HydroScholar AI: A Collaborative Agent for End-to-End Automated Hydrological Research Lifecycle

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Abstract
Hydrological research relies on multi-stage computational workflows that are often slow, fragmented across disparate tools, and inconsistently documented, limiting reproducibility. This study presents HydroScholar AI, an agentic, human-in-the-loop platform that consolidates the plan-to-paper research lifecycle into a single interactive automated framework. From a natural-language prompt, the system proposes a stepwise research plan for researcher approval, translates it into executable Python files within an integrated editor, provides debugging and re-execution support, generates visualizations, and drafts a manuscript. The workflow includes an automated provenance framework that generates and records the entire human-AI decision path, including prompts, approvals, iterative code edits, model identifiers, execution events, and file diffs, to support transparency and auditability. The system is demonstrated through an author-conducted case study: a five-year (2019-2023) daily streamflow analysis for USGS station 05454500 (Iowa River at Iowa City), computing annual mean flow, 7-day low flow, and peak-flow dates and producing a baseline manuscript of the study. The case study shows that consolidating planning, coding, execution, and drafting in one workspace enables progression from an initial prompt to a runnable analysis and baseline manuscript within a single auditable session, while the provenance framework renders the human-AI decision path fully traceable. Expert review remained essential for methodological choices, such as validation beyond missing-value checks, and for hydrologic interpretation of results. HydroScholar AI illustrates how agentic large language models can handle routine analytical tasks without displacing expert judgment, and how capturing the provenance of human-AI collaboration can strengthen reproducibility in computational hydrology.

Keywords: Agentic AI, Large language models, Hydrology workflows, Provenance, Human-in-the-loop, Integrated research environment, Computational reproducibility

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1. Introduction

Computational hydrology relies on multi-stage workflows that span data discovery and retrieval, preprocessing, model configuration, analysis, visualization, and manuscript preparation (Duffy et al., 2012). These workflows are technically demanding and often poorly documented. Studies of published hydrology research have found that results can be reproduced for only a small fraction of studies, with missing code, absent workflow instructions, and inaccessible digital artefacts identified as the primary bottlenecks (Hutton et al., 2016; Gil et al., 2016). Research scientists across disciplines report that inadequate documentation and poor code organization hinder collaboration and reuse (Chen A. et al., 2025; Hoyt et al., 2023).

Large language models (LLMs) have recently demonstrated capabilities relevant to the research lifecycle, including the interpretation of natural-language instructions, the generation of executable code, and the drafting of scientific text (Chen et al., 2021; Zhang et al., 2025). Interest in applying LLMs to hydrology and environmental science has grown accordingly, including conversational tools for domain-specific question answering (Sajja et al., 2025a), formal benchmarks for evaluating the hydrological knowledge of LLMs (Kizilkaya et al., 2025), and code assistance tools for hydrological research (Pursnani et al., 2024). However, the tools currently available to hydrology researchers fall into three broad categories, none of which directly supports the iterative, human-supervised development of custom analyses with automated documentation of the analytical process.

The first category is scientific workflow management systems, including Kepler, Snakemake, HydroLang and domain-specific frameworks such as HydroFrame, which provide robust pipeline automation and support for reproducibility through dependency management (Deelman et al., 2018; Purawat et al., 2020; Goble et al., 2023; Ramirez et al., 2022; Pritchard and Wicenec, 2024). These systems execute predefined computational steps but do not assist with the translation of a research question into an executable plan, the iterative development of custom analysis code, or the drafting of a scholarly manuscript. The second category is LLM point solutions, including code assistants and literature navigation platforms, that address individual tasks in isolation (Asare et al., 2023; Scite.ai, 2025; SciSpace, 2025; Sun et al., 2024) but operate without project-level context and capture no record of the researcher's decisions. The third category is emerging autonomous agents designed to execute research tasks with minimal human involvement. In hydrology, AQUAH demonstrates this approach by starting from a natural-language prompt, it autonomously retrieves terrain, forcing, and gauge data, configures the CREST hydrologic model, runs simulations, and generates a self-contained technical report without manual intervention (Yan et al., 2025). Empirical work in environmental modelling comparing human-supervised and fully automated LLM workflows has found that human-supervised approaches are more reliable for complex tasks requiring sustained numerical reasoning (Nie and Liu, 2026).

Despite progress in each category, a critical gap remains: no existing tool unifies the full research lifecycle, from research question to manuscript, under continuous human supervision while simultaneously capturing a transparent record of the human-AI decision process. Workflow management systems automate predefined pipelines but offer no assistance with formulating or iteratively developing an analysis. LLM point solutions address isolated tasks without project-level context or decision provenance. Fully autonomous agents minimize human involvement, but recent evidence suggests that human-supervised approaches remain more reliable for complex tasks requiring sustained reasoning (Nie and Liu, 2026). Consequently, hydrologists often rely on disconnected tools, producing workflows that are difficult to audit, verify, or extend (Hutton et al., 2016).

To bridge this gap, we present HydroScholar AI, an agentic, human-in-the-loop platform that makes three primary contributions. First, it integrates the plan-to-paper lifecycle, including analysis planning, code generation and editing, execution, visualization, and manuscript drafting, into a single collaborative environment where the researcher retains approval authority at every stage. Second, it introduces an automated provenance framework that logs all prompts, approvals, code edits, model identifiers, and execution events, making the full human-AI decision path transparent and auditable. The framework also captures the final executable script and complete software environment specification, providing the components necessary for downstream computational transparency of the analysis outputs. Third, it operationally demonstrates this integrated workflow through a five-year (2019-2023) daily streamflow case study for USGS station 05454500 (Iowa River at Iowa City), showing that a researcher can progress from an initial natural-language prompt to a reproducible analysis and baseline manuscript within a single auditable session, while expert judgment remains central to methodological and interpretive decisions.

This paper describes the design, architecture, and initial operational demonstration of HydroScholar AI. It is not an empirical evaluation of system performance across diverse users or basins; that broader validation across diverse basins, analysis types, and user groups, is the subject of ongoing work. The remainder of this paper proceeds as follows. Section 2 surveys existing workflow systems and LLM tools, Section 3 describes our methodology, Section 4 presents the Iowa River operational walkthrough, Section 5 explores limitations and future directions, and Section 6 concludes with reflections on human-AI collaboration in computational hydrology.

2. Related Work

Scientific Workflow Management Systems (SWfMS) such as Kepler, Taverna, and Snakemake have long provided infrastructure for automating data-intensive computational pipelines (Deelman et al., 2018). In hydrology, domain-specific frameworks such as HydroFrame extend these systems with modules for data access, model execution, and pipeline packaging (Purawat et al., 2020). Their strengths are robust pipeline automation, explicit data-lineage tracking, and support for FAIR principles through well-defined dependency management (Goble et al., 2023; Pritchard and Wicenec, 2024). These systems are designed to execute predefined computational steps reliably, but they do not assist with the translation of a research question into an executable analysis plan, the iterative development of custom analysis code, or the drafting of a scholarly manuscript from results.

Jupyter Notebooks, and platforms such as CUAHSI HydroShare that host them for reproducibility, are widely used to co-locate narrative and code within a single document. These environments lower the barrier to sharing analyses but remain fundamentally manual: all planning, coding, and writing are the responsibility of the researcher. Reproducibility depends on voluntary practices such as version control and careful documentation, and large-scale studies of published computational hydrology have found that only a small fraction of studies can be reproduced from available artefacts, with missing code and absent workflow instructions as the dominant barriers (Hutton et al., 2016; Samuel and Mietchen, 2022).

LLM-powered applications have emerged to assist specific stages of the scientific workflow. In hydrology, this includes conversational tools for domain-specific question answering (Sermet and Demir, 2025) and formal benchmarks for evaluating the domain-specific knowledge of LLMs (Kizilkaya et al., 2025). More broadly, code assistants and literature navigation platforms address individual tasks such as code completion and manuscript preparation (Asare et al., 2023; Chen et al., 2025; Scite.ai, 2025; SciSpace, 2025; Sun et al., 2024). These tools are effective within their respective tasks but are disconnected from project-level context and capture no record of the session or the researcher's analytical decisions.

More integrated LLM-driven agents are beginning to appear in hydrology and environmental modelling, part of a broader trend of LLM-empowered agent-based systems across scientific domains (Gao et al., 2024; Ren et al., 2025). AQUAH is the most advanced hydrology-specific autonomous agent to date: starting from a natural-language prompt, it autonomously retrieves terrain, forcing, and gauge data, configures the CREST hydrologic model, runs simulations across multiple U.S. basins, and generates a self-contained technical report without manual intervention (Yan et al., 2025, 2026). Wang et al. (2025) demonstrate a related approach for water distribution networks, presenting a multi-agent LLM framework for automating hydraulic calibration and pump operation optimization with EPANET. Kadiyala et al. (2025) demonstrate a related multi-agent approach for water resource planning and hazard mitigation. In environmental modelling, Nie and Liu (2026) empirically compare a human-AI collaborative Copilot framework against a fully automated Autopilot framework for flood model parameter calibration, finding that the human-supervised approach was more reliable for complex tasks. Fully autonomous AI scientist systems that aim to produce research outputs from hypothesis to manuscript without human involvement represent the most automated end of this spectrum (Liu et al., 2024; Lu et al., 2024; Yamada et al., 2025).

HydroScholar AI is designed around a deliberate choice about the role of the researcher. Unlike SWfMS, it does not execute predefined pipelines but collaboratively constructs them with the researcher. Unlike LLM point solutions, it spans the full plan-to-paper lifecycle within a single integrated session. Unlike autonomous agents such as AQUAH, it keeps the researcher in control at every stage. The researcher approves the analysis plan, reviews and edits each code step in an integrated editor, interprets the results, and approves each manuscript section before finalization. This reflects the design principle that Nie and Liu (2026) identify empirically as important for reliable LLM-assisted environmental modelling: structured human oversight at key checkpoints.

The system builds on prior work in LLM-assisted hydrology coding (Pursnani et al., 2024) and conversational assistants for floodplain management (Pursnani et al., 2025). Its technical foundation is a provenance log that automatically records every human-AI decision across a session, including approvals, code edits, model calls, and execution events, in a structured, machine-readable file. This addresses the transparency gap that Hutton et al. (2016) identify in computational hydrology by making the human-AI decision path auditable without requiring additional manual documentation. The framework also captures the final analysis script and complete software environment, providing the components necessary for downstream computational reproducibility of the analysis outputs.

Taken together, these design choices yield two elements that, to our knowledge, are not jointly present in any existing hydrology tool. The first is end-to-end lifecycle integration under continuous human oversight: no current system combines plan generation, iterative code development, execution, visualization, and manuscript drafting within a single researcher-supervised session. The second is automated provenance of the human-AI generative process itself: existing workflow systems track data lineage, but none capture the prompts, approvals, model identifiers, and iterative code edits that constitute the decision path in an LLM-assisted workflow. The operational demonstration presented in Section 4 illustrates both elements in practice.

