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 explored by Reed et al., (2010).

Large-scale parallelization of hydrological models has been studied using standards such as OpenMP and Open ACC for graphical processing units (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 generalized likelihood uncertainty estimation (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 spatio-

temporal data resolutions, allowing 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 & 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., 2022; Erazo et al., 2023). 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). Novel machine learning and artificial intelligence libraries allow for the creation of models that run on the client side. Examples of these libraries are TensorFlow, CoreML, ONNX, and MediaPipe (Sit & Demir, 2023). The continuous adoption of technologies allows for new and specialized implementations to be added to client-side environments. For instance, TensorFlow.js, a web-based implementation of TensorFlow, 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. Section 3 presents 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, and Section 5 provides a discussion on future work and conclusions.

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 applications. 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 explored 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, specifically using a directed acyclic graph, were set to analyze functional dependencies, while dynamic memory allocation through data movement instead of cloning in both the CPU and GPU optimized resource utilization. The implementation of parallel execution involving simultaneous processing of independent tasks and sequential execution, ensuring task order dependency (Rönngren & Ayani, 1997), was a primary focus during the development of the library. These computational techniques are found in hydrology, with parallel executions processing large datasets and complex models, while sequential execution handles interconnected modeling phenomena such as assessing flooding risks or hydrological routing (Zhou et al., 1998; Vivoni et al., 2011).

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 directives. 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 ensures security through its own memory management and execution context. Furthermore, WebAssembly enables the utilization of legacy low-level applications, allowing developers to scale systems by reusing existing code. This eliminates the need for complete application rewrites, leading to significant performance improvements, particularly in industries with computationally demanding applications.

WebRTC: WebRTC is a set of standards that allows peer-to-peer communication through a semantic API available in major web browsers (W3C, 2023b). It was released in 2011 with applications for video conferencing and peer communication leveraging the technology. The API contains methods that allow for large amounts of data to be shared among peers without the need for external servers to host and manage traffic for the data. An example of how the technology has been used in water research and education has been developed by Zhang et al. (2022), with a focus on flood modeling and simulation directly for democratized information sharing.

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; and (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 comprises two main approaches: a computational scheme driven by engines for JavaScript, Web Assembly, and WebGPU, and a data-sharing scheme driven by a WebRTC engine. These are managed through four primary layers: a connection layer for data sharing and configuration, an engine layer that switches to the required engine based on user inputs and also hosts the WebRTC handler, a threading layer for thread setting based on simulation requirements and keeping track of results, and the scripts layer that calls web workers to fetch scripts in specific directories based on the handlers for each engine. User control over these connections is centralized through the connection layer, as depicted in Figure 1, allowing users to make corrections to results or data handling and configuration as required. Figure 2 shows how to create different types of runs using the library, from initializing an instance to running a simulation. The configuration object passed into the library for a run contains the required specific and default arguments.

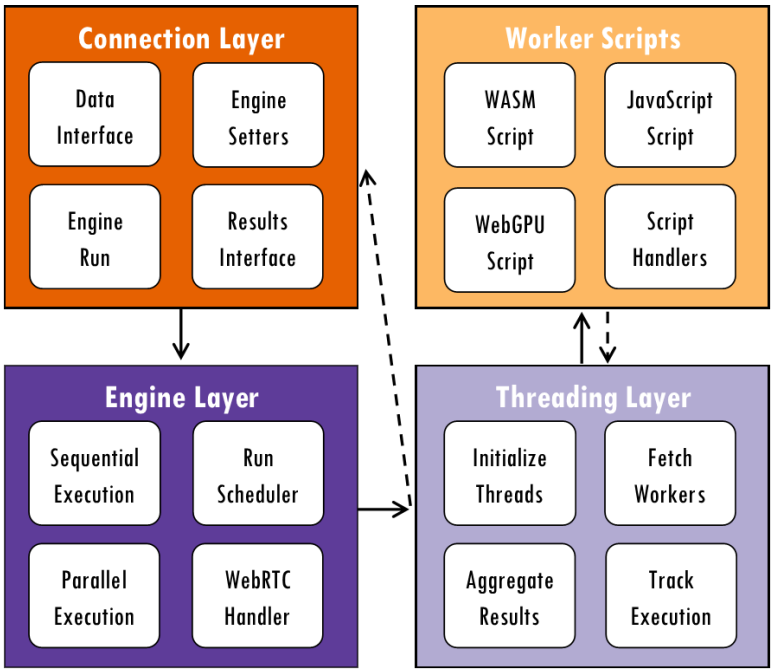


Figure 1. Architecture and components of the HydroCompute library. The results, once a simulation has finished, are temporarily saved in the threading layer and then transferred to the connection layer..

```
// Initialize a HydroCompute instance
const compute = new hydrocompute('engineName'); // Specify engine name
// or default to JS engine
const compute = new hydrocompute();

// Set simulation data by grabbing it from a file path as a JSON file
compute.data(dataFilePath);
// or save the dataset in the JS running environment
compute.data({ id: dataFileName, data: some2Dor1Darray });

// Run the library using functions found in the engine's scripts folder with dependencies
compute.run({
  functions:    [Array of functions per step],
  dataId:       [Array of Id names],
  dependencies: [Array of dependencies],
  funcArgs:     [Other arguments per function to use]
});

// Alternatively, use a script found in the local environment using a 'main' function
// interface and the data saved in the compute instance
compute.run('scriptFilePath');
```

Figure 2. Different modes of initializing a HydroCompute instance, setting simulation data, and running the library.

2.3.1. Connection Layer

The connection layer keeps track of the number of engines available for use, the number of 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. It is the main interface all the other engines interact with. The basic running requirements are saved and passed to the run function 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 use of the computation or the data sharing engines. These 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. Figure 3 shows the workflow for initializing a simulation run, specifically how the data is parsed and saved in the library's local storage context. 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, 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.

(3) Data Validation: The input data must not be an empty array or contain faulty characters or anything other than numbers, whether decimal or whole, that are intended for use in the simulation.

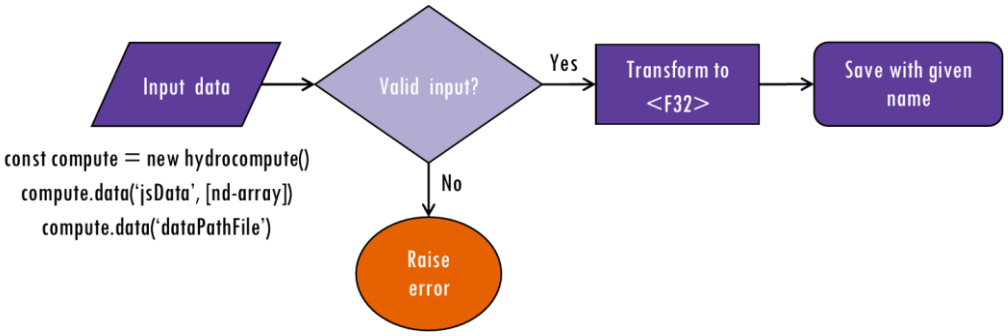


Figure 3. On initializing data for a run.

The data is then registered using a naming convention specified by the user or a random assignment of letters and numbers. Given that the domain of interest is hydrology and environmental sciences, float 32-byte numbers were considered to have 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 described in Table 1. Once all default requirements have been established, the `hydrocompute.run()` commands trigger an instance of the engine class to execute the simulation, following the flowchart shown in Figure 4. More discussion on what DAG represents and how it is used will be given in the following sections.

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.

