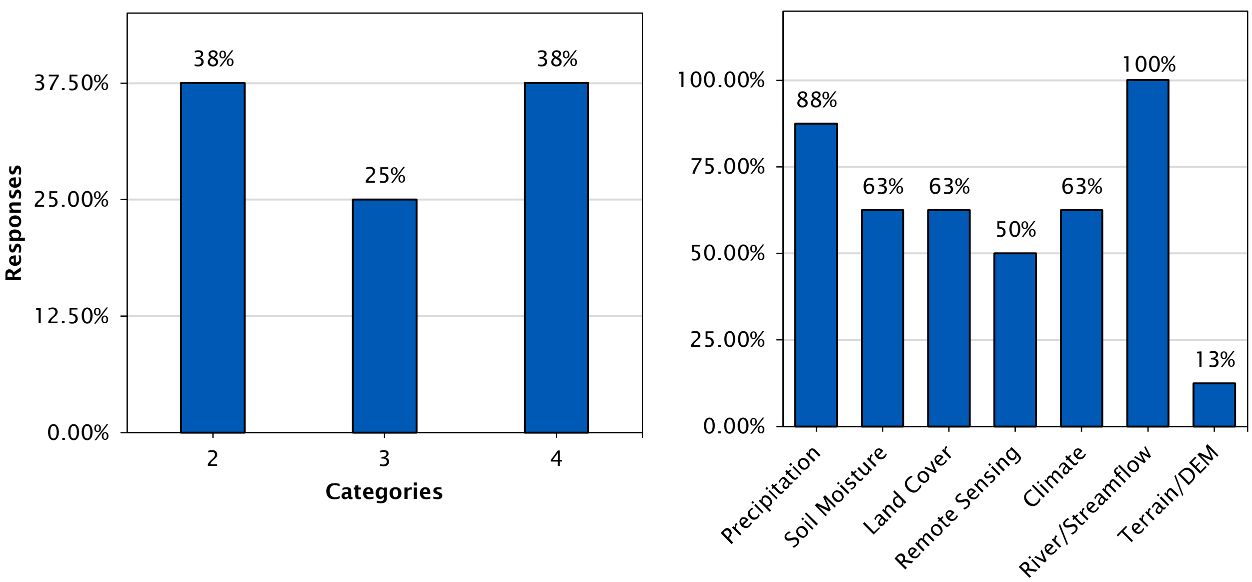
To assess the usability of the HydroCompute library and determine its potential benefits for research and education, a workshop and a presentation were conducted at a conference for developers and a department meeting, respectively. These sessions aimed to demonstrate the library's usage and capabilities, including the development of various case studies that showcased different features of the library, such as code migration from different programming languages, stepwise and functionwise executions, and integration with other web tools.

During and after the presentations, a survey was conducted to gather feedback from the participants. The survey included questions regarding the participants' backgrounds, understanding of the tool, and its usability across different domains. It also sought to assess the applicability and usability of the library's various features. The survey employed open-ended questions and a 5-point Likert scale style (1=Completely Disagree, 2=Somewhat Disagree, 3=Neutral, 4=Somewhat Agree, 5=Completely Agree) to gauge satisfaction and comprehension.



(a) (b)

Figure 18. Sample results for the queried stations for (a) Hoover Creek at Hoover National Historic Site, West Branch, IA and (b) WB Wapsinonoc Creek at College St at West Branch, IA highlighting reliability on available data.



(a) (b)

Figure 19. Usefulness rating of the library given by the participants. Questions (a) “On a scale 1-5 (1 being not useful at all and 5 being extremely useful), how would you rate the usefulness of HydroCompute for your field of work?” (b) “Which types of datasets or resources would you like to see processed with HydroCompute (Please select all that apply)”.