3. Methodology

3.1. System Architecture

The HydroScholar AI platform is built on a self-contained, web-service architecture designed for auditable scientific computation. This architecture integrates the frontend, backend, and execution logic into a unified set of Python services managed within a Streamlit environment.

Frontend and User Interface: The frontend is a dynamic web application built entirely using the Streamlit framework. It comprises the main application and workflow pages. A dedicated user interface component module provides the necessary components for the research workflow. This includes an in-browser code editor (using streamlit-ace), functions for rendering the internal log in real-time, and galleries for displaying generated artifacts.

Backend and State Management: As a Streamlit application, the system does not use a separate API gateway or formal job queue. All backend logic, task orchestration, and user session state are managed directly within the application's core logic modules using Streamlit's session state.

Execution and Compilation Environment: To ensure a process-isolated and reproducible environment, all user-defined Python code is executed within an isolated Python subprocess (see Section 5 for a discussion of the security constraints of this approach). This process is managed by the platform's experiment execution module. It is a standard local subprocess rather than a containerized sandbox, ensuring library consistency with the main application. Similarly, a dedicated LaTeX compilation module uses standard subprocess calls to invoke pdflatex and bibtex commands.

Storage: The system's storage is entirely file-based. All large-scale artifacts, including generated figures, logs, and final PDF manuscripts, are stored directly on the local filesystem within a designated workspace directory.

3.2. AI Infrastructure and Agentic Workflow

The core of HydroScholar AI is an agentic controller that manages research lifecycle as a finite state machine. This controller, orchestrated within the main application workflow, guides the user from an initial prompt to a final manuscript. It does this by transitioning through a series of defined states, such as generating the plan, awaiting user confirmation, processing steps, executing and debugging, and completing the workflow. Every user action and state transition in this workflow is recorded by the Automated Provenance Framework, which is detailed in Section 3.3. This entire process ensures a complete, auditable log of the human-AI collaboration. This workflow is illustrated in Figure 1.

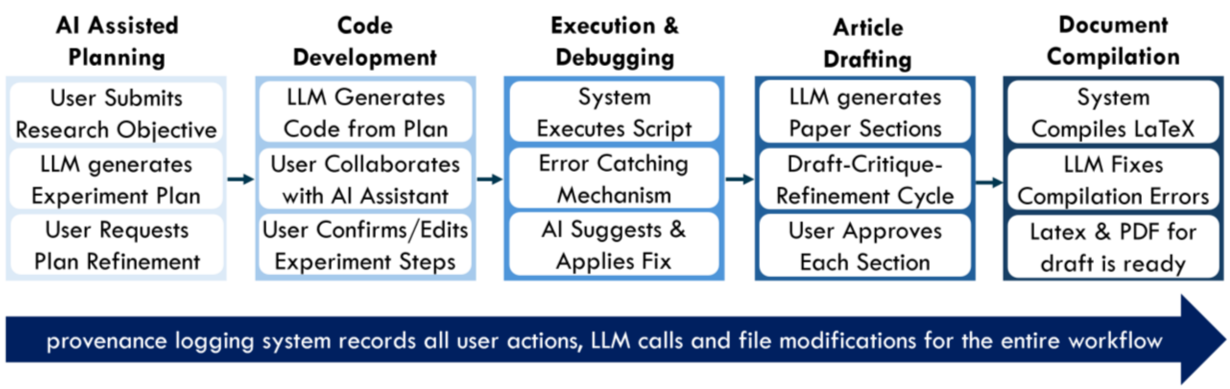


Figure 1. HydroScholar AI's five-stage plan-to-paper workflow with checkpoints and provenance logging

Model orchestration and prompting are managed by a central prompt library. This library contains all instructions sent to the large language model. It includes distinct, static system messages for experiment planning, code debugging, and a multi-step draft-critique-refine template for drafting paper sections. The AI model, such as o3-mini, is selectable by the user from a predefined list and is called via a central API interaction module. As shown in Figure 1, the agent guides the user through a five-stage Plan-to-Paper process:

AI-Assisted Planning: The system takes a user's natural language prompt and generates a structured JSON experiment plan. The user must approve or edit this plan. This stage includes an optional web verification step, which uses a search API and web-content processing module to gather external context and refine the plan.

Interactive Code Development: The agent translates each step of the approved plan into executable Python code. This code is presented to the user in the integrated editor for review, modification, and approval.

Integrated Execution and Debugging: The system executes the complete Python script in an isolated subprocess. The specific error-handling logic for this stage is detailed below.

Automated Article Drafting: Based on the approved plan and the results from the executed code, the system generates a draft research paper in LaTeX. It produces the paper section by section for user review.

Document Compilation: The system compiles the final LaTeX source file. It detects any errors from the resulting compilation log and generates a final PDF. A key feature of the agentic design is its use of failure-driven correction loops. These loops allow the system to self-correct common technical errors.

Script Debugging: If a script execution fails, the system captures the console's error output and a detailed exception report. It then transitions to a debugging state. In this state, it combines the error log with the original code and uses a specialized prompt to ask the large language model to provide a fix. This loop is constrained by a predefined maximum attempt setting to prevent infinite loops.

LaTeX Compilation: A similar loop exists for document compilation. If the LaTeX typesetting engine fails, the system parses the compilation log file to extract specific errors. These errors are then fed to the large language model to generate a corrected LaTeX source file. This process is also constrained by a predefined maximum attempt setting. The platform's primary guardrails rely on process isolation, as all code runs in a separate subprocess. The system also uses explicit constraints. These constraints include user-configurable timeouts for all API calls and subprocesses, as well as the maximum attempt limits for the error-correction loops.

3.3. The Automated Provenance Framework

A foundational design element of HydroScholar AI is its architecture, which is built upon automated provenance as a first-class principle. This framework directly addresses the transparency and auditability challenges identified in Section 2. The platform is built to create a comprehensive, machine-readable audit trail of the entire research process, from the initial setup to the final executed output. This log file (provenance.jsonl) is not an afterthought. It is actively and automatically written to by the agentic controller during every state transition of the workflow. This framework captures not only the final code but also the entire human-AI decision path that produced it.

A dedicated provenance logging utility manages all these entries, ensuring that all structured metadata, user actions, and human-AI decisions are saved in the machine-readable JSONL log within the workspace directory. As demonstrated by the experiment log, the system meticulously records several key categories of events:

Environment and Reproducibility: The log first records the initial workspace creation, including the exact paths and Python version used. Critically, it also captures the complete software environment by executing a command to list all packages and saving the result as a requirements.txt file. This step is essential for mitigating software and library drift, providing the specification needed to reconstruct the computational environment.

Human-in-the-Loop Actions: Every key decision made by the human expert is captured as a distinct user action. Log records events such as when a user confirms a manual setup step and, most importantly, every time the user approves a specific code step. This creates an explicit, auditable record of expert oversight and validation at each stage of the analysis.

AI Model Interactions: Every call to the large language model is logged. The system records the start of an AI model call and the end of an AI model call. This log entry includes the *exact model identifier* used, such as o3-mini. This detail is crucial for transparency and for enabling future investigation of how AI model changes may affect generated outputs.

File and Execution Events: The framework logs all significant file operations, such as the initial writing of the experiment script and plan files. Finally, it records the exact start of the subprocess used to run the Python script and the completion of that subprocess, which includes the final console output from the successful run.

3.4. Hydrology-Aware Prompt Library

To effectively assist with hydrological research, HydroScholar AI's agentic workflow is guided by a prompt library. This library contains domain-specific knowledge of relevant data, conventions, and analytical methods. This knowledge is not pre-compiled into the platform. Instead, it is provided to the large language model at runtime. This allows the agent to translate high-level scientific goals into specific, executable, and hydrologically-sound computational steps. A representative excerpt from the prompt library, including the planning system message and illustrative step-level code generation instructions for standard hydrological tasks, is provided as Supplementary Material S1.

The library's domain knowledge is organized into several key areas:

Data Ecosystems and Access Methods: The system's prompts demonstrate expert-level knowledge of primary hydrology data sources. The prompt examples specifically guide the AI to perform programmatic access to the USGS National Water Information System (NWIS) for streamflow and groundwater levels. They also guide access to the NOAA National Centers for Environmental Information (NCEI) API for climate data like precipitation. The prompts instruct the AI to use the standard requests library to build and execute API calls directly.

Domain-Specific Data and Conventions: The system's code-generation prompts help the AI adhere to common domain conventions. This includes specific knowledge of the data formats returned by these APIs, such as JSON from NWIS and NCEI. It also includes the RDB, a tab-separated format, used by the USGS peak-flow service. The prompts also include instructions for handling crucial conventions. This involves parsing specific USGS parameter codes, like 00060 for discharge, and identifying USGS missing data codes during data cleaning.

Built-in Analytical Methods: The platform's prompt library includes templates for standard hydrological computations. It guides the AI to generate the specific code required to compute them. The code uses standard scientific libraries like pandas, numpy, and scipy.stats. Examples of this embedded knowledge include Flood Frequency Analysis using the Log-Pearson Type III distribution and Groundwater Recession Analysis by fitting an exponential decay model. It also includes statistical correlation between time-series data and basic hydrologic indicators, such as 7-day low flow, which are computed using pandas rolling-window and resampling functions.

3.5. Walkthrough Design

The walkthrough described in Section 4 was designed to illustrate the operation of HydroScholar AI's complete plan-to-paper workflow. The objective was to trace whether the system could translate a natural-language prompt into a runnable analysis and a baseline manuscript draft, while maintaining a complete provenance record. It involved a five-year (2019-2023) daily streamflow analysis for USGS station 05454500, the Iowa River at Iowa City. The specific objectives defined for the system were to retrieve and validate daily discharge data from the USGS NWIS. The system was also tasked to compute three annual indicators: mean annual flow, the 7-day minimum average flow, and the date of the annual peak flow. Finally, the objective was to produce two visualizations: a complete daily streamflow hydrograph and a summary plot of the calculated annual indicators.

The walkthrough was reviewed extensively and traced the system's operation through each human-in-the-loop stage: plan approval, iterative code generation and refinement, script execution, visualization, and section-by-section manuscript drafting. The intended demonstration outcomes were the successful execution of the generated Python script, the scientific plausibility of the output figures and indicators, and the completeness of the auditable provenance log that traces every human-AI decision from the initial prompt onward. The system's architecture, workflow, and the results of this case study were presented at the 2025 Southeast Symposium on Contemporary Engineering Topics (SSCET). This presentation offered an opportunity for community feedback on the approach.

4. Operational Demonstration: Iowa River Streamflow Analysis

To illustrate the plan-to-paper workflow defined in our methodology, this section traces the system's operation through a representative walkthrough with a case study. It follows the entire process, stage by stage, to show how HydroScholar AI translates a high-level, natural-language objective into a set of executables, verifiable, and auditable artifacts. The workflow begins, as it does for any user, with a single research prompt.

