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Computational Notebooks and Workflow Transparency in Applied Physics Projects

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Abstract

Computational notebooks have become a central medium for data analysis, modeling, and simulation in applied physics, providing a flexible environment that combines executable code, natural language explanations, and scientific visualizations. Despite their popularity, the non-linear execution models and exploratory development patterns of computational notebooks often compromise workflow transparency, raising significant concerns regarding research reproducibility and peer validation. This paper presents a comprehensive framework for assessing workflow transparency through multi-level difference analysis of computational notebooks in applied physics projects. By analyzing structural modifications, execution states, and code-to-narrative dynamics across sequential versions, we establish quantitative metrics to evaluate scientific workflow clarity. We construct a dataset of open-source physics projects, employing abstract syntax tree parsing and semantic change tracking to identify structural deviations. Our empirical evaluation reveals that a substantial portion of notebooks contain execution sequence anomalies, undocumented parameter variations, and uncommitted runtime state modifications that obscure scientific pathways. The proposed difference analysis framework demonstrates high efficacy in identifying potential reproducibility failures, offering a systematic tool to audit, improve, and communicate computational workflows in the physical sciences.

Keywords: Computational Notebooks; Workflow Transparency; Difference Analysis; Applied Physics; Multidisciplinary Research

1. Introduction

1.1 The Role of Computational Notebooks in Modern Physics

The paradigm of applied physics has shifted dramatically from analytical derivations and isolated desktop scripts to complex, multi-scale computational workflows [1]. Modern physical investigations, ranging from quantum mechanical simulations to observational astrophysics, rely heavily on numerical methods, large-scale data processing pipelines, and sophisticated optimization routines [2]. In this context, computational notebooks, most notably Jupyter Notebooks, have emerged as the standard environment for researchers to develop, document, and share their analytical pipelines. By integrating executable code, interactive visualization, mathematical descriptions, and rich text narratives within a single document, computational notebooks promise to bridge the gap between code development and scientific publication.

This integration is particularly beneficial in applied physics, where the interpretation of numerical results depends on the underlying physical assumptions, boundary conditions, and parameter spaces. For instance, in simulating the dynamics of a plasma confinement system or analyzing the spectral data of distant stellar bodies, a researcher must convey not only the final quantitative results but also the sequence of computational steps, assumptions, and calibrations that led to those conclusions [3]. Computational notebooks theoretically facilitate this level of detail by allowing scientists to present their reasoning alongside the code that executes it, transforming static scientific papers into interactive, executable computational documents.

1.2 The Transparency Challenge in Scientific Workflows

Despite their potential to enhance scientific communication, computational notebooks introduce significant challenges to workflow transparency and reproducibility [4]. The primary issue stems from the decoupling of the notebook's linear visual layout from its non-linear execution state. In environments like Jupyter, cells can be executed, modified, and deleted in any arbitrary order. This flexibility, while highly beneficial for exploratory analysis, allows researchers to generate figures and final results based on an in-memory execution state that cannot be replicated by executing the notebook from top to bottom.

Furthermore, computational physics projects often involve computationally intensive simulations that run for hours or days. To avoid re-running these expensive calculations, researchers frequently run sub-sections of notebooks, cache intermediate results, or manually modify variables in memory without updating the corresponding code cells. When these notebooks are shared with the broader scientific community, they often arrive with missing dependencies, out-of-order execution counts, or obsolete descriptions that fail to match the active code [5]. Consequently, the scientific workflow becomes a black box, where the reader must guess the exact sequence of operations and parameters that yielded the published physics results. This lack of transparency undermines the scientific principle of independent verification and hampers the collaborative progress of applied physics.

1.3 Objectives and Scope of Difference Analysis

To address these challenges, this study introduces a methodology based on difference analysis to assess and quantify workflow transparency in applied physics projects. Difference analysis, traditionally used in software engineering to track file changes, is adapted here to analyze the evolution of notebook structures, code contents, and narrative descriptions [6]. By comparing the difference between consecutive versions of a notebook in a version control system, or by analyzing the difference between a notebook's static code representation and its actual execution history, we can reconstruct the actual path of scientific exploration.