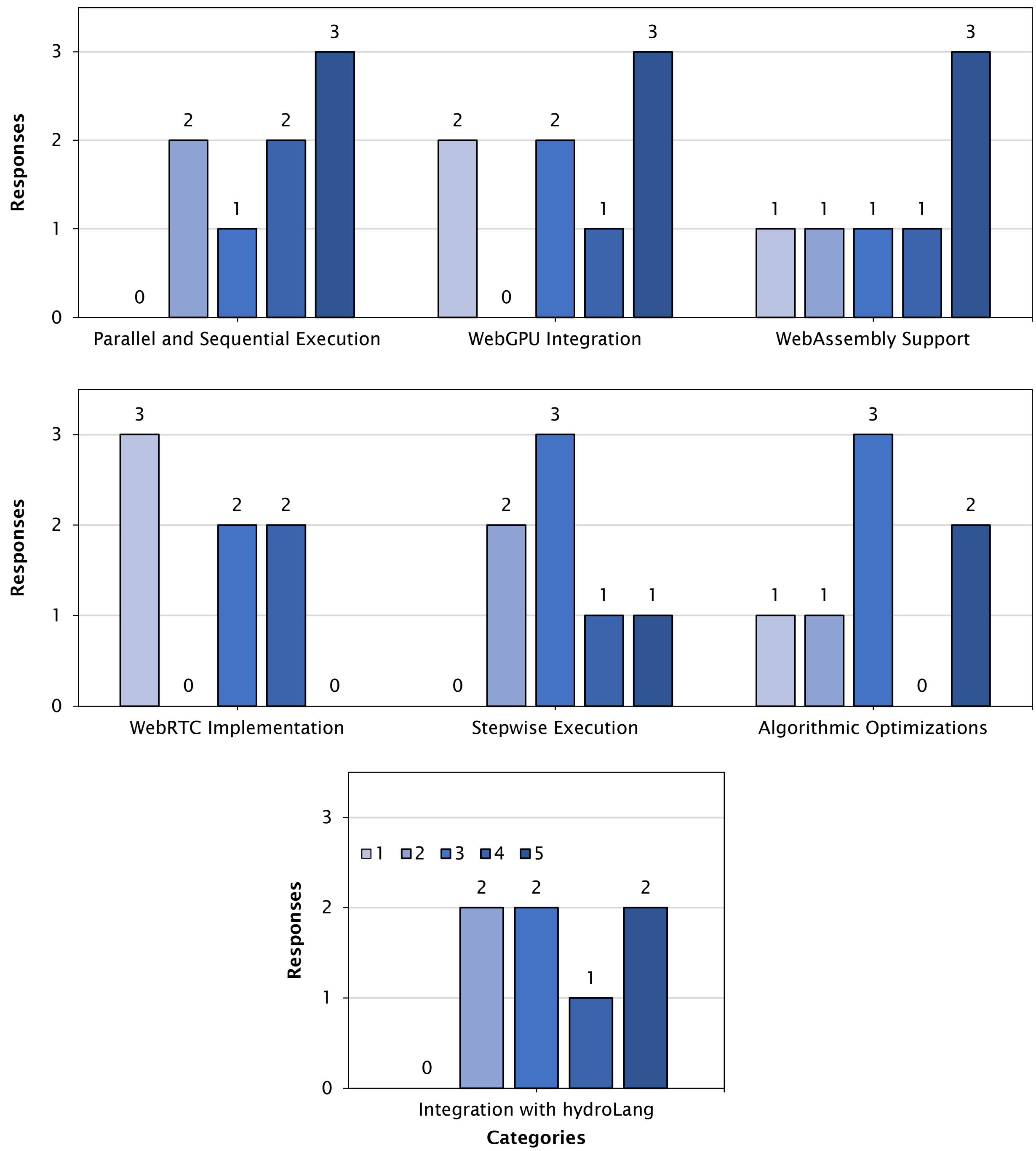


Figure 20. Results of survey utility of functionalities in the HydroCompute library. Question: “Please rate the utility of the following functionalities of HydroCompute on a scale of 1-5 (1 being not useful at all and 5 being extremely useful)”

The survey provided valuable insights into the library's applicability and user experience. Out of the participants (n=8), approximately 38% had backgrounds in hydrology and hydroinformatics. They highlighted the library's suitability for web application development, particularly with datasets related to precipitation, soil moisture, land cover, remote sensing, river and streamflow. Participants expressed interest in utilizing the library for tasks like flood forecasting, drought monitoring, surface water modeling, hydrological data management, and real-time monitoring systems. Regarding usability, 50% and 75% of participants expressed neutrality or agreement with the library's usability, respectively (Figure 19). Participants expressed a desire for higher levels of abstraction to simplify library implementation and emphasized the importance of including the library in public repositories for easy accessibility.

Functionalities like parallel and sequential execution, integration of new technologies, and integration with libraries such as HydroLang were given high valuation, as shown in Figure 20. Overall, the positive insights gleaned from the survey will be used to improve future iterations of the library and workshops, enabling the creation of enhanced features that cater to a wider audience.

4. Discussions

The HydroCompute library presents a promising solution to address computational challenges in hydrology and environmental sciences by leveraging cutting-edge web technologies and offering a flexible, user-friendly, and high-performance computational platform. Despite its advantages, there are potential challenges and limitations that need to be addressed to ensure the successful implementation and adoption of the library. Some of these challenges are discussed below.

Different execution times were observed from the test case evaluations for each of the engines implemented. These differences can be attributed to optimization techniques used by the compiler when understanding the reading executions required for each run. The optimization done by the compiler is largely dependent on the code provided and the different techniques utilized. Performance issues were observed when running the WebGPU's with the different benchmarking tests, specifically in the web worker environment. The WebGPU performance is heavily constrained by the device type running the application that is available to the user. When running different simulations, the devices and adapters got lost in integrated circuits when performing other operations in the machine. The combinations of CPU and GPU tasks running on a worker also heavily influenced the termination of an execution.

During the development of the project, computer bitwise organization, or endianness, was not thoroughly considered due to uncertainty in the interactions between the different types of data saved within the framework and the compilation types for each engine. This topic will be addressed in future releases of the project.

There are two topics that limited the full in-browser portability of the library during the development process: the underlying engine that transpiles the JavaScript code (for example, Chromium V8 in Google Chrome and Edge or SpiderMokey in Mozilla) and the full compatibility of the technologies used (in particular, Web Assembly and WebGPU). The first topic refers to the full implementation of ES6 modules and classes, while the latter represents a more difficult issue in terms of how these technologies are being adopted within specific browser vendors. Nevertheless, the library has been developed with the anticipation that all these standards will be universally adopted in the near future across all web browsers, thereby ensuring full compatibility.