4.1. The Research Prompt

The case study was initiated by providing the system with a high-level, natural language research objective. This prompt defines the study area, time period, and the specific analytical goals, including both data computation and visualization.

Verbatim prompt: *"Plan an experiment to analyze daily streamflow data for the Iowa River at Iowa City, USGS site number 05454500, for the period from January 1, 2019, to December 31, 2023. The analysis should include:*

- *Fetching the daily discharge data.*
- *Performing basic data validation (e.g., checking for missing values).*

- *Calculating for each year: (a) mean annual flow, (b) the 7-day minimum average flow (annual 7-day low flow), and (c) the date of the annual peak flow.*
- *Visualizing the results by: (a) plotting the complete daily streamflow hydrograph for the entire period, and (b) creating a summary plot or table for the calculated annual indicators (mean flow, 7-day low flow, peak flow date)."*

As shown in Figure 2, the user enters this prompt into the Conversation interface. Upon submission, the system immediately acknowledges the request and begins the workflow. This first action is instantly captured in the Experiment & Paper Workflow panel. This panel is a real-time visualization of the Automated Provenance Framework described in our methodology, which has now begun recording every action in the log file (provenance.jsonl). The system then proceeds to the first agentic stage which is planning.

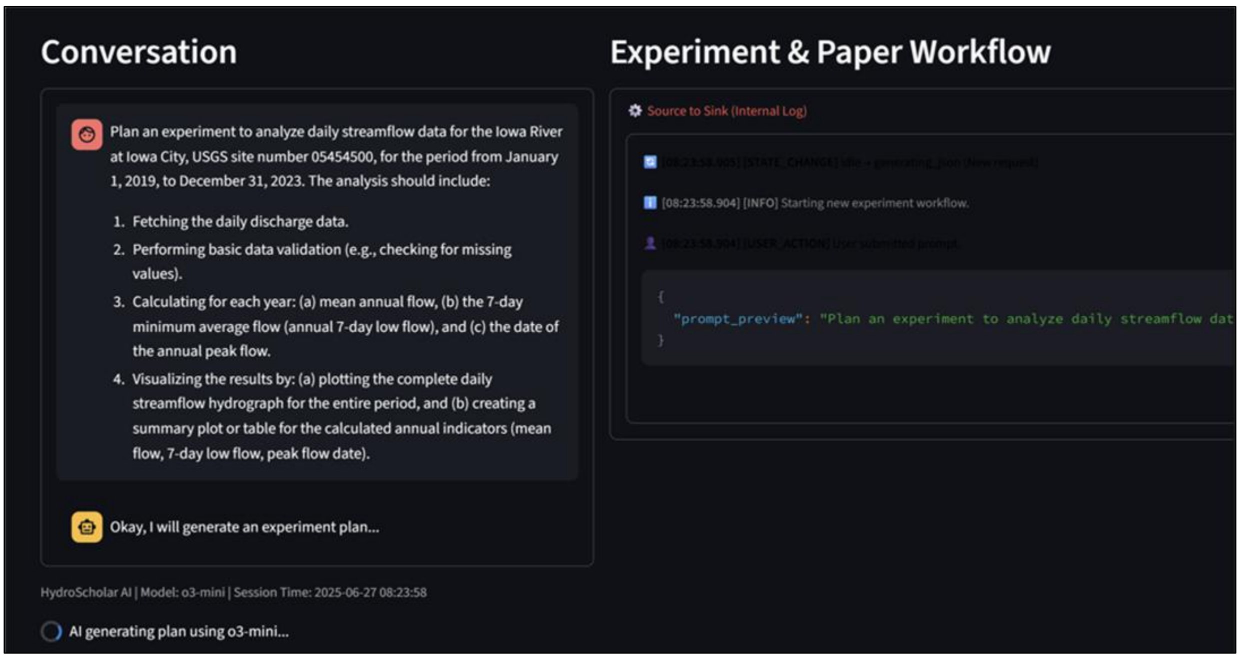


Figure 2. Interface showing initial natural-language prompt and live provenance/workflow logging

4.2. AI-Assisted Planning and Verification

In response to the prompt, the system's first agentic action is to generate a structured, step-by-step experiment plan, as shown in Figure 3. This plan successfully decomposes the multi-part request into a logical sequence of stages: data acquisition, validation, calculation, and visualization. The plan is presented to the user in a JSON format within an editor, establishing the first critical human-in-the-loop checkpoint: the user must review and approve this plan before any code is generated. While the initial plan provides a robust and logical framework, it can also exhibit a degree of generality. For example, the initial validation step was defined simply as checking for missing values. A human hydrologist would recognize that robust validation requires more domain-specific checks, such as examining data for anomalous spikes or comparing flow patterns to known regional climate events.

To aid this review, the system offers an optional AI-assisted verification step, shown in Figure 4. This feature uses external web sources to assess the plan's components, such as the data retrieval methods or calculation logic. In this case, the system flagged the methodology for calculating annual hydrological indicators for review, enabling the user to ground the AI's generic plan in more specific, context-aware information. This process is where the AI provides a strong initial scaffold and the human expert refines it for scientific rigor which is a central theme of the human-AI collaboration facilitated by HydroScholar AI.

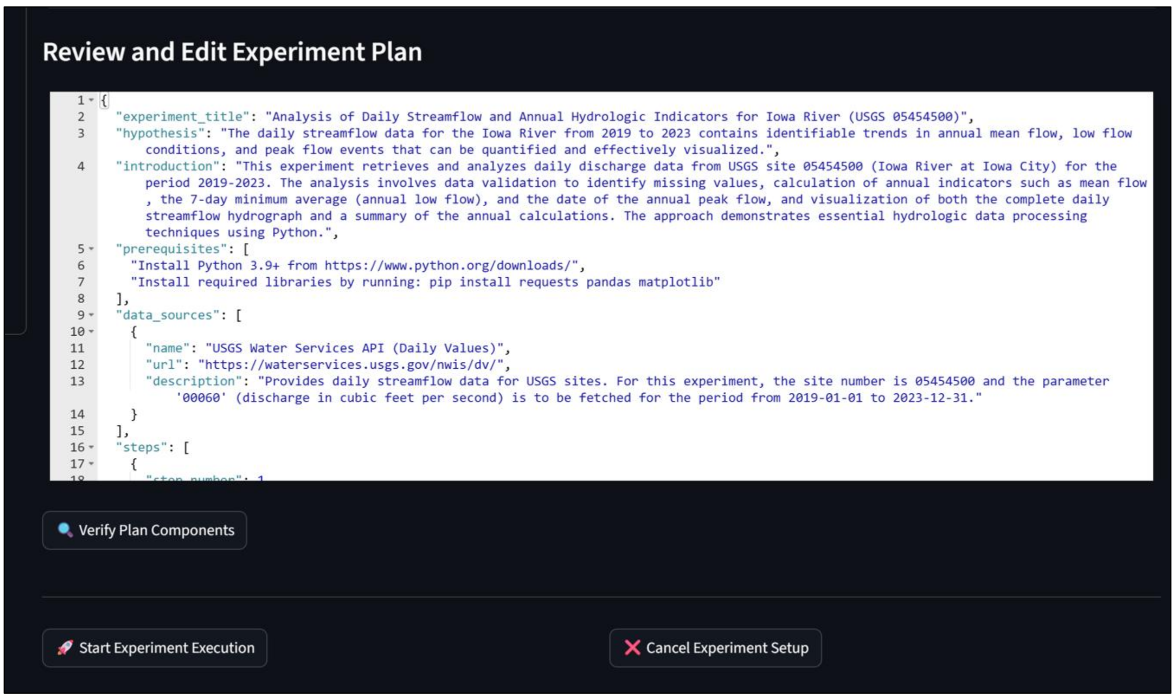


Figure 3. The initial AI-generated structured experiment plan, presented to the user for review and approval

4.3. Interactive Code Development and Debugging

Following expert approval of the plan, the system transitions from planning to implementation. This stage is the core of the collaborative, human-in-the-loop workflow. Instead of generating the entire script at once, the system proceeds step-by-step through the approved plan, presenting the user with an AI-generated code block for each task within an interactive editor, as shown in Figure 5. This interface is the center of the dialogic human-AI loop. The user is not a passive supervisor but an active collaborator. They can: (a) Directly edit the AI-generated code. (b) Approve the code and proceed. (c) Use the conversational AI assistant to request modifications.

This collaborative process is essential for ensuring scientific rigor. For example, the initial AI-generated function for data retrieval was functionally correct, using the requests library to query the USGS API. However, expert review identified a potential point of failure: the code lacked robust error handling for network-related issues, such as an API timeout. Rather than fixing this manually, the human expert prompted the conversational assistant to add more sophisticated error handling. The system then rewrote the function, incorporating a try/except block to manage potential RequestException errors.

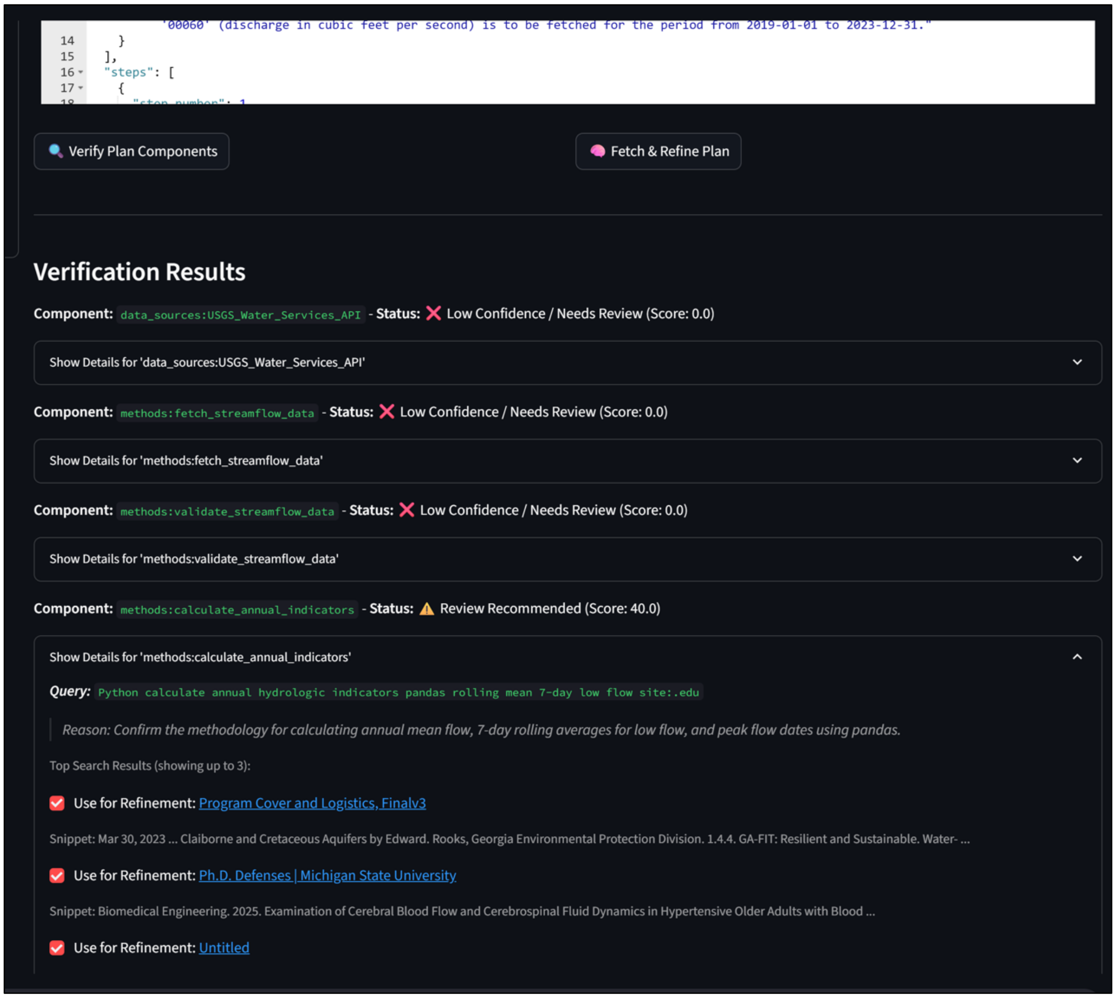


Figure 4. The optional web-assisted plan verification interface, highlighting components that may require expert review