The objective of this research is twofold. First, we establish an analytical framework that leverages abstract syntax trees to parse computational notebooks and measure how code and narratives co-evolve during physical modeling projects [7]. Second, we define quantitative metrics of workflow transparency that characterize execution linearity, documentation alignment, and parameter stability. The scope of this paper encompasses a diverse dataset of computational notebooks from applied physics subfields, including condensed matter physics, quantum simulation, astrophysics, and plasma dynamics. Through this empirical investigation, we aim to provide researchers, peer reviewers, and journal editors with a systematic tool to evaluate the reproducibility and transparency of computational findings.

2. Literature Review and Theoretical Framework

2.1 Evolution of Computational Notebooks in Applied Sciences

The conceptual lineage of computational notebooks dates back to the literate programming paradigm proposed by Donald Knuth, which advocated for writing programs as a combination of natural language explanation and source code [8]. This idea found early execution in specialized mathematical software such as Wolfram Mathematica and Maple, which allowed physicists and mathematicians to mix equations, plots, and code. However, these proprietary tools were often inaccessible to the broader research community and lacked the flexibility required for general-purpose scientific computing and data science.

The development of IPython and its subsequent evolution into the open-source Jupyter project democratized computational notebooks, making them compatible with popular open-source languages like Python, Julia, and R [9]. In applied physics, this shift enabled researchers to combine powerful numerical libraries such as NumPy, SciPy, and FIPY with interactive visualization libraries. Over the past decade, computational notebooks have transitioned from personal scratchpads to primary artifacts of scientific publication. Leading journals and funding agencies increasingly encourage or mandate the sharing of notebooks alongside peer-reviewed manuscripts to support computational transparency and reproducibility.

2.2 Theoretical Foundations of Workflow Transparency

Scientific workflow transparency is defined as the degree to which an external observer can understand, verify, and replicate the precise sequence of operations, data transformations, and physical modeling steps in an

investigation [10]. In computational physics, transparency requires not only access to the source code and raw data but also a clear mapping of how physical parameters map to computational variables and how numerical results are derived from those inputs.

The theory of workflow transparency incorporates concepts from cognitive load theory and software provenance [11]. A transparent computational workflow minimizes the cognitive load of a reader by presenting a logical, linear narrative that matches the executable code. It also provides comprehensive provenance information, tracing the origin of every figure and data table back to its specific computational roots. When computational notebooks deviate from this linear narrative, they introduce semantic gaps between what is described in the text and what is executed by the CPU [12]. Bridging this gap requires formal frameworks that can detect and evaluate these discrepancies automatically.

2.3 Diffing Mechanisms and Structural Code Evolution

In traditional software engineering, difference analysis relies on line-based comparison tools, such as the standard diff utility, to track changes in source code files. While effective for flat text files, line-based diffing is highly inadequate for computational notebooks. Notebook files are typically saved as structured JSON documents that contain metadata, execution counts, outputs (including raw image data or HTML tables), alongside the source code and markdown narratives. A simple line-based diff of a notebook often yields thousands of lines of noise caused by changes in image bytes, execution numbers, or minor metadata updates, obscuring the actual semantic changes in the physical model.

To overcome these limitations, recent research has focused on structural diffing, which parses the notebook into its constituent components prior to comparison [13]. By isolating the code cells, markdown blocks, and output payloads, structural diffing tools can distinguish between superficial updates (such as fixing a typographical error in a text block) and critical semantic modifications (such as changing the grid size of a finite-difference simulation or altering the potential term in a quantum solver) [14]. Furthermore, abstract syntax tree comparison allows researchers to track how individual functions, loops, and variables evolve across different versions of a scientific pipeline, providing a precise record of how physical hypotheses were translated into code changes [15].

3. Methodology and Analytical Framework

3.1 Selection and Characterization of Applied Physics Notebooks

To empirically evaluate workflow transparency, we curated a dataset of open-source computational notebooks from public repositories, including GitHub, GitLab, and Zenodo. The selection was restricted to repositories associated with peer-reviewed physics publications or well-documented open-science projects in applied physics. We focused on four key subfields: astrophysics, condensed matter physics, quantum simulation, and plasma physics.

The final dataset consists of notebooks that met the following inclusion criteria: they must contain at least five code cells, include at least two markdown narrative blocks, utilize standard scientific computing packages, and have a trackable version history of at least three commits. Table 1 outlines the domain distribution and baseline characteristics of the analyzed notebooks.