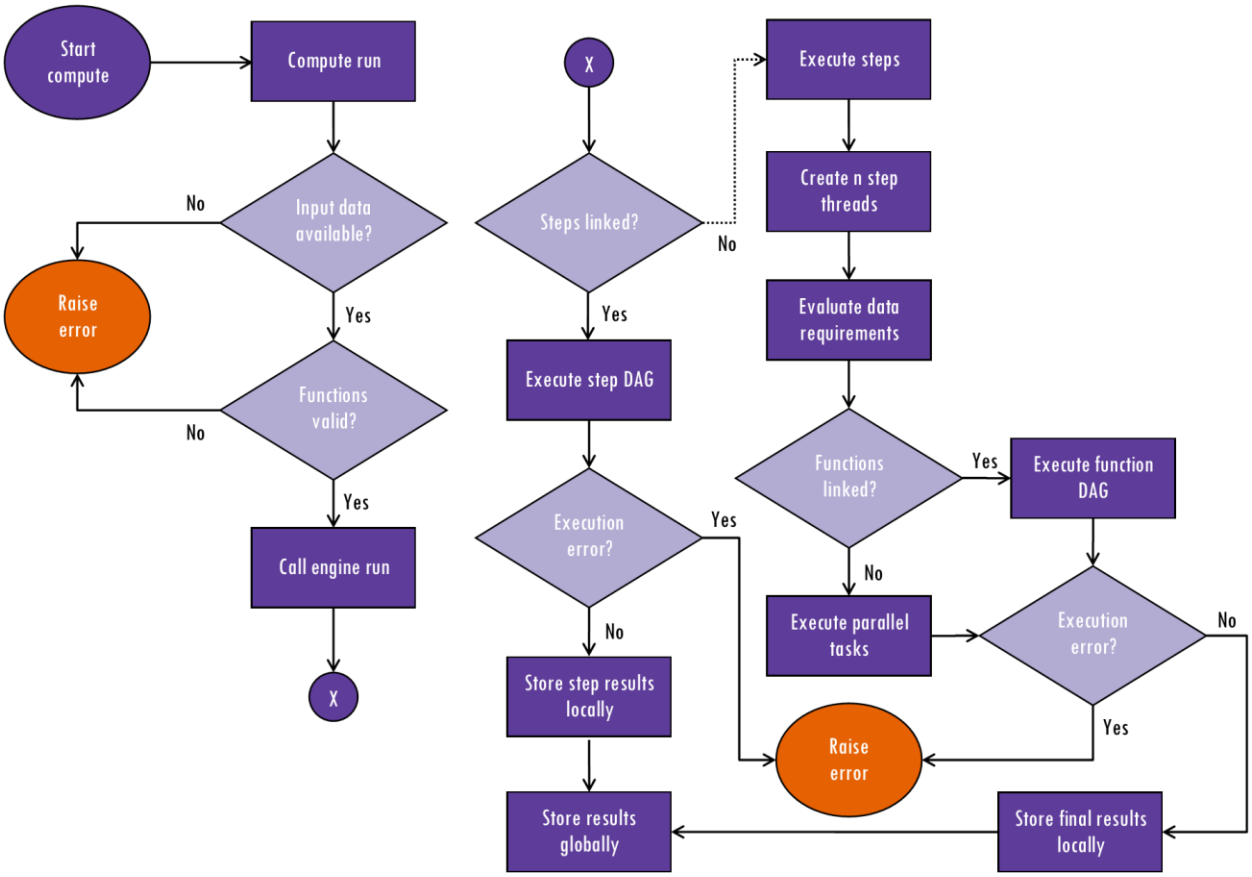


Figure 4. Flowchart of running a simulation.

2.3.2. Engine Management

The engine class serves as the fundamental driver for executing the available APIs within the HydroCompute library. Figure 4 shows how initializing an engine switches between the different engine types. The methods in the layer 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.

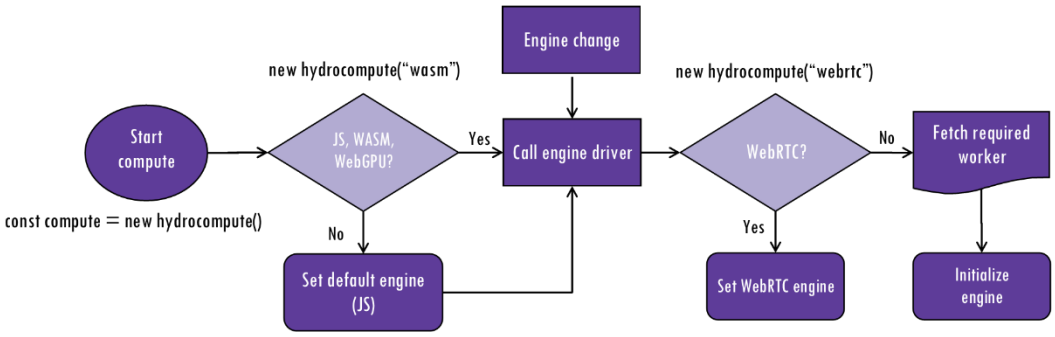


Figure 5. Flowchart of initializing the library or changing engines.

The scheduling of each thread is determined by the number of functions to run, their dependencies, and the data size. This is achieved either by partitioning the input data among the available engines or by assigning multiple functions to the same data using threshold functions implemented in the library that are accessible through the API. These functions include arbitrary partition sizes given by the users. 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 graph algorithm is implemented to ensure efficient thread coordination. After each task is completed, the results are combined into a single result space, which is interfaced within 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 using a directed acyclic graph implementation with promise-based executions for steps with dependencies and sequential executions for steps without dependencies. This approach ensures execution based on dependencies and linkage requirements.

Parallel Execution: A promise-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 6. The number of threads set to run is limited by the 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 6. Parallel execution of a set of functions for a given step.

By limiting the number of threads per batch to the total number of available 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 thread engine.

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 tasks that will execute in the given order of the results required down the line (Figure 7). This workload is then submitted to run under the set 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, fun-
cArgs: 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 7. 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 8. 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 8 and 9). The algorithm is provided with an input object that includes the functions, a dependency array in DAG format, additional arguments, and the type of execution (stepwise or functionwise). Promises are used to execute the functions, resolving all functions once they have completed their respective executions. The values returned from each function are stored in an array and passed as arguments to subsequent functions as specified by the dependency list. The precedence

of each function is assumed within the algorithm, and parallel execution occurs when a function call has no dependencies.

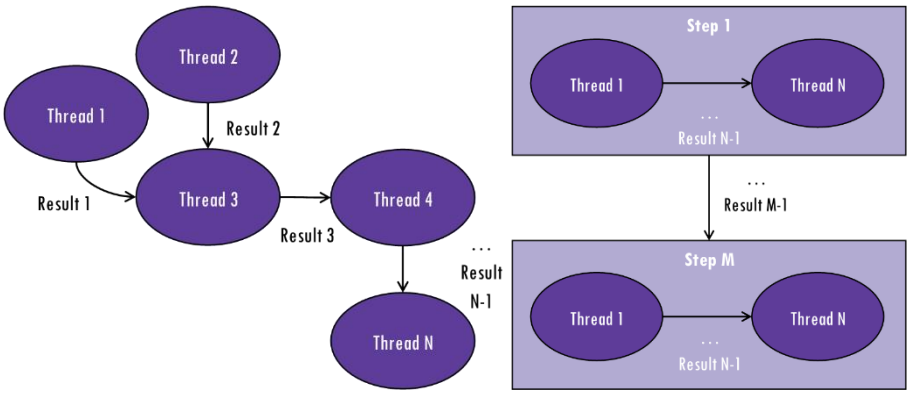


Figure 9. Execution for a single step DAG (a) and execution for a multiple steps DAG (b).

2.3.4. Thread Manager

The thread manager class creates a scaffold containing specific running implementations for each thread requirement (Figure 10). It contains local 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.