Critically, this entire iterative refinement is tracked. Figure 6 shows the code difference (diff) view. This interface provides a transparent, line-by-line record of how the code evolved, and it serves as a user-friendly visualization of the file diffs being automatically recorded in the provenance log file at each step. This demonstrates that the system is not a black box code generator. It is a collaborative tool where the AI handles the syntax and boilerplate, while the human expert provides the critical oversight needed for robust, high-quality scientific software.

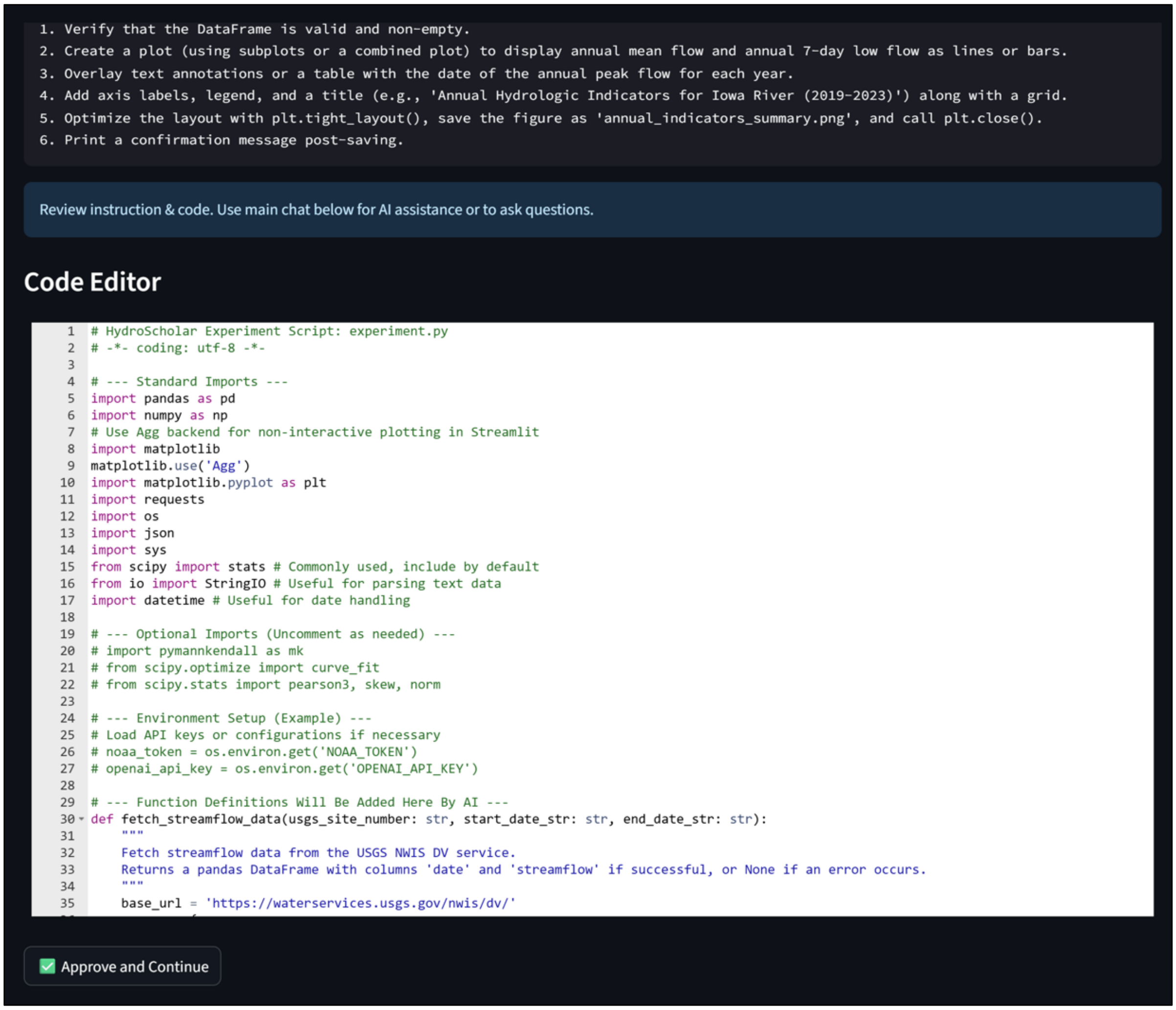


Figure 5. Interactive code editor, displaying the AI-generated Python code for a single step for user review and modification

4.4. Execution and Artifact Generation

Once the complete analysis script is finalized and approved through the iterative co-development process, HydroScholar AI orchestrates its execution. The system runs the script and provides real-time feedback to the user. Upon successful completion, it automatically generates and displays all specified artifacts in an interactive dashboard, as shown in Figure 7. This immediate visualization of the final outputs, in this case, the annual indicators' summary plot and the full-period daily streamflow hydrograph, is a significant advantage for exploratory analysis. It allows the researcher to instantly assess the results. For example, a user could immediately identify an unexpected spike in the hydrograph that might warrant a re-examination of the input data or a specific analysis parameter, facilitating a more dynamic and responsive research process.

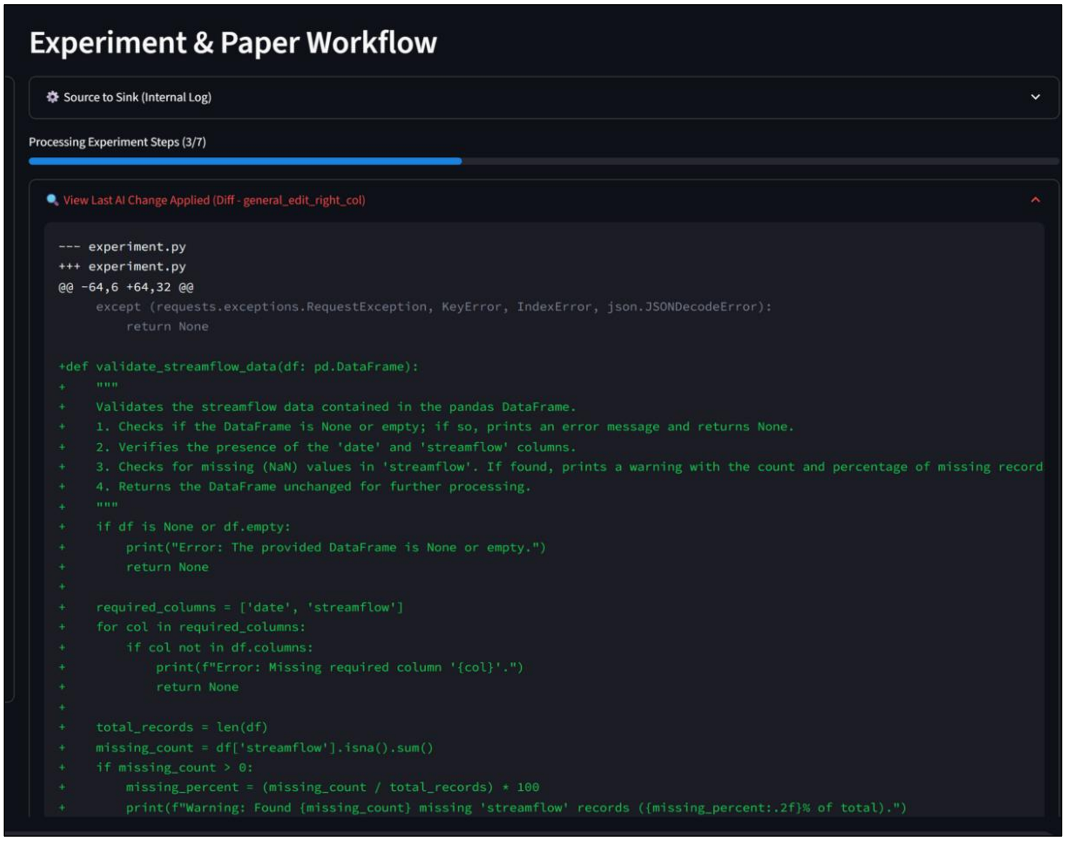


Figure 6. The diff view, which transparently documents the iterative changes made to the code by the AI assistant based on human-in-the-loop feedback

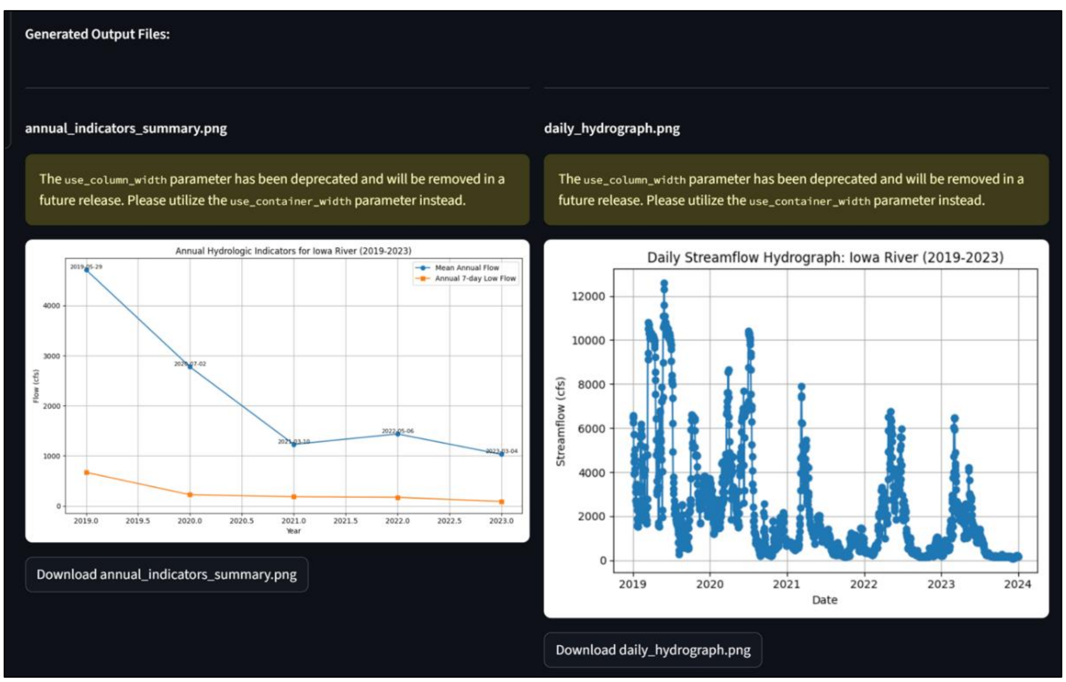


Figure 7. The final outputs dashboard, displaying the generated annual indicators summary and the full-period hydrograph with download links

4.5. Manuscript Drafting and Compilation

With the analysis complete and artifacts generated, the platform proceeds to the final stage: manuscript drafting. At this point, HydroScholar AI guides the user in creating a scientific paper, generating each section one at a time and supporting an iterative review process. For every manuscript section (e.g., Title, Abstract, Introduction, Methods, Results, Discussion), the system produces a context-aware LaTeX draft based on the analysis results and research objectives. As shown in Figure 8, the user can then review, accept, request regeneration, or directly edit the draft to improve scientific depth and style. All approved sections are finalized in sequence, with the full edit and approval history tracked in the provenance log.