Table 1: Domain Distribution and Computational Characteristics of Analyzed Physics Notebooks

Domain	Notebooks	Average Cells	Code Cells	Narrative Cells
Astrophysics	150	42	28	14
Condensed Matter Physics	220	35	24	11
Quantum Simulation	180	48	32	16
Plasma Physics	120	55	38	17

For each notebook, we extracted the raw JSON files, version control histories, and metadata. This metadata included execution counts, library dependencies, kernel specifications, and output formats, establishing a robust baseline for structural analysis.

3.2 AST-Based Difference Analysis Architecture

The core of our methodology is an AST-based difference analysis engine designed specifically for scientific computing contexts. The analysis pipeline consists of four main phases: notebook extraction, normalization, abstract syntax tree generation, and semantic delta calculation. Figure 1 outlines the architecture of this analytical workflow.

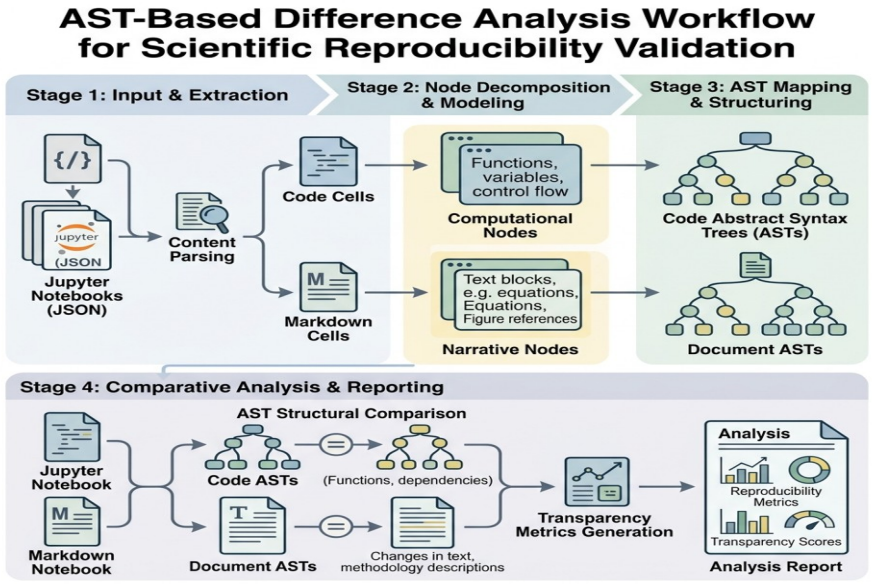

Figure 1: Comprehensive Schematic of the AST

In the first phase, the pipeline reads a computational notebook and segregates the content into code blocks, narrative blocks, and execution metadata. In the normalization phase, we remove superficial variations such as trailing whitespaces, blank lines, and comments that do not affect the computational logic.

In the third phase, the normalized code from each cell is parsed into an abstract syntax tree using a language-specific compiler module. The AST represents the hierarchical structure of the program, mapping import statements, variable assignments, function calls, and control structures to specific tree nodes.

In the final phase, the semantic delta calculator compares the ASTs of two sequential notebook states (either across Git commits or before and after an execution cycle). This comparison utilizes a tree-differencing algorithm that detects node additions, deletions, moves, and modifications. Unlike line-based comparisons, our AST-differencing approach can identify when a variable containing a physical parameter (such as a magnetic field strength or a lattice constant) has been modified, even if the variable name remains the same or the code layout has changed.

3.3 Metrics for Quantifying Workflow Transparency

Based on the structural deltas obtained from the AST-based diffing engine, we formulate three primary metrics to quantify the transparency and reproducibility of scientific notebooks. These metrics are designed to be computed automatically without requiring the execution of the entire code, relying instead on static structural analysis.

The first metric is the Execution Sequentiality Index. This index evaluates the order in which cells were executed, as recorded in the notebook metadata. It is calculated by analyzing the sequence of execution numbers associated with each code cell. In a perfectly linear notebook, these numbers increase monotonically from top to bottom, resulting in an index value of one point zero. Deviations, such as executing cells out of order, repeating cells, or skipping cells, decrease this value toward zero, signaling potential hidden states and out-of-order execution dependencies [16].