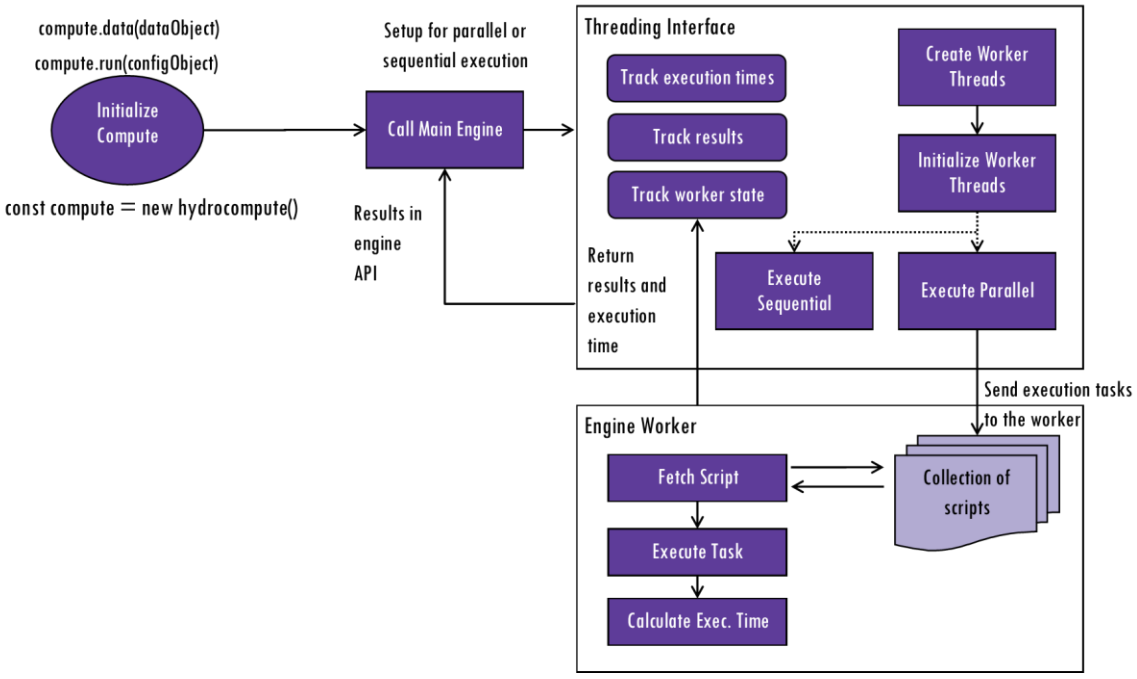


Figure 10. Thread initializer and executioner.

When an engine initializes the class, the location of where each worker is as well as the name of the engine are provided in order to run the execution context. 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.

Given the class declaration of ES6 modules, the architecture allows for multiple instances to run simultaneously, allowing for separation of interests when possible. This also means that the engines can be changed according to their functions using the library. All engines are driven by worker scripts that contain ready-set methods for manipulating the input data. The worker structure searches for the required function execution name in the collection of scripts available per engine. The function scripts are user-tailored and can be saved either in the specified folder for scripts for each engine or in the library's local directory for direct calls. Figure 10 shows the specific structure for each of the available engines. The JavaScript and WebGPU scripts have an object structure with all the defined function names for interfacing, while the WASM-compiled code uses the glue code generated by the specific language compiler—i.e., EMSCRIPTEN for C/C++—to interface with the binary code generated.

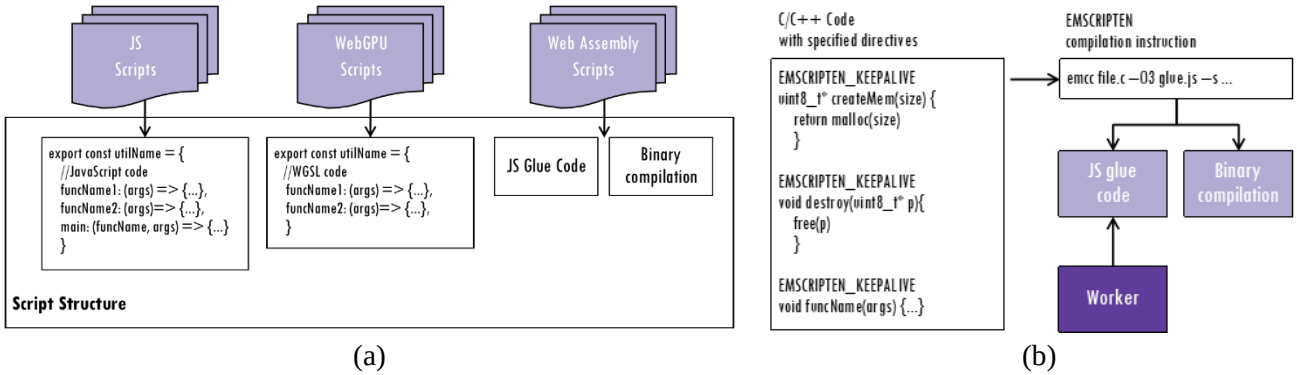


Figure 11. (a) Structure of the worker scripts for each engine and (b) structure of the EMSCRIPTEN compiled code from C/C++ with required directives for in-browser manipulation.

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.

WebGPU Worker: The WebGPU worker leverages the WebGPU API through different methods that call GPU adapters and devices available on the machine running the browser. The adapter is specific to the web browser engine and has native memory growth and allocation. The WebGPU worker is best suited for analyzing large-scale data and becomes inefficient with

smaller data since the architecture of GPU adapters allows for native parallelization. Similar to the JavaScript worker, the scripts are kept as objects containing the required GSLS shading code provided by a specific name definition within the object. Buffers and shaders are created as modules that are dispatched to the device to be copied from the CPU to the GPU and back, clearing the data as it is moved from one point to another to avoid memory leaks or unnecessary storage.

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 from the browser, the engine allows the execution of different types of Web Assembly-compliant code under the same scope. As an initial step for this project, two Web 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 allows for easy compiling through EMSCRIPTEN, outputting fast and small-sized bundles. AssemblyScript, on the other hand, is a TypeScript(TS)-like subset for Web Assembly that enables web developers to easily transition to writing code from a JS or TS mindset.

WebRTC Implementation: The WebRTC engine creates a wrapper around the WebRTC features for efficient data transfer, such as results from simulations on another machine or transfers from a peer's local machine, given the tasks are run on the same network. It provides ready-set methods to save large data sizes directly into the available sources object, leveraging the shared structure within the library. During initialization, the engine sets up connection parameters, such as the maximum message size (65 kB), required data 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. Case Studies

Two case studies were developed to evaluate the performance of data-driven heavy computation: a classic benchmarking case using naïve matrix multiplication and a time series analysis with

real-time data from gauging stations across Iowa. The implementation was executed on a machine 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,Microsoft Edge v.110.0.1587.56, and Mozilla Firefox v.118.0.1. The Chrome browser was used for WebGPU executions, and the other two were used for WASM and JS executions. Limitations found when running different types of executions in the Firefox browser, specifically in regards to the WebGPU engine, are mentioned in the Discussions section. The case studies can be found in the GitHub repository, with descriptions of how to run them in each respective folder as well as the respective routines used for each.

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 equation solvers (Volkov & Demmel, 2008). Moreover, the case study allowed for the setting of thresholds for the usage of specific engines based on the number of operations required. To test the engines, square matrices of varying sizes (ranging from 4^2 to 5625^2) were generated and filled with random numbers between 0 and 1000. To evaluate worst-case scenarios and performance trends in the web browser environment for the implemented engines, we implemented a naïve matrix algorithm as scripts for all engines with both $O(n^3)$ complexity and floating-point operations (FLOPs) count, as detailed in Hunger (2007). This algorithm involves three nested loops for matrix calculations, resulting in $O(n^3)$ multiplications for square matrices. Notably, WASM and JS use CPU resources, while WebGPU employs a GPU multicore architecture, leading to different transactional operations. For large square matrices, JS or WASM multiplications are roughly n^3-n^2, while WebGPU divides transactions into predefined workgroup sizes, resulting in $(2n^3)/64$ transactions. These estimates do not account for factors like memory caching, CPU speed, and hardware/software specifics, which can significantly affect the actual transaction counts.

