

LLM-GUARD: Large Language Model-Based Detection and Repair of Bugs and Security Vulnerabilities in C++ and Python

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Abstract—Large Language Models (LLMs) such as ChatGPT-4, Claude 3, and LLaMA 4 are increasingly embedded in software/application development, supporting tasks from code generation to debugging. Yet, their real-world effectiveness in detecting diverse software bugs, particularly complex, security-relevant vulnerabilities, remains underexplored. This study presents a systematic, empirical evaluation of these three leading LLMs using a benchmark of foundational programming errors, classic security flaws, and advanced, production-grade bugs in C++ and Python. The dataset integrates real code from SEED Labs, OpenSSL (via the Suresoft GLaDOS database), and PyBugHive, validated through local compilation and testing pipelines. A novel multi-stage, context-aware prompting protocol simulates realistic debugging scenarios, while a graded rubric measures detection accuracy, reasoning depth, and remediation quality. Our results show that all models excel at identifying syntactic and semantic issues in well-scoped code, making them promising for educational use and as first-pass reviewers in automated code auditing. Performance diminishes in scenarios involving complex security vulnerabilities and large-scale production code, with ChatGPT-4 and Claude 3 generally providing more nuanced contextual analyses than LLaMA 4. This highlights both the promise and the present constraints of LLMs in serving as reliable code analysis tools.

Index Terms—Artificial Intelligence (AI), LLMs, Code, Software Development, Security.

I. INTRODUCTION

Large Language Models (LLMs) are a class of Machine Learning (ML) models that have revolutionized natural language understanding and generation [1]. Models such as ChatGPT [2], Claude [3], GitHub Copilot [4], LLaMA [5], and BERT [6] have become dominant tools in software development scenarios, where these tools are used for tasks ranging from translating natural language instructions into code to performing debugging and answering code-related queries [7]–[9]. Their utility has exploded rapidly on various platforms such as Integrated Development Environments (IDE), educational platforms, and enterprise DevOps pipelines, accelerating programming workflows and lowering barriers to entry for novice developers [10]. However, the usage of these models, the accuracy of LLMs' potential, especially when applied to diverse, realistic software bugs, remains underexplored. This

gap is critical, as undetected bugs can lead to functional failures, security breaches, and substantial maintenance costs in modern software systems.

This study addresses this critical question by conducting a systematic, empirical evaluation of three cutting-edge LLMs such as ChatGPT-4, Claude 3 (Sonnet 3.7), and LLaMA 4 (maverick) on their ability to detect and explain a broad spectrum of software bugs. Our investigation spans foundational programming mistakes, classic security vulnerabilities, and advanced, real-world bugs drawn from widely-used open-source systems. The code samples include C++ snippets from SEED Labs and OpenSSL (via the Suresoft GLaDOS bug database), as well as Python bugs from the PyBugHive repository [11], covering libraries like NumPy and Pandas. Unlike prior studies that often rely on synthetic or narrowly-scoped examples, our dataset integrates checking codes and validating bugs. Moreover, our methodology includes rigorous local validation of each bug, multi-stage prompting to simulate real-world debugging, and a graded detection rubric to measure not just correctness, but also depth of reasoning and remediation quality. This multifaceted evaluation allows us to expose both the strengths and limitations of current LLMs when operating as static and dynamic code analyzers under varied code complexity levels and programming paradigms.

The novelty of this research lies in its holistic and context-aware framework for assessing LLM performance across multiple layers of code reasoning, from shallow syntax-based flaws to deeper semantic, contextual, and security-related vulnerabilities. This work is motivated by the increasing dependence on LLMs in automated code review pipelines, educational tools for programming instruction, and even security auditing processes.

The main contributions of this paper are as follows:

- Developed a comprehensive benchmark composed of foundational, security, and advanced real-world bugs across C++ and Python, validated through local compilation and testing pipelines.
- Designed and implemented a novel, multi-stage, context-aware prompting protocol to mimic realistic developer

interaction and debugging workflows.

- Conducted a comparative, fine-grained analysis of three leading LLMs (ChatGPT-4, Claude 3, and LLaMA 4), assessing detection accuracy, reasoning depth, and suggestion quality using a standardized rubric.

The remainder of this paper is organized as follows. Section II presents the literature review on vulnerability detection using LLMs. We present the methodology of this work in Section III. Various types of bugs and their detection are discussed in Section IV. Advanced work on bug detection of C++ and Python is presented in Section V and Section VI respectively. Discussion and Conclusion are discussed in Section VIII.