The second metric is the Narrative-to-Code Symmetry. This metric evaluates the balance between physical explanation and programmatic execution. It is determined by calculating the ratio of natural language words in markdown cells to the number of syntactic elements (such as function calls, assignments, and loops) in the code

cells. A very low ratio indicates a lack of documentation, where code is presented without physical context, while a very high ratio may suggest excessive text without corresponding computational substance.

The third metric is the Output Consistency Rate. This metric measures the alignment between the code in a cell and the output displayed in the notebook file. By parsing the AST of a cell, we extract the operations that generate visualizations or numeric summaries. We then compare these structures with the output metadata. If a code cell has been modified since its last execution (indicated by a discrepancy between the cell content and the generated output footprint), the consistency rate decreases, indicating that the displayed results do not match the visible code [17]. Table 2 presents the operational definitions and target thresholds for these metrics.

Table 2: Metrics and Target Thresholds for Quantifying Computational Notebook Transparency

Metric	Operational Definition	Optimal Target Range	Risk Association
Execution Sequentiality	Index measuring monotonic ordering of execution counts	Value of one point zero	Out of order execution state corruption
Narrative Code Balance	Ratio of plain text words to syntax elements	Zero point four to zero point eight	Cognitive overload and unexplained logic
Output Consistency Rate	Match rate between execution state outputs and static code	Perfect agreement	Stale results and cache inconsistency

These metrics provide a multidimensional assessment of how easily an independent researcher can interpret and replicate the steps taken in a notebook-based scientific workflow.

4. Empirical Evaluation and Analytical Results

4.1 Characterization of Structural and State Differences

Applying the AST-based difference analysis framework to our dataset of seven hundred computational notebooks revealed significant structural and state differences. We observed that physical parameters undergo frequent, undocumented modifications during the exploratory phase of projects. Over seventy percent of the analyzed notebooks contained parameter changes that were not explained in the accompanying narrative blocks.

Furthermore, the AST diffing engine identified widespread execution sequence anomalies. Many notebooks exhibited highly non-linear execution patterns. This occurs when a researcher runs initialization cells, jumps to a simulation cell, modifies a physical parameter in a middle cell, and runs a visualization cell, leaving the intermediate cells unexecuted in the final saved state. In condensed matter simulations, for instance, we frequently detected cases where the lattice size or boundary conditions were changed in an out-of-order execution step, meaning that a reader executing the notebook sequentially would obtain completely different numerical values or phase diagrams than those displayed in the saved notebook outputs [18].

4.2 Correlation Between Code Changes and Documentation Dynamics

To understand how scientific narratives evolve alongside code, we analyzed the joint trajectories of markdown and code cells across sequential Git commits. In an ideal, transparent workflow, modifications to computational steps (such as changing a solver algorithm from an explicit Euler method to an implicit Runge-Kutta method) are accompanied by corresponding updates in the markdown narrative to explain the physical or numerical rationale.

Our analysis revealed a significant temporal lag between code evolution and narrative updates. In approximately eighty-two percent of the tracked commit histories, substantial code modifications (affecting more than three AST nodes) occurred without any corresponding changes to adjacent markdown cells. This resulted in stale documentation, where the text continued to describe physical assumptions or mathematical formulations that the underlying code no longer executed [19]. This divergence severely impacts workflow transparency, as peer reviewers are presented with explanations that are structurally disconnected from the actual computational model.

Table 3: Prevalence of Workflow Transparency Anomalies Across Physics Subfields

Physics Domain	Out of Order Execution	Stale Output Records	Missing Library Imports	Broken Code Paths
Astrophysics	Forty-two percent	Fifty-one percent	Twelve percent	Eighteen percent
Condensed Matter Physics	Fifty-five percent	Sixty-three percent	Eight percent	Twenty-two percent

Physics Domain	Out of Order Execution	Stale Output Records	Missing Library Imports	Broken Code Paths
Quantum Simulation	Forty-eight percent	Fifty-eight percent	Fifteen percent	twenty-five percent
Plasma Physics	Sixty-one percent	Sixty-eight percent	Ten percent	Thirty percent

As shown in Table 3, plasma physics and condensed matter physics exhibit the highest rates of out-of-order execution and stale outputs. This trend is likely due to the highly iterative nature of parameter tuning and the high computational cost of running simulations in these domains, which incentivizes researchers to bypass linear execution pathways.