Three scenarios were analyzed to assess engine performance. The first involved running a single thread for increasing matrix sizes,; the second used multiple threads for smaller size matrices; and the last explored the difference in workgroups for large matrices using the WebGPU engine.

Scenario 1 shows similar behavior for all engines for matrices smaller than 16^2, and a clear trend toward an increase for the three engines, with WebGPU performing best for larger matrix computations as shown in Figure 12.

Scenario 2 runs an n-number of threads in parallel, each representing the maximum number of data allocated within the running environment without forceful stoppage by the browser. Once a thread is finished, the result is aggregated into the library's result space, where the execution times for each of the threads are recorded. Figure 13(a) shows matrix sizes from 16^2 to 128^2 as a

set of floating-point operations (FLOPs) in thread counts of 2000, 4000, 8000, and 16000. The values for FLOPs and the execution time were normalized using the thread counts by dividing both axes by the number of threads, and the same procedure is done for larger matrices from 240^2 to 1024^2 for thread counts of 100, 200, and 400 as shown in Figure 12(b). From this, thresholds were found for when to use which engine; specifically, JS and WASM are more efficient for matrix sizes below 124^2, and WASM for matrix sizes below 318^2. Afterwards, the WebGPU engine has the best performance.

Scenario 3 evaluates the limits of the WebGPU engine in terms of maximum FLOPs; testing was done with matrices of sizes $1{,}024^2$ through $5{,}625^2$. The calculation used a single instruction—one thread—and a log-linear tendency was observed for very large matrix sizes. Different workgroups were used to study the relationship between the WebGPU switching mechanisms and the hardware limits. Figure 15 shows how different workgroups compare as single workers are submitted for execution for workgroups of 1 through 64 instructions. As stated in the WebGPU specification at W3C (2023a), workgroups represent the size of shaders that are to be computed in the x,y, and z directions and default to 64 if not given to the function. The sizes, then, represent the multiplication of all the instructions required to drive a computation, i.e., 8x8x1 = 64 instructions, which can be written in code as `@workgroup(8)` or `@workgroup(8,8,1)`. Given the naïve implementation, workgroup size 1 yields the best results in terms of performance. This is in accordance with how the concurrency of the GPU through the WebGPU API allocates tasks. The instruction was cheaper to run on a single workgroup than to partition the data into multiple chunks. There was a non-linear increasing tendency in the data for all the tested sizes. Throughout the given workgroups, there was a significant execution time jump at size 4096, which is linked to the data allocation driven by the device's hardware, maximum paging size available per instruction, and number of cores per device. After 4096, a switch in data allocation was performed by the device, which then showed the same increasing behavior as previously stated. It is important to mention that this mechanism is highly dependent on the device's memory management and a specific vendor's GPU schemes.

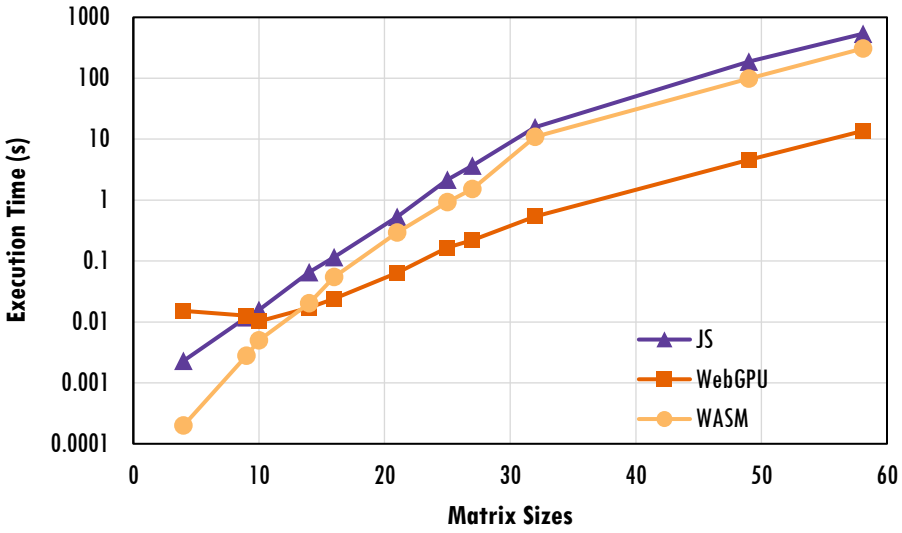
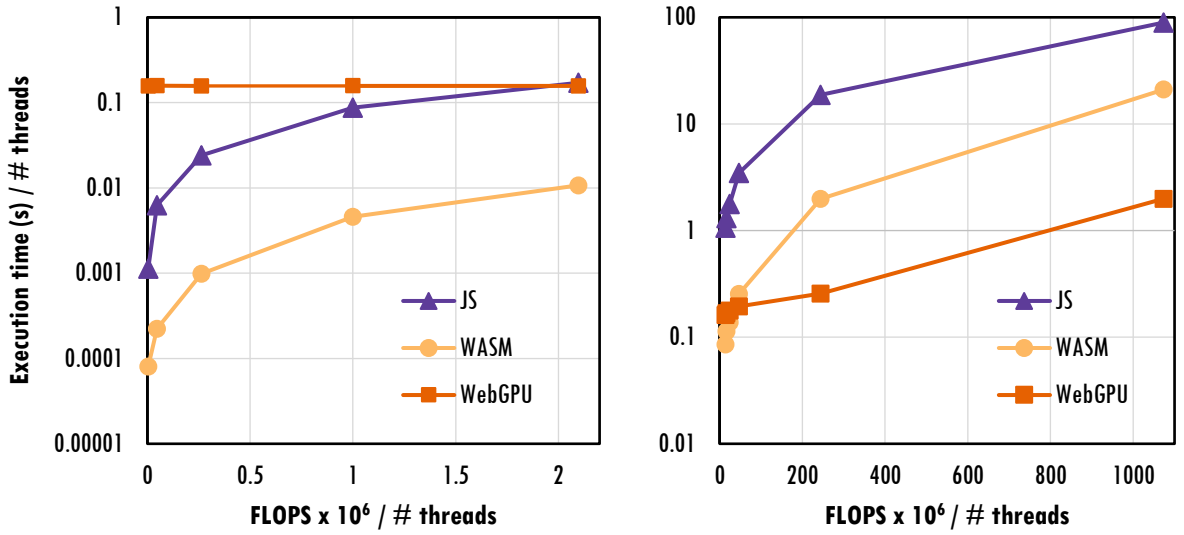


Figure 12. Results from using a single thread on multiple matrix sizes ranging from 4^2 to 60^2 in semi-log scale base 10.