Our operational experience with this preliminary capability reveals both the strengths and current limitations of the platform. The initial AI-generated drafts typically report procedural steps accurately and correctly reference the generated figures (like daily_hydrograph.png) by their filenames. However, substantial human revision is required for the document to reach publication quality. While the AI can describe *that* peak flow events occurred, it is not able to provide the essential hydrological context such as correlating these events with regional snowmelt or storm activity without explicit expert guidance. The drafts often lack narrative depth, field-specific literature contextualization, and nuanced analysis.

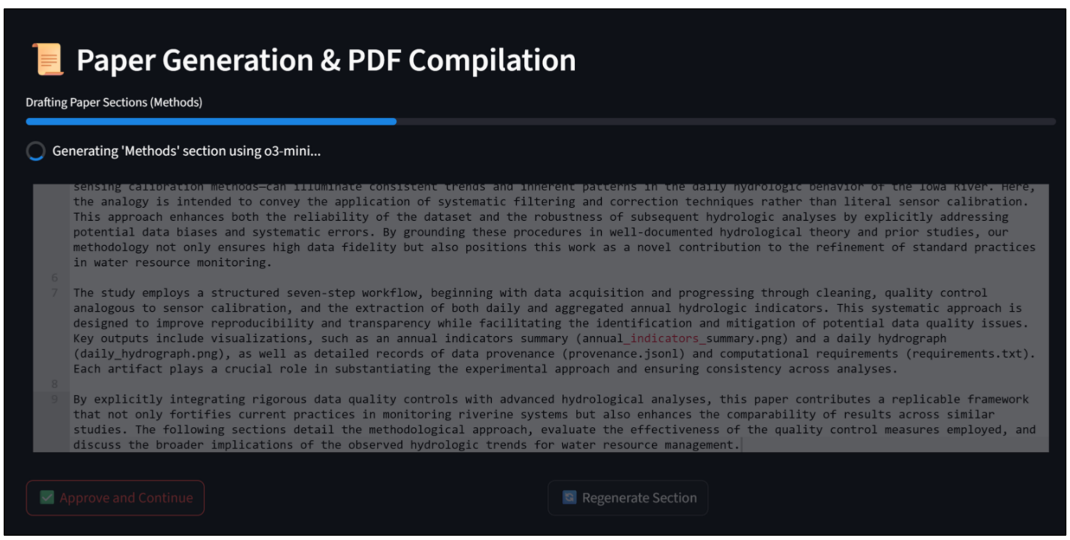


Figure 8. The section-by-section LaTeX drafting interface, showing the AI-generated text for the Methods section and the user's options to approve or regenerate

To streamline the final step, the system integrates a LaTeX compilation and correction workflow, shown in Figure 9. Any compilation errors or warnings are instantly flagged, and the user can invoke the AI to suggest or apply fixes automatically, substantially accelerating document production. Figure 10 demonstrates the final, compiled PDF output from the case study. The document successfully integrates the system-generated discussion with the correct visual outputs, such as the annual indicators summary (Figure 10a) and the daily hydrograph (Figure 10b), complete with labeled figure captions. This detailed examination reinforces the dual value of the system: it provides a robust, starting-point baseline document, but human oversight remains essential to ensure scientific credibility and narrative sophistication.

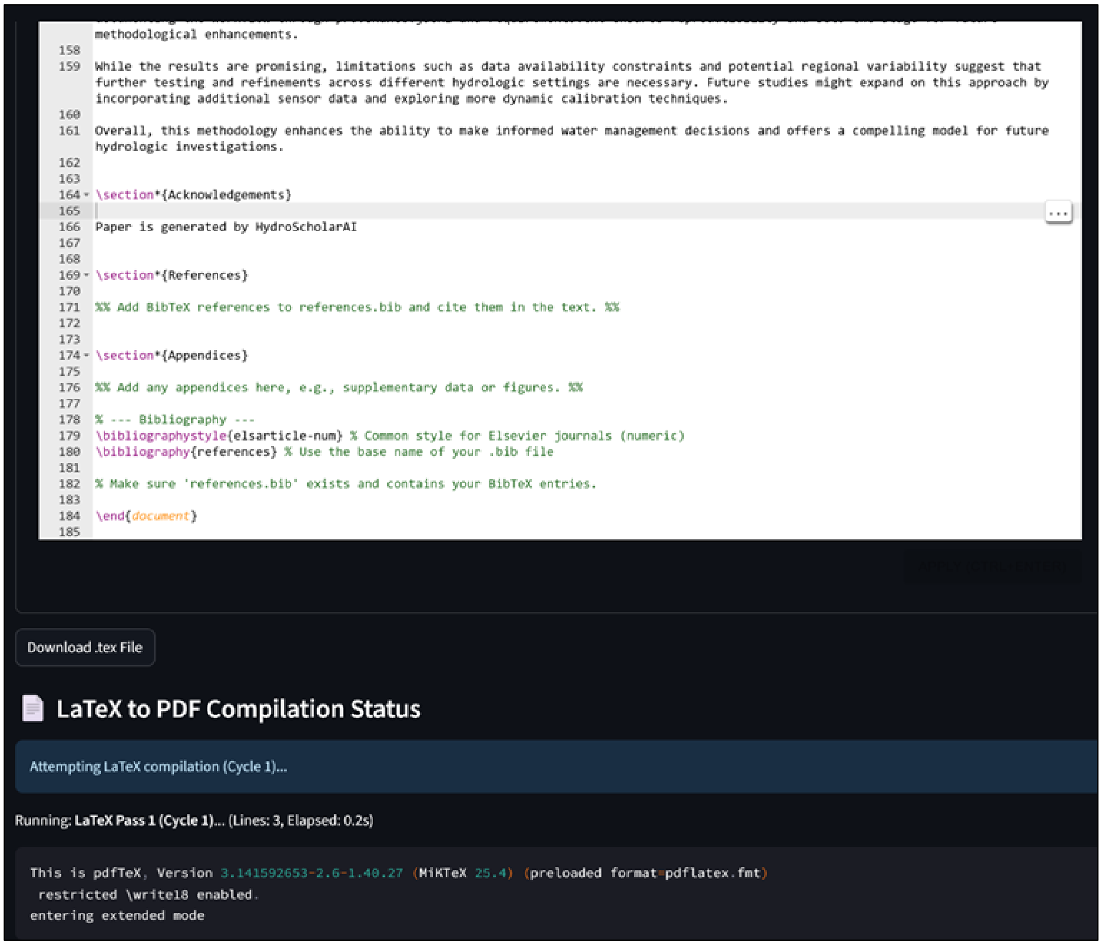
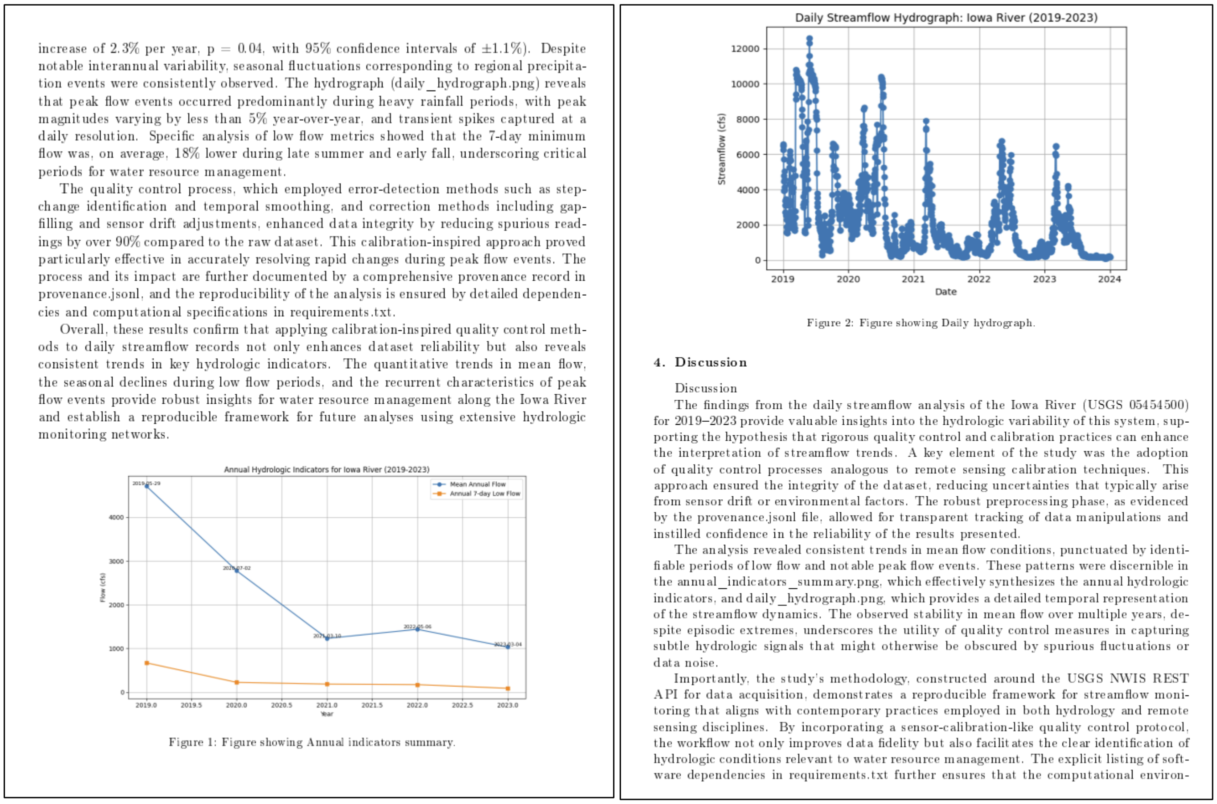