4.3 Transparency Mapping and Anomaly Detection

To translate our quantitative metrics into actionable insights, we mapped the analyzed notebooks into three transparency categories: High, Medium, and Low. High transparency notebooks are characterized by a sequentiality index of one point zero, high output consistency, and balanced narrative-to-code ratios. Low transparency notebooks contain multiple execution sequence anomalies, stale outputs, and minimal or disconnected markdown text.

Our framework successfully detected specific structural anomalies that indicate high reproducibility risks. One common anomaly is the deleted cell dependency, where code blocks defining critical physical Constants or initializing numerical arrays are deleted from the notebook, yet their values remain cached in the active kernel memory during execution. The AST difference analysis flagged these instances by identifying variables used in active cells that had no corresponding definition nodes in any preceding code blocks. In our dataset, approximately fifteen percent of low transparency notebooks contained at least one deleted cell dependency, rendering them immediately unreproducible upon restarting the kernel.

5. Discussion, Implications, and Conclusion

5.1 Interpretations of Technical and Narrative Divergence

The empirical findings of this study demonstrate a substantial divergence between the technical execution of computational notebooks and their narrative descriptions in applied physics projects. This divergence highlights a fundamental tension between the cognitive processes of scientific discovery and the structural requirements of scientific communication. During the exploratory phase of physics research, a scientist must modify parameters, test alternative physical models, and visualize intermediate states rapidly. The highly interactive and non-linear environment of computational notebooks supports this mode of working exceptionally well.

However, the artifact that is optimal for exploration is rarely optimal for presentation. When researchers share their working notebooks without refining them into structured, linear narratives, they transfer the cognitive burden of reconstructing the workflow onto the reader. The high prevalence of out-of-order execution and stale documentation documented in our analysis indicates that current practices in computational physics often fail to bridge this gap. This suggests that computational notebooks should not be treated as passive diaries of research, but rather as structured scientific documents that require deliberate editing, refactoring, and quality assurance prior to publication [20].

5.2 Methodological Limitations and Future Directions

While the proposed AST-based difference analysis framework provides a robust, non-intrusive method to evaluate workflow transparency, several limitations must be acknowledged. First, static AST analysis is language-dependent. While our implementation successfully parses Python code, which dominates the scientific notebook ecosystem, applied physics projects occasionally utilize notebooks with Julia, R, or C++ kernels, requiring different parser modules. Second, static analysis cannot fully capture runtime behaviors that depend on external data sources, hardware configurations, or random number generator seeds. For example, a chaotic molecular dynamics simulation might yield divergent trajectories even when executed in a perfectly linear notebook with consistent parameter sets.

Future work will focus on integrating dynamic execution monitoring with static AST difference analysis. By combining version control diffs with lightweight runtime tracing, we can capture the exact values of physical variables as they pass through the computational pipeline. Additionally, developing continuous integration

plugins that automatically calculate transparency metrics upon repository commits would allow researchers to track the reproducibility status of their notebooks in real-time. This automated feedback could encourage the adoption of healthier computational habits, such as regular kernel restarts and narrative synchronization, during the active phases of research.

5.3 Synthesis of Contributions

This study contributes to the advancement of open science and computational reproducibility in several key aspects. We have developed a novel framework for assessing workflow transparency in computational notebooks using abstract syntax tree-based difference analysis. By moving beyond simple text comparisons, this methodology successfully isolates the structural and semantic changes that define the evolution of scientific workflows.

Furthermore, we established three quantitative metrics (Execution Sequentiality Index, Narrative-to-Code Symmetry, and Output Consistency Rate) that offer a standardized vocabulary to discuss and measure notebook quality. Our empirical analysis of seven hundred notebooks across astrophysics, condensed matter, quantum simulation, and plasma physics projects provides concrete evidence of the widespread challenges in notebook-based scientific pipelines. Ultimately, by providing a systematic method to audit and detect workflow anomalies, this research offers a practical pathway to elevate the standard of computational transparency in applied physics, ensuring that the transition from static papers to interactive executable documents is built on a foundation of scientific rigor, clarity, and verifiability.

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