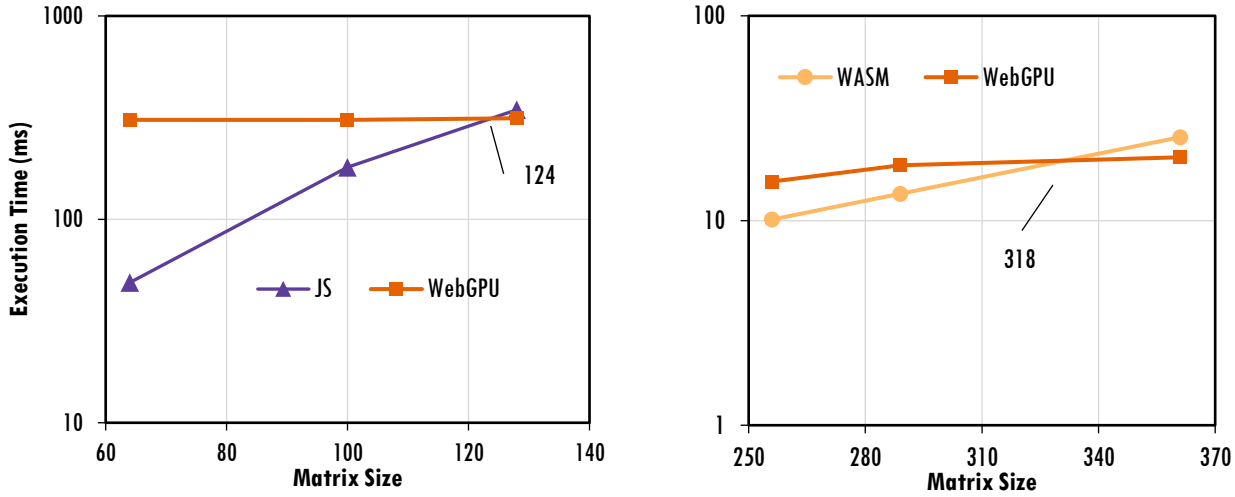
The evaluation of the engines' performance revealed that significant differences exist in terms of running time across the different implementations of the operation. While the WASM and JS code demonstrated faster performance for smaller-sized matrices, WebGPU proved to be more efficient for larger matrices. 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 efforts by the GPU device. Furthermore, suboptimal memory access patterns for small-sized operations result in higher memory access latencies and lower performance. The implemented WebGPU shading code becomes increasingly important when dealing with large data chunks that require managing the massive parallelism of the GPU and leveraging its memory bandwidth and caching capabilities.

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 task running in the background. For example, whenever a click event or switching tabs with a video rendering or similar happened, the adapter that the WebGPU API connected to got lost with no reconnection. This behavior was seen whenever running either the multithread tasks or when running a single thread with large matrices.



(a) (b)

Figure 13. (a) FLOPx10^6 vs. execution time in seconds for 2,000, 4,000, 8,000, and 16,000 threads for matrices of sizes 16^2 through 128^2 and (b) FLOPx10^6 vs. execution time in seconds for 100, 200, and 400 for matrices of sizes 240^2 through 1024^2. Each execution FLOP value and execution was divided by the corresponding thread in semi-log scale base 10.



(a) (b)

Figure 14. Cutoff for JS and WASM engines in comparison to the WebGPU, at sizes (a) <124 and (b) <318 respectively.

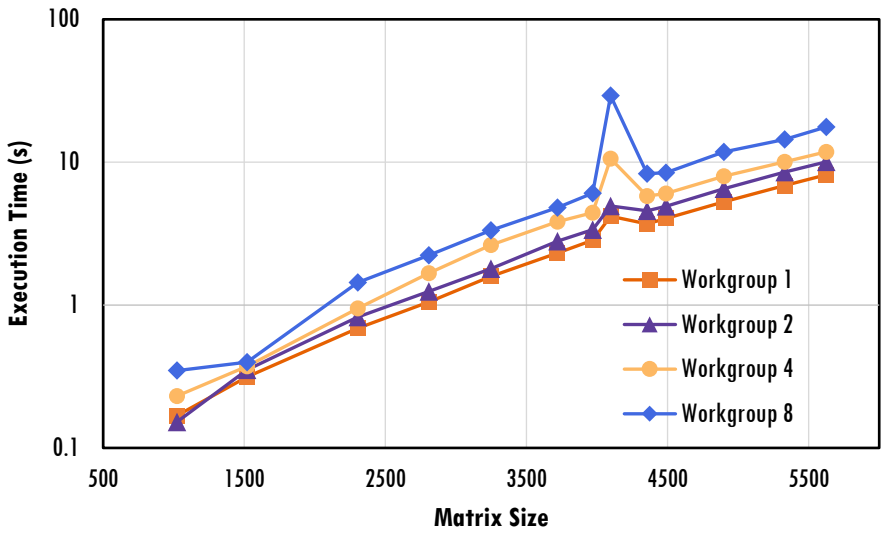


Figure 15. Testing for different workgroup sizes for matrices from 1024^2 to 5625^2 using the WebGPU engine. The jump at 4096 represents a switch in data allocation done by the GPU device.

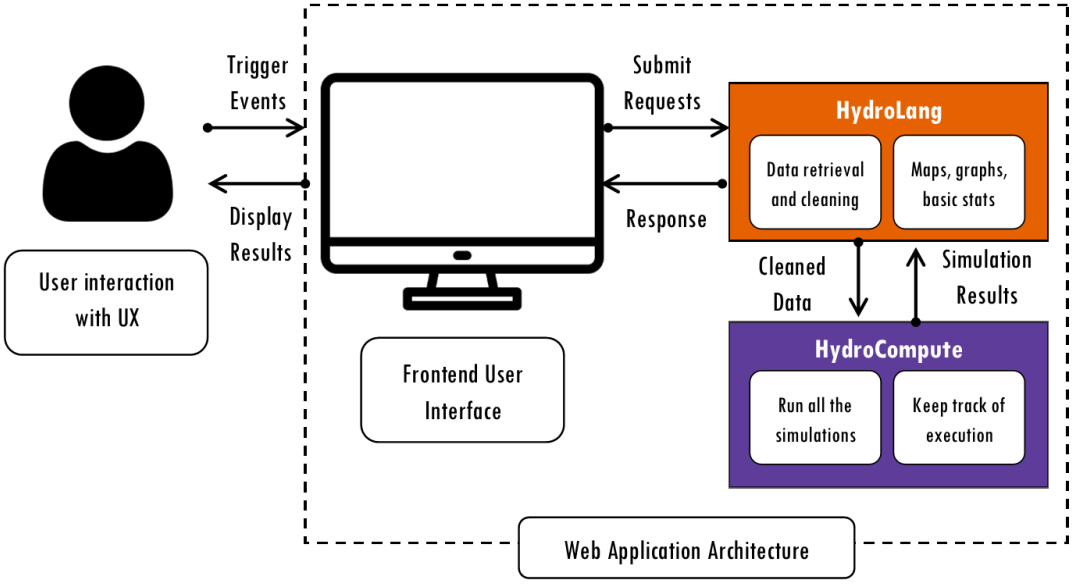


Figure 16. Architecture of the web application. HydroLang works as a front-end developing tool and data connection, HydroCompute works as a heavy computing client-side library running external scripts in the background.