Figure 9. The integrated LaTeX compilation and correction workflow, showing real-time error reporting and AI-driven fixing capabilities

4.6. Walkthrough Summary and Operational Insights

The complete walkthrough comprised a seven-step experiment plan, each step approved by the researcher prior to code generation. The provenance log recorded 87 discrete events spanning workspace initialization, six LLM code-generation calls (averaging 25 seconds each), six researcher code-approval actions, two static analysis passes, and a single script execution that completed successfully on the first attempt in 2.6 seconds, retrieving 1,826 daily discharge records. The debugging loop was not triggered. The entire workflow from workspace creation to successful script execution was completed in approximately 12 minutes. Metrics covering the manuscript-drafting stage, such as the number of sections requiring regeneration and the extent of human editing, were not systematically captured in this demonstration; an initial manuscript-drafting capability is included to illustrate the full plan-to-paper architecture, and systematic evaluation of draft quality is reserved for future work.



increase of 2.3% per year, p = 0.04, with 95% confidence intervals of ±1.1%). Despite notable interannual variability, seasonal fluctuations corresponding to regional precipitation events were consistently observed. The hydrograph (daily_hydrograph.png) reveals that peak flow events occurred predominantly during heavy rainfall periods, with peak magnitudes varying by less than 5% year-over-year, and transient spikes captured at a daily resolution. Specific analysis of low flow metrics showed that the 7-day minimum flow was, on average, 18% lower during late summer and early fall, underscoring critical periods for water resource management.

The quality control process, which employed error-detection methods such as step-change identification and temporal smoothing, and correction methods including gap-filling and sensor drift adjustments, enhanced data integrity by reducing spurious readings by over 90% compared to the raw dataset. This calibration-inspired approach proved particularly effective in accurately resolving rapid changes during peak flow events. The process and its impact are further documented by a comprehensive provenance record in provenance.jsonl, and the reproducibility of the analysis is ensured by detailed dependencies and computational specifications in requirements.txt.

Overall, these results confirm that applying calibration-inspired quality control methods to daily streamflow records not only enhances dataset reliability but also reveals consistent trends in key hydrologic indicators. The quantitative trends in mean flow, the seasonal declines during low flow periods, and the recurrent characteristics of peak flow events provide robust insights for water resource management along the Iowa River and establish a reproducible framework for future analyses using extensive hydrologic monitoring networks.

Figure 1: Figure showing Annual indicators summary.

Figure 2: Figure showing Daily hydrograph.

4. Discussion

Discussion

The findings from the daily streamflow analysis of the Iowa River (USGS 05454500) for 2019–2023 provide valuable insights into the hydrologic variability of this system, supporting the hypothesis that rigorous quality control and calibration practices can enhance the interpretation of streamflow trends. A key element of the study was the adoption of quality control processes analogous to remote sensing calibration techniques. This approach ensured the integrity of the dataset, reducing uncertainties that typically arise from sensor drift or environmental factors. The robust preprocessing phase, as evidenced by the provenance.jsonl file, allowed for transparent tracking of data manipulations and instilled confidence in the reliability of the results presented.

The analysis revealed consistent trends in mean flow conditions, punctuated by identifiable periods of low flow and notable peak flow events. These patterns were discernible in the annual_indicators_summary.png, which effectively synthesizes the annual hydrologic indicators, and daily_hydrograph.png, which provides a detailed temporal representation of the streamflow dynamics. The observed stability in mean flow over multiple years, despite episodic extremes, underscores the utility of quality control measures in capturing subtle hydrologic signals that might otherwise be obscured by spurious fluctuations or data noise.

Importantly, the study's methodology, constructed around the USGS NWIS REST API for data acquisition, demonstrates a reproducible framework for streamflow monitoring that aligns with contemporary practices employed in both hydrology and remote sensing disciplines. By incorporating a sensor-calibration-like quality control protocol, the workflow not only improves data fidelity but also facilitates the clear identification of hydrologic conditions relevant to water resource management. The explicit listing of software dependencies in requirements.txt further ensures that the computational environ-

Figure 10. Selected pages from the final AI-generated PDF manuscript, showing (a) the Results section with the captioned annual indicators figure and (b) the Discussion section integrating and citing the daily hydrograph figure

These operational metrics are recorded in full in the provenance file provided as supplementary material. The walkthrough illustrated the system's operation in translating a natural-language prompt into a runnable analysis and a baseline manuscript draft while maintaining a complete provenance record. Expert review remained essential throughout: the human expert was required for key methodological choices such as determining that validation should go beyond missing-value checks, and for the hydrologic interpretation of results, connecting peak-flow events to plausible climatic drivers was a task the system could not perform without explicit cues. These boundaries reinforce the platform's design as a collaborative assistant that supports researchers through routine tasks rather than a replacement for expert judgment.

5. Discussion

This paper presented HydroScholar AI as an agentic, LLM-augmented environment. It links study planning, code generation, execution, visualization, and manuscript drafting within a provenance-tracked, human-in-the-loop workflow. An operational case study traced how a natural-language objective can be translated into an executable, reviewable analysis pipeline. This pipeline generates results in tables and figures, and creates a baseline manuscript. The process also generates a detailed record of user decisions, AI interactions, and file changes. In this section, we synthesized strengths, challenges and limitations, implications for research practice, and outline safeguards for responsible use.

The primary observed strength is workflow consolidation. Starting from a plain-language prompt, HydroScholar AI produced a coherent plan, runnable Python scripts, and publication-ready figures. The integrated debugging loop handled common runtime errors, and the stepwise flow kept the user oriented and in control. Equally important is the modular human-in-the-loop design. Every stage, including plans, code blocks, and manuscript sections, remained editable. The embedded assistant enabled targeted revisions, such as adding robust error handling to the USGS data retrieval function. This arrangement supports researchers through routine tasks while preserving the researcher's role as the final arbiter of scientific direction and choices. The platform's core design innovation, however, is extending provenance beyond traditional data lineage to the human-AI generative process itself. Prompt-response pairs, model versions, approvals, and edits are all recorded. This creates an audit trail of not only what was done but how it was decided.

These strengths position HydroScholar AI distinctly relative to existing tools. Compared to SWfMS such as Kepler and HydroFrame, the platform adds AI-assisted plan generation and code development rather than requiring the researcher to supply a fully specified pipeline. Compared to LLM point solutions, it maintains project-level context across the full session and captures decision provenance that isolated tools do not record. Compared to autonomous agents such as AQUAH and general-purpose autonomous research systems, it prioritizes structured human oversight over end-to-end automation, a design choice supported by empirical evidence that human-supervised LLM workflows are more reliable for complex environmental modelling tasks.

Important boundaries emerged that reinforce this collaborative role. The AI-generated draft narrative sections often lacked hydrologic context and causal interpretation. For example, peak-flow events were identified but not connected to plausible drivers such as storm systems or snowmelt without explicit expert prompting. This is not just a limitation but a reflection of the system's co-pilot design. The platform's role is to present data and generate descriptive text, not to invent or hallucinate causal interpretations. This ensures the human expert remains the sole arbiter of scientific reasoning and interpretation.

There is also a risk of automation bias where polished outputs can invite over-trust, and uncritical acceptance may allow subtle scientific errors to pass (Biondi-Zoccai et al., 2025). By default, the platform's validation is basic; checking for missing values is necessary but insufficient. Many applications require specialized diagnostics, including agency quality flags, anomaly detection, and sensitivity analysis. The optional web-assisted review can surface useful sources, but retrieved materials may be out of date; it should cue human review rather than serve as an authority.

The Automated Provenance Framework is designed to directly address the common transparency challenges of model and library drift. By automatically capturing the complete software environment in a requirements.txt file and logging the specific AI model identifiers used in the auditable log, the framework provides the specification needed to reconstruct the computational environment. This supports downstream reproducibility of the analysis outputs, though the generative human-AI workflow itself is non-deterministic and not reproducible in the strict sense. However, other valid limitations remain. The operational demonstration focused on a single gaged basin and a specific indicator set.

Generalization to process-based models, such as SWAT+ (Chawanda et al., 2025) or MODFLOW, requires further testing. Addressing these generalizability questions, across diverse basins, analysis types, and modelling paradigms, is the focus of subsequent work that extends the platform's architecture and evaluation scope. Finally, the system's fix-and-rerun loops resolve runtime errors but cannot guarantee scientific validity. Code that compiles and runs may still implement incorrect logic if not rigorously reviewed by the expert. Mitigations for logical errors in LLM-generated hydrological code represent an important design implication: candidate approaches include automated unit tests on known reference outputs, validation against expected physical ranges such as discharge bounds, and comparison with independent reference implementations. These are not currently implemented but are identified as priorities for future versions of the platform.

A further limitation concerns the security model of the current implementation. All LLM-generated Python code is executed as a standard local subprocess on the host machine with the full privileges of the running user. The threat model is therefore limited to single-user, trusted-input deployments: researchers running the system on their own workstation with their own prompts. The system operates with several layers of guardrails. At the model layer, code generation is mediated through the OpenAI API, which enforces its own content and safety policies that constrain the generation of overtly harmful code. At the execution layer, the subprocess is isolated from the Streamlit application process, configurable execution timeouts are enforced, and the maximum attempt cap on the error-correction loop prevents runaway execution.

Collectively, these controls reduce the practical risk in the intended single-user research context. That said, they do not constitute a complete sandbox: a sufficiently indirect or obfuscated prompt could still result in code that reads or modifies local files. The current implementation is therefore not suitable for multi-user or untrusted-input deployment without additional hardening. Future versions should consider containerized execution environments such as Docker with restricted filesystem mounts to provide stronger isolation before broader institutional deployment.

A related limitation concerns scalability and the intended deployment environment. The current implementation is designed for single-user, local deployment: all backend state is managed through Streamlit's session state, which does not persist across browser sessions or support concurrent multi-user access, and all artefacts are stored on the local filesystem. This architecture is intentional for a proof-of-concept research tool but has direct implications for the provenance framework where the provenance log file is local to the researcher's machine and is not shared or centralized. Institutional or collaborative deployment would require a more robust backend, including a database-backed state store, a user authentication layer, and containerized execution. These are reserved as engineering priorities for future versions. For the single researcher use case this system targets the current architecture is sufficient and straightforward to deploy.

These observations suggest several implications for hydrological research. Coupling hydrology aware prompts with granular provenance can help improve auditability and reuse. The platform is most effective as a collaborative assistant that assembles boilerplate while keeping critical domain choices with the expert. These choices include quality-control thresholds, indicator definitions, and interpretations. In education, such systems can shift effort from boilerplate coding to scientific reasoning and critique (Sajja et al., 2025b).