It is important to assess the validity and applicability of the underlying algorithms that will be executed using the compute framework. During the implementation of ARMA processes for the case study, low reliability was observed in the forecasting results due to incorrect implementation, which was later corrected. Given the open nature of development, it is crucial to clearly define the problem statement to effectively leverage the capabilities of the library. Although the case study provides some examples, the ability to port code from different programming languages to web browsers necessitates a clear understanding of the intended purpose of the code once it is implemented in the HydroCompute's engine. Any issues with the simulation run, such as undefined instruction definitions, uncaught or unhandled memory leaks, or other implementation details, can arise from unclear instruction definitions or improper use of the engines.

Finally, while the HydroCompute library has demonstrated its capabilities in handling large-scale computations, there may be limitations when dealing with extremely large datasets. The performance and efficiency of the library can be affected by factors such as available memory, processing power, and network bandwidth on the user's device. In some cases, the library may not be suitable for applications that require processing massive datasets or running complex simulations that exceed the available resources on the user's device. To address this challenge, future work will focus on optimizing the library's memory management and computational efficiency while exploring innovative solutions that can harness the power of distributed computing to handle extremely large datasets. One such solution is to leverage WebRTC, a technology already integrated within the HydroCompute library for peer-to-peer communication, to enable distributed computing across multiple devices.

5. Conclusions

In conclusion, the HydroCompute library offers a powerful and versatile solution for addressing computational challenges in hydrology and environmental sciences. By leveraging cutting-edge web technologies, such as Web Workers, WebGPU, Web Assembly, and WebRTC, the library enables users to perform efficient and scalable computations within client-side web applications. The modular architecture, integration with existing frameworks, and compatibility with different programming languages enhance the library's adaptability and applicability across a wide range of hydrological and environmental applications. The case studies demonstrate the library's performance capabilities and highlight its potential to contribute to the advancement of hydrological and environmental sciences through improved data processing, analysis, and decision-making. By providing an open-source, user-friendly, and high-performance computational library, HydroCompute aims to foster a community of users and developers that will contribute to its growth and improvement, ultimately benefiting researchers, practitioners, and educators in the fields of hydrology and environmental sciences.

Future work will focus on the addition of new specialized scripts that contain heavily used and computationally expensive routines, which will enhance the library's functionality and promote better integration with hydrological sciences. This will involve incorporating new algorithms and techniques that are specific to hydrological sciences, as well as expanding the library's compatibility with different programming languages and platforms. In addition, in-browser transpilation using bundlers such as WebPack and Babel will be utilized to package the library and host it in package managers so the library can be used in development environments such as Node.js or port directly into the browser using a content delivery network. Furthermore, efforts will be made to optimize the framework's performance, particularly in terms of reducing execution times and minimizing resource utilization. This will involve exploring new optimization techniques, as well as leveraging advancements in hardware technology to further enhance the library's capabilities.

Another promising future work is to utilize WebRTC for distributed computing, which can allow the HydroCompute library to segment and distribute processing tasks among a network of devices, such as personal computers, smartphones, or tablets. This approach would allow users to share their computational resources to collaboratively process large datasets or run complex simulations that would otherwise be unfeasible on a single device. Implementing adaptive algorithms that dynamically allocate resources based on the size of the dataset and the capabilities of the participating devices could further optimize the overall performance and efficiency of the distributed computing network.

Abbreviations

API	Application Programming Interface
ARMA	Autoregressive Moving Average
BMI	Basic Modelling Interface
CSS	Cascading Style Sheets
C/C++	C-based Programming Language
CPU	Central Processing Unit
CUDA	Compute Unified Device Architecture
CUAHSI	Consortium of Universities for the Advancement of Hydrologic Science
DAG	Directed Acyclic Graph
DOM	Document Object Model
ES6	ECMAScript 6
XML	Extensible Markup Language
FLOP	Floating Point Operations
GLUE	Generalized Likelihood Uncertainty Estimations
GPU	Graphics Processing Unit
HPC	High-Performance Computing
HTML	Hypertext Markup Language
JSON	JavaScript Object Notation
MPI	Message Passing Interface
MOPEX	Model Parameter Estimation Experiment
NOAA	National Oceanic and Atmospheric Administration

NOAA GHCN	NOAA Global Historical Climatology Network
NaN	Not a number
OpenACC	Open Accelerators
OpenMP	Open Multi-Processing
EMSCRIPTEN	Open source compiler for C/C++
TypeScript	Programming Langauge, subset of JavaScript
FORTRAN	Programming Language
Rust	Programming Language
AssemblyScript	Programming Language
JavaScript (JS)	Programming Language
WebAssembly (WASM)	Programming Standard
Tensorflow.js	TensorFlow for JavaScript
USGS	United States Geological Survey
UI	User Interface
WebGL	Web Graphics Library
WebRTC	Web Real Time Communication
W3C	World Wide Web Consortium

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