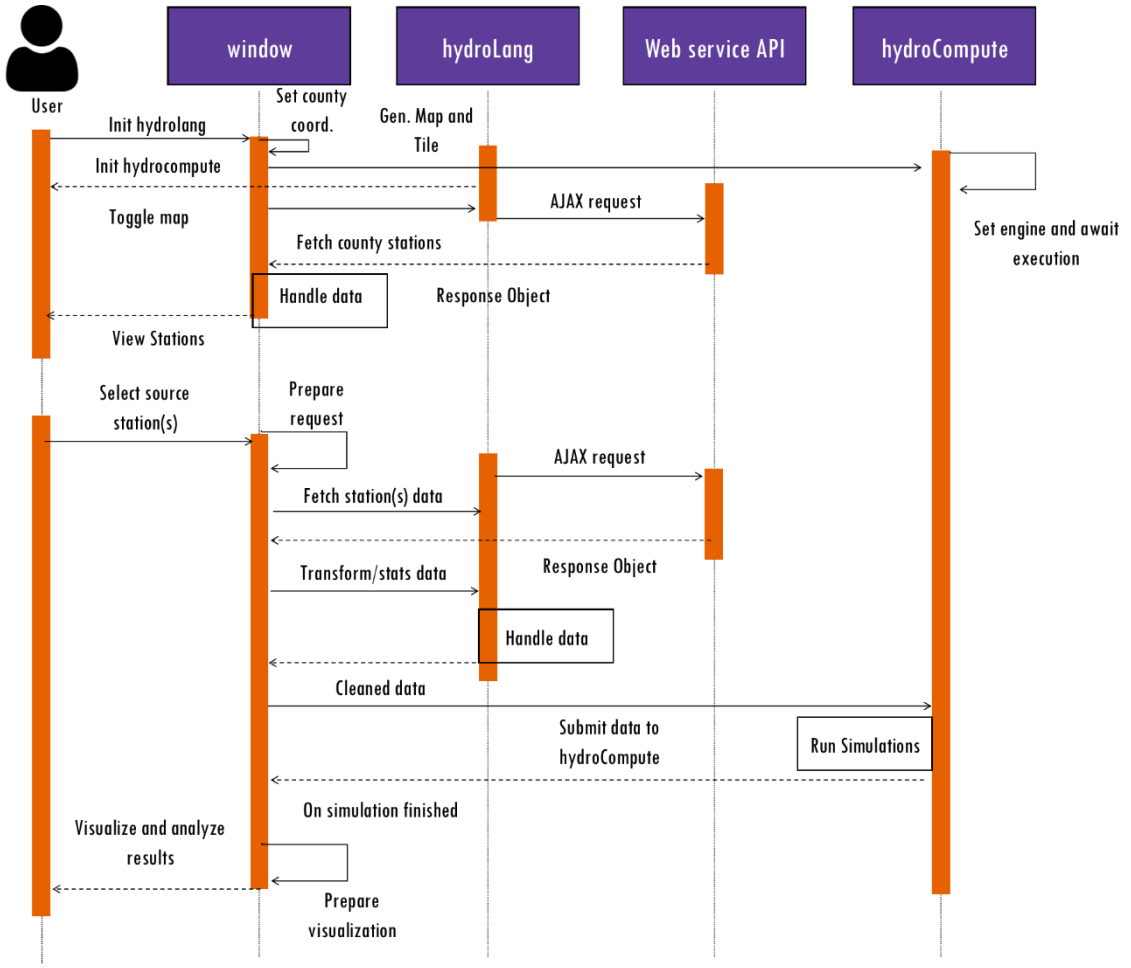


Figure 17. Sequence diagram for the case study.

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

To highlight the usage of the library, 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 showcase the development pipeline using the library alongside complementary web-based tools. This is represented in the application architecture and sequence diagram shown in Figures 16 and 17, respectively, and the user interface of the application shown in Figure 18. The application connects through statewide rectangular coordinates per county or per rectangular selection on screen to CUAHSI WaterOneFlow services (Castranova et.al, 2018) for daily values from USGS (USGS, 2023), MOPEX (Shaake et al., 2009), and NOAA GHCN (Peterson et al., 1997) to query and obtain all the available streamflow stations with daily readings falling within the set boundary from 1900 through the day of analysis. This is done using the web-based hydrological framework HydroLang (Erazo et al., 2022), which retrieves and cleans streamflow data, and the HydroCompute library used to predict timebound streamflow using autocorrelation functions, the auto-regressive moving average (ARMA) process, and simple and exponential moving averages, following a similar pathway as Vecchia (1985).

The design of the dashboard leverages the tools found within the HydroLang framework, including data retrieval, cleaning, maps, and graphs. These are the less computationally expensive tasks, while all the heavy lifting for the analytical part is done by HydroCompute using a collection of time series analysis functions implemented to work specifically for the case study. The functions used for the analysis were written in JavaScript (exponential and simple moving averages) and in C code compiled in EMSCRIPTEN (ARMA, moving averages, transformations, and autocorrelation functions). These functions were written using (Kottegoda & Rosso, 2008) and can be found in the supplementary materials of this manuscript and the library's repository in the scripts folder for the JS and WASM engines. For each required simulation, the HydroCompute main engine was switched to fetch the external scripts provided for the analysis, initiating with the JS engine for the first two simulations and the WASM engine after. The user interface is kept organized for further data manipulation and cleaning while the compute framework handles the heavy workload on the backend, meaning that the user is able to read the data information and basic statistics while the analysis processes are running out of the main thread.

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 strictly 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 conditions that would categorize the data as faulty. The number of executions varied by station, as the implemented analysis functions depended on the number of executions per algorithm and the number of required transactions. For example, stations in or near rivers or streams that are used in cities have more records available since 1900 in comparison to stations near small streams or remote areas. Since the main task is to obtain daily values, data sizes per station varied from 0 records to over 40,000, and whichever amount was obtained was used to run the simulations as required. Specifically, there were 33 algorithmic function calls per station done on the HydroCompute library, as described in Table 2.

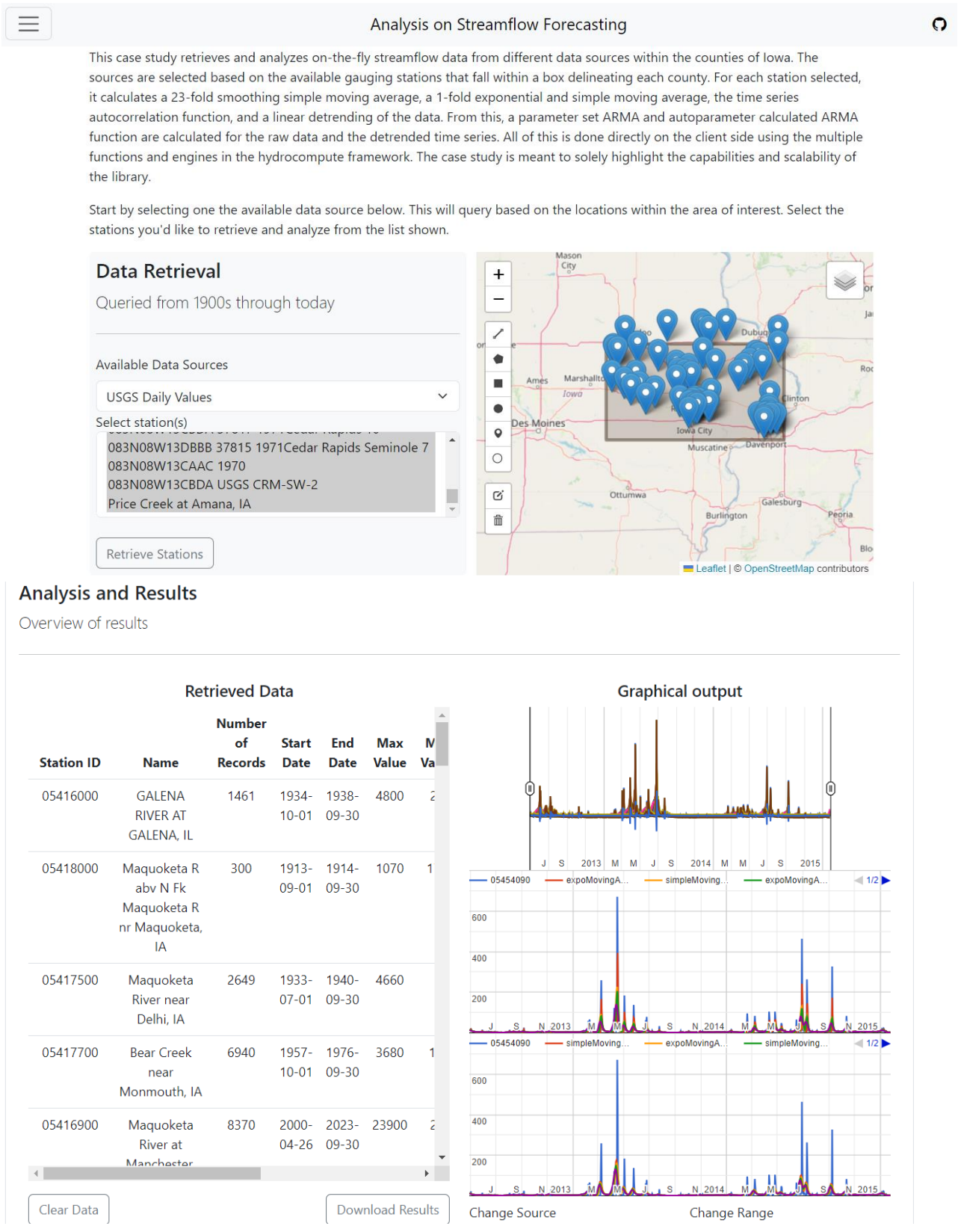


Figure 18. Screenshot of the web dashboard for streamflow time series analysis for real time USGS gauge stations in eastern Iowa.