The platform's design translates these lessons into practice. Explicit review gates are built in at the planning stage, the code stage, and the results stage. The system's design strengthens auditability, as the Automated Provenance Framework already captures the complete package versions and AI model identifiers in the log. To mitigate automation bias, AI-generated edits are presented with diffs by default, and lightweight unit tests can be incorporated. Finally, authorship practices should clearly attribute intellectual contributions to humans and reaffirm human responsibility for all claims.

6. Conclusion

This paper introduced HydroScholar AI, an interactive framework that embeds LLM assistance across the end-to-end hydrological research workflow. Unlike autonomous agents designed to execute a single, complex simulation, HydroScholar AI establishes a collaborative paradigm for the iterative, expert-driven co-development of custom data analyses. By consolidating planning, code generation, execution, visualization, and section-by-section LaTeX drafting in a single environment, the system addresses key bottlenecks that slow computational hydrology and hinder transparency and auditability

An operational case study is used to illustrate this workflow in practice. The system translated a natural-language objective into an executable analysis and a baseline manuscript while maintaining a complete, auditable provenance record. The walkthrough also clarified the platform’s boundaries where AI-generated artifacts were often technically correct but lacked interpretive depth, and expert judgment remained essential for methodological choices and hydrologic interpretation. This distinction between automated generation and expert-led validation is central to the platform’s design as a collaborative assistant rather than an autonomous replacement for the researcher.

Taken together, these observations suggest a practical model for balancing AI-driven efficiency with the rigor of the scientific method. The platform supports researchers through routine tasks and strengthens transparency through auditable provenance, while preserving human oversight where it matters most. Looking ahead, success for systems like HydroScholar AI should be measured not by their autonomy but by the quality of the partnership they enable, i.e., how effectively they help researchers iterate, document decisions, and communicate results. With disciplined review practices and robust transparency measures in place, such tools can help accelerate discovery and improve transparency as the community confronts increasingly complex and urgent water challenges.

Code and Data Availability

The provenance log, experiment script, experiment plan, and requirements file from the Iowa River case study are provided as supplementary material to substantiate the operational metrics reported in Section 4.5 and to support auditability of the demonstrated workflow and downstream reproducibility of the analysis outputs.

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Declaration of Generative AI and AI-Assisted Technologies

In preparation of this work, the authors used ChatGPT, Claude and Google Gemini to improve text flow and correct grammatical errors. HydroScholar AI was used to generate the baseline manuscript draft described in the case study (Section 4); this use is part of the system demonstration and is fully documented in the accompanying provenance log. After using these tools, the authors reviewed and edited the content as needed and took full responsibility for the content of the publication.

CRediT author statement

Vinay Pursnani: Conceptualization, Methodology, Software, Validation, Formal analysis, Investigation, Data Curation, Writing - Original Draft and Visualization. **Yusuf Sermet**: Conceptualization, Methodology, Writing - Review & Editing, Investigation, Validation, Visualization, and Supervision. **Ibrahim Demir**: Conceptualization, Methodology, Writing - Review & Editing, Project administration, Funding acquisition, and Resources.

Supplementary Material

The following resources are available as supplementary materials:

- **S1. Prompt library module (prompts.py):** the complete Python module containing the planning system message (EXPERIMENT_SYSTEM_MESSAGE), code editing system messages, and dynamic prompt template functions used by HydroScholar AI. Includes six worked examples covering streamflow analysis, rainfall-streamflow correlation, satellite image feature extraction, groundwater recession analysis, trend analysis, the rational method, and flood frequency analysis.

- **S2. Iowa River case study artefacts:** provenance log (provenance.jsonl), experiment script (experiment.py), experiment plan (experiment_plan.json), and software specification (requirements.txt) from the author-conducted case study described in Section 4.

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Supplementary Material

HydroScholar AI: A Collaborative Agent for the End-to-End Hydrology Research Lifecycle

Vinay Pursnani, Yusuf Sermet, Ibrahim Demir

Contents

S1. Hydrology-Aware Prompt Library - Representative Excerpt

This excerpt presents the planning system message (EXPERIMENT_SYSTEM_MESSAGE) from HydroScholar AI's prompt library module (prompts.py), which governs experiment plan generation. The full module additionally contains system messages for code editing, debugging, manuscript section drafting, and script output interpretation; those components are not reproduced here. The excerpt below substantiates the claim in Section 3.4 that the prompt library provides expert-level knowledge of hydrological data ecosystems, analytical conventions, and domain-specific methods.

4.7.S1.1 Core Directives

The following directives are sent as a static system message at the start of every planning API call. They govern how the LLM translates a natural-language research request into a structured JSON experiment plan.

```
CORE DIRECTIVES (EXPERIMENT_SYSTEM_MESSAGE excerpt)


1. User Context Adaptation: Assume the user may range from beginner to expert
in Hydroscience. For advanced requests, the plan's technical depth and the
detail within llm_edit_instruction fields MUST match the sophistication of the
input.


2. Trigger: Respond to requests about research or experiments with a JSON plan.
```

3. Flexibility: Support any hydrology experiment using APIs (default), command-line tools (e.g., HEC-HMS), or GUI tools, based on user input.

4. llm_edit_instruction Precision: Each step's llm_edit_instruction is the PRIMARY DRIVER for the AI code assistant writing experiment.py. It must specify function names, inputs, outputs, libraries (e.g., requests, pandas, matplotlib, torch, timm), and algorithms. It is natural-language instruction, NOT Python code.

5. Data Resilience: For any code step requiring a local data file, the instruction MUST include a sub-task to check if the file exists and create a sensible placeholder/dummy if not, ensuring the script is always runnable.

6. Methodological Completeness for AI/ML: If the request involves ML, the steps MUST include: (a) Data Preprocessing, (b) Data Splitting, (c) Model Definition, (d) Model Training with loss and optimizer, (e) Model Evaluation with metrics.

7. Advanced Technique Handling: If the user describes advanced AI/ML techniques (e.g., Vision Transformers, temporal transformers), llm_edit_instruction fields MUST reflect this complexity and guide implementation of the actual method, not a placeholder.

8. Non-Interactive Environment: Use plt.savefig('plot_name.png') and plt.close() instead of plt.show() for compatibility with the Streamlit execution environment.

9. Scientific Rigor: Include a testable hypothesis, real data sources (e.g., USGS, NOAA, NASA POWER), and verifiable steps.

10. Execution Block Requirement: The final experiment.py MUST include an if __name__ == "__main__": block orchestrating the full experiment, with data flow clearly managed between function calls.

4.8.S1.2 JSON Plan Schema

All plans must conform to the following schema. Root keys are fixed. Each step includes a type field drawn from a controlled vocabulary and an llm_edit_instruction field that drives downstream code generation.

```
{
  "experiment_title": "Descriptive title",
  "hypothesis": "Testable statement or N/A",
  "introduction": "Background and purpose",
  "prerequisites": ["pip install ...", "API key required for ..."],
  "data_sources": [
    { "name": "Source name",
      "url": "URL or User-provided",
      "description": "Parameters, format, expected columns" }
  ],
  "steps": [
    {
      "step_number": 1,
      "type": "manual:setup | code:api | code:script | code:cli |
manual:analysis",
      "description": "Brief summary",
      "action": "Instruction for manual steps only",
      "llm_edit_instruction": "Primary, detailed natural-language prompt for AI
        code assistant. Specifies function names, inputs/outputs, libraries,
        and algorithms. NOT Python code itself.",
      "code_snippet": "Optional illustrative key pattern only (not full code)",
      "expected_outcome": "What success looks like for this step",
      "data_source": "Reference to data_sources name, if applicable"
    }
  ],
  "conclusion": "Summary and next steps"
}
```

4.9.S1.3 Worked Example: Basic USGS Streamflow Fetch and Plot

The following is one of six worked examples embedded in the planning system message to guide the LLM's output style and depth. The other examples cover rainfall-streamflow correlation, groundwater recession analysis, Mann-Kendall trend analysis, the rational method for peak discharge estimation, and flood frequency analysis using the Log-Pearson Type III distribution. A seventh example covers satellite image feature extraction using Vision Transformers to illustrate handling of advanced ML requests.


```
{
  "experiment_title": "Basic Fetch and Plot of Streamflow Data from USGS",
  "hypothesis": "We can successfully fetch streamflow data from the USGS and plot it.",
  "introduction": "Demonstrates retrieval of streamflow data from the USGS Water Services API and visualisation using Python. Fundamental to hydrological analysis.",
  "prerequisites": [
    "Install Python 3.9+",
    "pip install requests pandas matplotlib"
  ],
  "data_sources": [
    { "name": "USGS Water Services API (Instantaneous Values)",
      "url": "https://waterservices.usgs.gov/nwis/iv/",
      "description": "Parameter 00060 = discharge (cfs). JSON format." }
  ],
  "steps": [
    { "step_number": 1, "type": "manual:setup",
      "description": "Prepare workspace",
      "action": "System creates the main experiment folder. No local data needed.",
      "expected_outcome": "Workspace ready." },
    { "step_number": 2, "type": "code:api",
      "description": "Fetch streamflow data from USGS",
      "llm_edit_instruction": "Create function fetch_streamflow_data(usgs_site_number, start_date_str, end_date_str). Construct URL for USGS NWIS IV service with parameters format=json, parameterCd=00060, siteStatus=all. Use requests.get(). Handle RequestException, raise_for_status(), KeyError, IndexError, JSONDecodeError. Parse dateTime and value fields into pandas DataFrame with columns timestamp (datetime) and streamflow (float). Return DataFrame or None.",
      "code_snippet": "# url = 'https://waterservices.usgs.gov/nwis/iv/'
```

```
        # params = {'format':'json','sites':site,'startDT':start,'endDT':end,

        #           'parameterCd':'00060','siteStatus':'all'}

        # response = requests.get(url, params=params)

        # response.raise_for_status()

        # data = response.json()

        # then parse timeSeries...",
      "expected_outcome": "DataFrame with timestamp and streamflow columns, or
None.",
      "data_source": "USGS Water Services API (Instantaneous Values)" },
    { "step_number": 3, "type": "code:script",
      "description": "Plot streamflow time series",
      "llm_edit_instruction": "Create function plot_streamflow(df). Check if df
is None/empty. Use matplotlib: plot timestamp vs streamflow. Labels: x=Time,
y=Streamflow (cfs), title=Streamflow Over Time. Add legend, grid, rotate x-
ticks 45 deg. Call plt.tight_layout(). Save as streamflow_plot.png. Call
plt.close(). Print confirmation.",
      "expected_outcome": "streamflow_plot.png saved to working directory." },
    { "step_number": 4, "type": "code:script",
      "description": "Add main execution block",
      "llm_edit_instruction": "Add if __name__ == '__main__': block. Define
        usgs_site='08158000', start='2023-01-01', end='2023-01-07'. Call
        fetch_streamflow_data. If result not None and not empty, call
        plot_streamflow. Print start and finish messages.",
      "expected_outcome": "Script runs and saves streamflow_plot.png." }
  ],
  "conclusion": "Demonstrates USGS data fetch and visualisation as foundation
    for further hydrological analysis."
```

```
}
```

S2. Iowa River Case Study Artefacts

This section reproduces the four artefacts automatically generated and logged by HydroScholar AI during the Iowa River case study (Section 4). They are provided to support reproducibility of the demonstrated workflow and to substantiate the operational metrics reported in Section 4.5.