Table 2: Simulation methods for the case study.

Simulation	Description
#1	Compute exponential moving averages (alpha = 0.5) and simple moving averages (window size = 5) an arbitrary number of times (23) and observe a gradual smoothing of results with each iteration running sequentially, written in JavaScript
#2	Compute simple moving averages (window size = 5) and exponential moving averages (alpha = 0.5) in parallel, 1 of each written in JavaScript.
#3	Compute the autocorrelation function, Box-Cox transformation, linear de-trended time series and ARMA with auto parameter update in parallel, 1 of each written in C and compiled using EMSCRIPTEN.
#4	Compute de-trended linear time series, and ARMA with auto parameter update using the previous results running sequentially, 1 of each written in C and compiled using EMSCRIPTEN.
#5	Compute exponential moving average (alpha = 0.5) and ARMA with auto parameter update using the previous results running sequentially, 1 of each written in C and compiled using EMSCRIPTEN.

To test the application, stations across different counties in the state were queried through a rectangular selection tool implemented in the map interface. Separate from the map interface, a drop-down selection button was added containing the names of the counties in the state, so the user can explore which stations are available in specific locations. The results of execution time show a linear relationship between time, the number of data points available at each station, and the number of stations within the selected area. Figure 19 shows running the 33 functions in both parallel and sequential modes. Querying a quarter of the state (around 250 stations in the northwestern part of the state) and data retrieval and cleaning took approximately 9 minutes, including around 3 minutes for the data retrieval and cleaning and 6 minutes for the analysis.

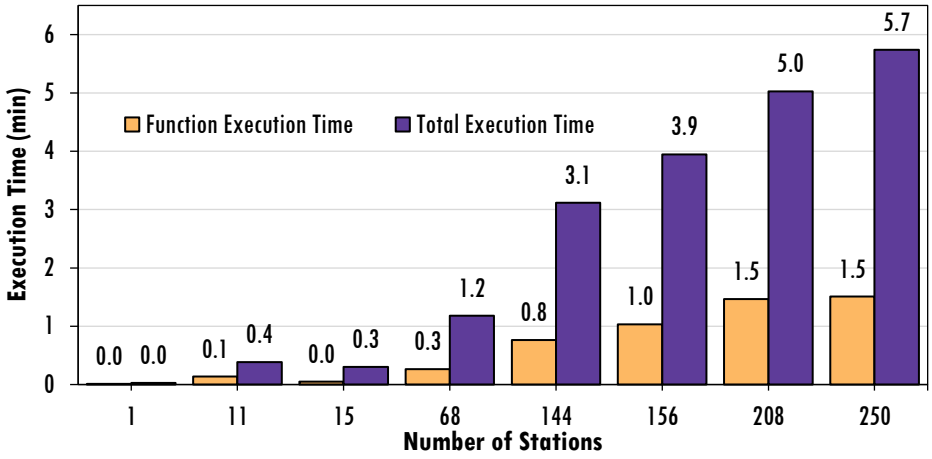


Figure 19. Elapsed time for executions at 250 stations in the case study.

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 20 shows the different results obtained for different stations in the same area, highlighting how the results from specific stations vary largely depending on data availability and time constraints. The stepping-like features in graph (b) represent a repetition in values that cannot be guaranteed to be accounted for either in the case study development or the incoming location values.

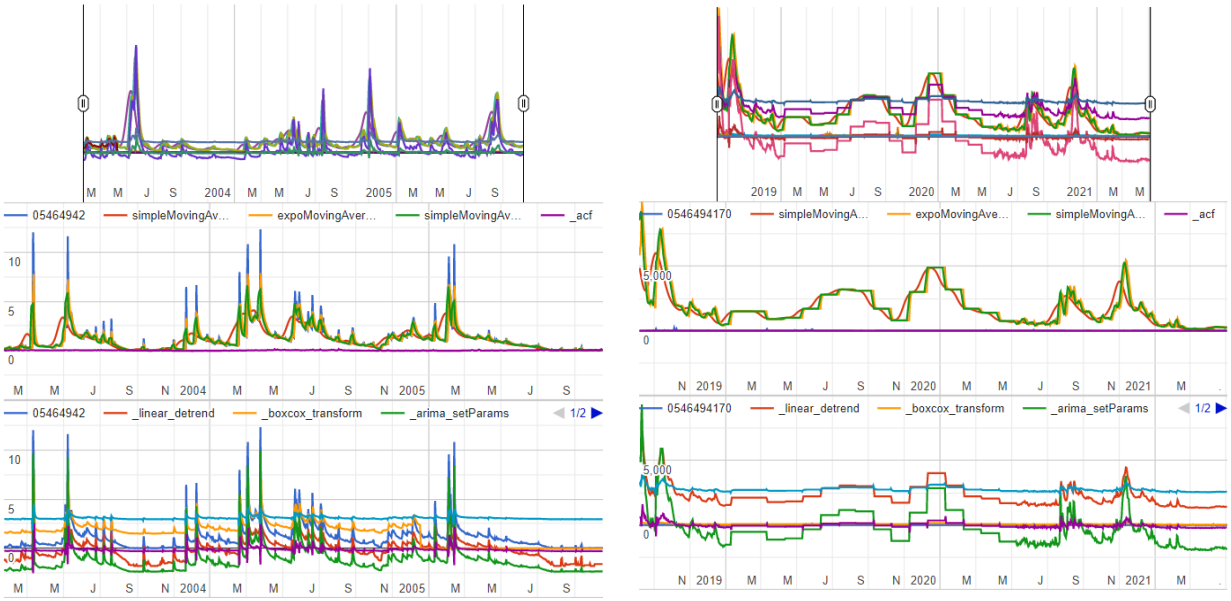
The execution times for each of the tested browsers showed a difference. Running the analysis for the same 10 stations around Iowa City area using Mozilla yielded a total execution time of 34221 ms, Chrome took 17176.5 ms, and Edge took 19412 ms. This difference can be attributed to the different just-in-time (JIT) engines for JavaScript in Mozilla (Spider Monkey) and Chrome/Edge (Chromium V8) (Rossberg et al., 2018). These differences, however, do not reflect poor performance in either browser and can be accounted for as negligible for small datasets.

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 by the developers at a hydrological domain conference and a department meeting at the University of Iowa. 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.