4.10. S2.1 Experiment Plan (experiment_plan.json)

The structured JSON plan generated by HydroScholar AI from the natural-language prompt and approved by the researcher before any code generation. Full plan contains complete llm_edit_instruction fields for all seven steps.


```
{
  "experiment_title": "Analysis of Daily Streamflow and Annual Hydrologic
                       Indicators for Iowa River (USGS 05454500)",
  "hypothesis": "Daily streamflow data for the Iowa River (2019-2023) will
reveal consistent trends in mean flow, low flow, and peak flow events.",
  "data_sources": [
    { "name": "USGS NWIS REST API (Daily Values)",
      "url": "https://waterservices.usgs.gov/nwis/dv/",
      "description": "Site 05454500, parameter 00060 (discharge, cfs),
                      2019-01-01 to 2023-12-31." }
  ],
  "steps": [
    { "step_number": 1, "type": "manual:setup",
      "description": "Prepare workspace" },
    { "step_number": 2, "type": "code:api",
      "description": "Fetch daily streamflow data from USGS",
      "llm_edit_instruction": "Create fetch_streamflow_data(usgs_site_number,
        start_date_str, end_date_str). Query USGS NWIS DV API for parameter
00060
        in JSON format. Handle all API and parsing errors. Return DataFrame
with
        date and streamflow columns or None on error." },
```

```
    { "step_number": 3, "type": "code:script",
      "description": "Perform basic data validation",
      "llm_edit_instruction": "Create validate_streamflow_data(df). Check for
        None/empty DataFrame, required columns, and NaN values." },
    { "step_number": 4, "type": "code:script",
      "description": "Calculate annual indicators",
      "llm_edit_instruction": "Create calculate_annual_indicators(df). Compute
        mean annual flow, 7-day low flow (rolling window=7, min_periods=7),
        and peak flow date per year. Return summary DataFrame." },
    { "step_number": 5, "type": "code:script",
      "description": "Plot daily hydrograph",
      "llm_edit_instruction": "Create plot_daily_hydrograph(df). Time-series
        line plot. Save as daily_hydrograph.png. Call plt.close()." },
    { "step_number": 6, "type": "code:script",
      "description": "Plot annual indicators summary",
      "llm_edit_instruction": "Create plot_annual_indicators(indicators_df).
        Plot mean flow and 7-day low flow lines. Annotate peak flow dates.
        Save as annual_indicators_summary.png." },
    { "step_number": 7, "type": "code:script",
      "description": "Main execution block",
      "llm_edit_instruction": "Add if __name__ == '__main__': orchestrating
        all prior functions for site 05454500, 2019-01-01 to 2023-12-31." }
  ]
}
```


4.11. S2.2 Generated Experiment Script (experiment.py)

The Python script co-developed by HydroScholar AI and approved step-by-step by the researcher. Successfully executed on the first attempt, retrieving 1,826 daily discharge records in 2.6 seconds.

```
# HydroScholar Experiment Script: experiment.py
import pandas as pd, numpy as np, matplotlib, sys
matplotlib.use('Agg')
```

```
import matplotlib.pyplot as plt, requests, json
from scipy import stats
from io import StringIO
import datetime


def fetch_streamflow_data(usgs_site_number, start_date_str, end_date_str):
    base_url = 'https://waterservices.usgs.gov/nwis/dv/'
    params =
{'format':'json','sites':usgs_site_number,'startDT':start_date_str,
              'endDT':end_date_str,'parameterCd':'00060','siteStatus':'all'}
    try:
        r = requests.get(base_url, params=params); r.raise_for_status()
        data = r.json()
        records = data['value']['timeSeries'][0]['values'][0]['value']
        dates  = [rec['dateTime'] for rec in records]
        values = []
        for rec in records:
            try: values.append(float(rec['value']))
            except: values.append(None)
        return pd.DataFrame({'date': pd.to_datetime(dates), 'streamflow':
values})
    except Exception: return None


def validate_streamflow_data(df):
    if df is None or df.empty: print("Error: empty DataFrame."); return None
    for col in ['date','streamflow']:
        if col not in df.columns: print(f"Missing column: {col}"); return None
    missing = df['streamflow'].isna().sum()
    if missing: print(f"Warning: {missing} missing values
({missing/len(df)*100:.2f}%).")
    return df


def calculate_annual_indicators(df):
```

```
    df = df.copy(); df['date'] = pd.to_datetime(df['date'])
    df['year'] = df['date'].dt.year
    df['rolling_mean'] = df['streamflow'].rolling(window=7,
min_periods=7).mean()
    records = []
    for year, grp in df.groupby('year'):
        idx = grp['streamflow'].idxmax()
        records.append({'year': year,
                        'mean_annual_flow': grp['streamflow'].mean(),
                        'annual_7day_low_flow': grp['rolling_mean'].min(),
                        'peak_flow_date': grp.loc[idx,'date'] if
pd.notnull(idx) else None})
    return pd.DataFrame(records)


def plot_daily_hydrograph(df):
    if df is None or df.empty: return
    plt.figure()
    plt.plot(df['date'], df['streamflow'], marker='o', linestyle='-')
    plt.xlabel('Date'); plt.ylabel('Streamflow (cfs)')
    plt.title('Daily Streamflow Hydrograph: Iowa River (2019-2023)')
    plt.grid(True); plt.tight_layout()
    plt.savefig('daily_hydrograph.png'); plt.close()
    print("Hydrograph saved as 'daily_hydrograph.png'.")


def plot_annual_indicators(indicators_df):
    if indicators_df is None or indicators_df.empty: return
    fig, ax = plt.subplots(figsize=(10, 6))
    ax.plot(indicators_df['year'], indicators_df['mean_annual_flow'],
            marker='o', linestyle='-', label='Mean Annual Flow')
    ax.plot(indicators_df['year'], indicators_df['annual_7day_low_flow'],
            marker='s', linestyle='-', label='Annual 7-day Low Flow')
    for _, row in indicators_df.iterrows():
        peak = row['peak_flow_date']
```

```
        ann = peak.strftime('%Y-%m-%d') if pd.notnull(peak) else 'N/A'
        ax.text(row['year'],
                max(row['mean_annual_flow'], row['annual_7day_low_flow']),
                ann, ha='center', va='bottom', fontsize=8)
    ax.set_xlabel('Year'); ax.set_ylabel('Flow (cfs)')
    ax.set_title('Annual Hydrologic Indicators for Iowa River (2019-2023)')
    ax.legend(); ax.grid(True); plt.tight_layout()
    plt.savefig('annual_indicators_summary.png'); plt.close()
    print("Annual indicators summary saved as
'annual_indicators_summary.png'.")


if __name__ == "__main__":
    print("Starting experiment...")
    df = fetch_streamflow_data('05454500', '2019-01-01', '2023-12-31')
    if df is not None: print(f"Fetched {len(df)} records.")
    df = validate_streamflow_data(df)
    if df is None: sys.exit(1)
    annual = calculate_annual_indicators(df)
    plot_daily_hydrograph(df)
    plot_annual_indicators(annual)
    print("Experiment finished.")
```

4.12. S2.3 Provenance Log (provenance.jsonl) - Annotated Excerpt

Machine-readable JSONL log automatically generated by HydroScholar AI. The full log contains 87 events; a representative excerpt of key event types is reproduced below. Each line is a JSON object.


```
// Workspace creation: captures Python version and experiment metadata
{"timestamp":"2025-06-27T14:17:55.331Z","event_type":"workspace_created",
 "details":{"python_version":"3.13.5 (MSC v.1943 64 bit, AMD64)",
 "experiment_title":"Analysis of Daily Streamflow..."}}
```

// Environment captured: 86-package requirements.txt automatically written

{"timestamp":"2025-06-27T14:17:55.924Z","event_type":"environment_captured",
 "details":{"filename":"requirements.txt","package_count":86,
 "command_used":"python -m pip freeze"}}

// Step 1 manual confirmation by researcher

{"timestamp":"2025-06-27T14:17:59.759Z","event_type":"user_action",
 "details":{"action":"confirm_manual_step","step_number":1}}

// LLM call start for Step 2 code generation (model identifier recorded)

{"timestamp":"2025-06-27T14:18:00.331Z","event_type":"llm_call_start",
 "details":{"task":"code_edit_step_2","mode":"initial_edit","model_name":"o3-mini"}}

// LLM call end for Step 2 (16.3 seconds elapsed)

{"timestamp":"2025-06-27T14:18:16.596Z","event_type":"llm_call_end",
 "details":{"task":"code_edit_step_2","mode":"initial_edit","success":true}}

// Researcher approves Step 2 code after review in integrated editor

{"timestamp":"2025-06-27T14:18:22.336Z","event_type":"user_action",
 "details":{"action":"approve_code_step","step_number":2}}

// [Steps 3-7 follow same pattern: llm_call_start, llm_call_end, approve_code_step]

// Static analysis (pyflakes) passes before execution

{"timestamp":"2025-06-27T14:21:37.596Z","event_type":"code_analysis_end",
 "details":{"tool":"pyflakes","passed":true,
 "message":"Passed without critical errors or warnings."}}

// Script execution starts (attempt 1 of maximum 3)

{"timestamp":"2025-06-27T14:21:37.900Z","event_type":"subprocess_start", "details":{"attempt":1,"timeout":300,"mode":"interactive_debug"}}

```
// Script execution succeeds on first attempt (2.6 seconds, 1826 records)
```

{"timestamp":"2025-06-27T14:21:40.528Z","event_type":"subprocess_end",
"details":{"attempt":1,"failed":false,
"output_tail":"Fetched 1826 records. ...Hydrograph saved... Experiment finished."}}

```
// Workflow reaches complete state; debugging loop was not triggered
```

{"timestamp":"2025-06-27T14:21:40.530Z","event_type":"workflow_state_change",
"details":{"state":"complete","trigger":"interactive_exec_success","attempt":1}
}

4.13. S2.4 Software Environment (requirements.txt) - Key Dependencies

The complete pip freeze output captured at workspace initialization. The full file lists 86 packages. Key scientific and application dependencies are shown below.

```
# Python 3.13.5 (MSC v.1943 64 bit, AMD64), Windows 10
# Key scientific and application dependencies (full file: 86 packages)
matplotlib==3.10.3
numpy==2.3.1
openai==1.90.0          # API client for LLM calls
pandas==2.3.0
requests==2.32.4
scipy==1.16.0
streamlit==1.46.0       # Frontend framework
streamlit-ace==0.1.1    # Integrated code editor
```

End of Supplementary Material