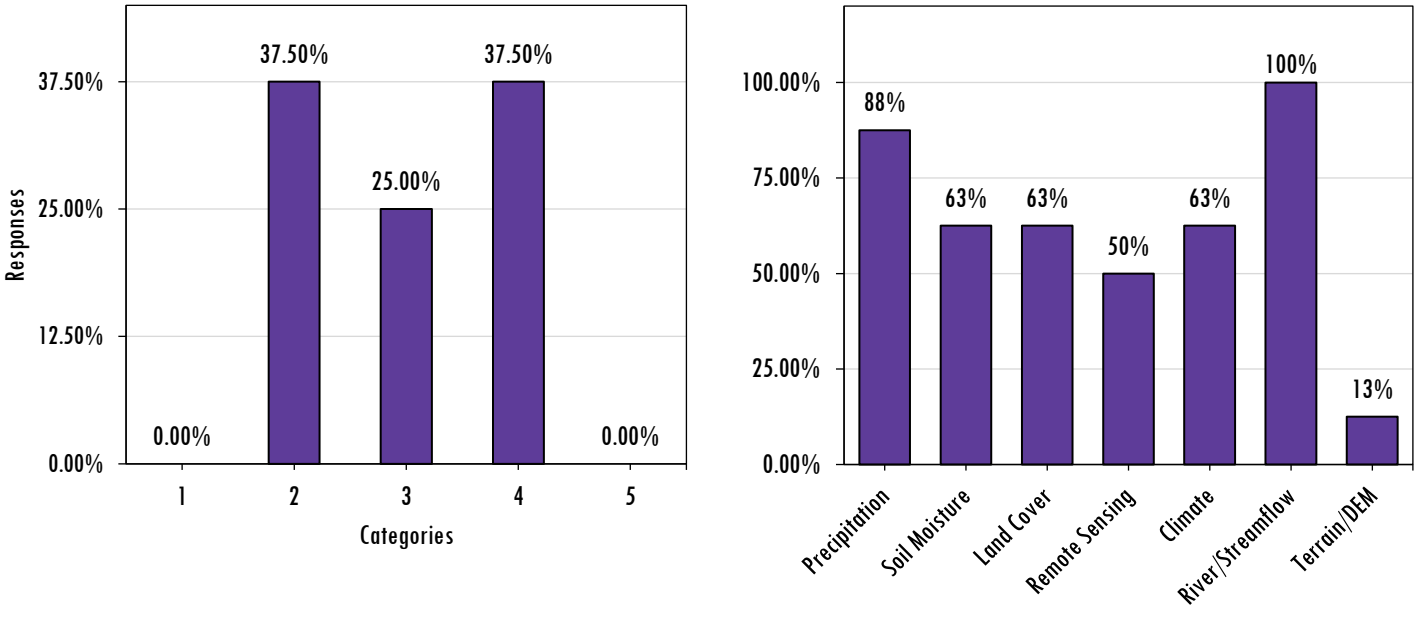
During and after the presentations, a survey was conducted to gather feedback from the participants. The survey included questions regarding the participants' backgrounds, understanding of the tool, and its usability across different domains. It also sought to assess the applicability and usability of 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 20. 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 21. 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)”.

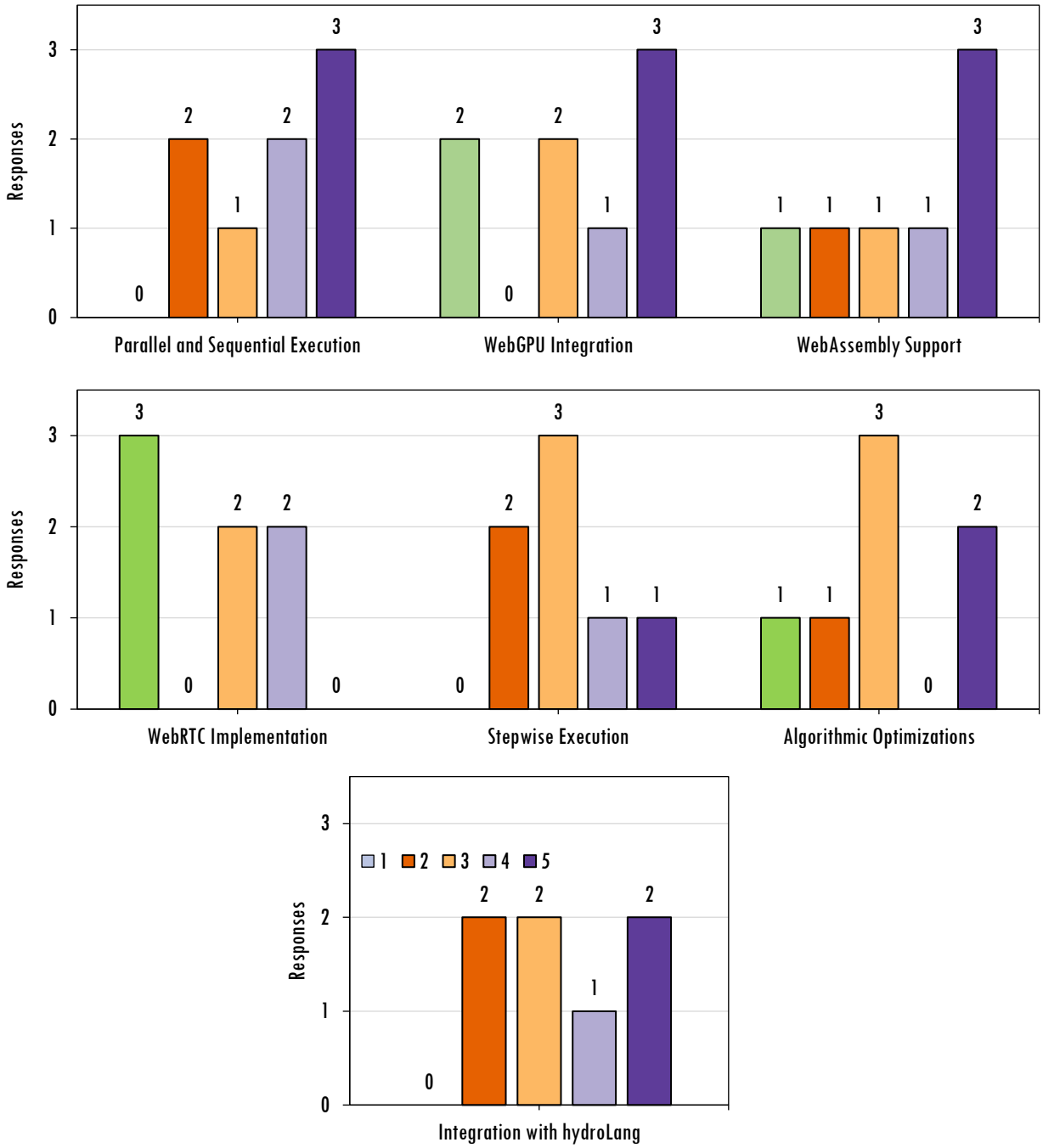


Figure 22. Results of survey utility of functionalities in the HydroCompute library. Question: “Please rate the utility of the following functionalities of HydroCompute on a scale of 1-5 (1 being not useful at all and 5 being extremely useful)”

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, rivers, 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 (Figure 21). 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 22. 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 implemented engines. These differences can be attributed to optimization techniques used by the compiler when interpreting the executions required for each run. The optimization done by the compiler is largely dependent on the provided code and the different techniques utilized. Performance issues were observed when running WebGPU's with the different benchmarking tests, specifically within the web worker environment. The WebGPU's performance is heavily constrained by the device type running the application available to the user. When running different simulations, the integrated GPU adapter lost connection with the WebGPU API when trying to perform separate graphical operations on the machine. The combinations of CPU and GPU tasks running on a worker also heavily influenced the execution time.

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). Both engines have implemented the ES6 module standard that has been adopted for code portability,

but the WebGPU implementation has not been fully implemented. 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 library. 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 requires a clear understanding of the intended purpose of the code once it is added for usage in the library. 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 on the client side in terms of tens of gigabytes (Gbs). 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. These can be managed through either processing a large number of the tasks on the server side and doing part of the computations on the client side and implementation of in-browser database mechanisms.

Future work will focus on the development of examples of specialized scripts that contain heavily used and computationally expensive routines, which will enhance the library's functionality and promote better integration with hydrological sciences. The functions utilized throughout the manuscript for both case studies can be found in the supplementary materials and on the library's GitHub repository. Aside from the exploration of new algorithms, there will be a focus on expanding the library's compatibility with different programming languages and platforms. Currently, the library has handlers for porting code from JavaScript, WebGPU, C, and AssemblyScript-compiled code and the repository contains the framework to follow so users can port their code into the library. However, there are several programming languages that are continuously improving the compilation mechanisms to run in the Web Assembly environment.

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.

5. Conclusions

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 through the WebAssembly standard 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. The library is able to read and manage code written in different programming languages by providing directives on structure and compilation that allow for fast deployment of web applications.

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

Declaration of generative AI and AI-assisted technologies in the writing process

During the preparation of this work the author(s) used ChatGPT 3.5 in order to improve grammar and spelling. After using this tool/service, the author(s) reviewed and edited the content as needed and take(s) full responsibility for the content of the publication.

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