II. RELATED WORK

With respect to vulnerability detection, the following work has been done: CodeQwen1.5, DeepSeek-Coder, CodeGemma, Starcoder-2, and CodeLlama were explored to find vulnerabilities in Python, Java, and Javascript [12]; *LProtector* used ChatGPT to analyze C++ code [13]; and *FuncVul* was used to analyze C/C++ [14]. Vulnerable code found on *Stack Overflow* was injected to Claude 3, GPT-4, and Llama 3 to determine if the model detects whether the code is secure or not [15]. Another topic of interest is Automated Program Repair (APR) with LLMs. However, the automation is not part of this work yet. *RepairAgent* uses autonomous agents based on a large language model (LLM) to find bugs and fix them [16]. *SRepair* fixes multi-function bugs and demonstrates cost efficiency with US\$0.029/Fixed Bug [17]. A Systematic Literature Review of LLMs in Code Security is provided in [18]. Automated code repair is surveyed here [19].

III. METHODOLOGY

This research examines the capacity of LLMs to detect software bugs, ranging from foundational programming errors to advanced real-world issues in widely-used open-source systems. We evaluate three cutting-edge LLMs—ChatGPT-4, Claude 3, and LLaMA 4—against a diverse set of C++ and Python code snippets, using a consistent evaluation protocol to assess diagnostic accuracy and fix-suggestion performance.

Dataset and Bug Categories

The dataset is stratified into three main categories:

- **Easy Bugs (C++ and Python):** These include fundamental issues commonly encountered in early computer science coursework—such as uninitialized variables, incorrect parameter passing, memory mismanagement, logical oversights, and pointer misuse. These examples are reflective of what students encounter in introductory programming courses at universities and colleges and were selected to assess LLMs’ ability to detect foundational errors with minimal context.
- **Security Vulnerabilities (C++):** This category includes snippets exhibiting classic security flaws such as race conditions, format string vulnerabilities, buffer overflows, unsafe memory access, and privilege escalation vectors. These examples were primarily drawn from SEED Labs,

an academic platform for hands-on cybersecurity education.

• Advanced Real-World Bugs:

- *C/C++ Bugs:* Extracted from real issues documented in the OpenSSL project and archived in the Suresoft GLaDOS bug database¹. These bugs include memory safety violations, cryptographic misconfigurations, and type inference issues.
- *Python Bugs:* Sourced from PyBugHive², a database of manually validated bugs in mainstream Python libraries, particularly NumPy and Pandas. These include internal state inconsistencies, API misuse, data structure conflicts, and edge-case behaviors relevant to scientific computing workflows.

Validation and Local Execution

All easy bug snippets were manually compiled and executed on local machines using C++ compilers (GCC 7.5) and Python 3.7 interpreters to validate their runtime behavior and confirm the presence of the expected compile-time, runtime, or logical errors.

For advanced bugs, the corresponding open-source repositories were cloned, and bugs were reproduced using the pre-patch versions, as verified through commit history and issue discussions. Associated unit tests and test cases were run locally to confirm that the buggy behavior was both reproducible and verifiable. The buggy version of the code along with minimal contextual dependencies was then provided to the LLMs as input.

Prompting and Interaction Protocol

For each snippet, a fresh chat session was initiated to prevent context carryover or bias from previous prompts. This was especially important to avoid situations where the model would focus solely on one type of bug (*e.g.*, memory leaks) even when the actual issue was logical or structural.

For easy bugs, the following standardized prompt was used:

Are there any compile-time, runtime, logical errors, or vulnerabilities in the following code? List them with the lines where they occur.

This minimal prompting approach assessed the LLMs’ baseline ability to reason about standalone code.

For advanced bugs, the prompt was extended with relevant auxiliary context, such as reduced versions of dependent files or known interfaces.

¹<https://github.com/Suresoft-GLaDOS>

²<https://pybughive.github.io/>

GCC	7.5	Python	3.7	numpy	1.23.4	pandas	0.19.2
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TABLE I: Compiler and software versions used in the study.

<p>Identify all internal logical errors, edge cases, and potential defects within the PyArray_FillWithScalar function, as well as those that may arise from its usage.</p> <hr/> <p>Based on the following test case, evaluate where PyArray_FillWithScalar could fail and cause an issue.</p> <pre>def test_fill_readonly(self): a = np.zeros(11) a.setflags(write=False) with pytest.raises(ValueError, match=".*read-only"): a.fill(0)</pre>

If the LLM’s first response listed a candidate issue or line, the next prompt would explicitly reference that function or line to probe for a deeper analysis or partial identification. When the LLM failed to surface meaningful results, we further introduced unit test descriptions or inputs, simulating how developers would triangulate buggy behavior using the test suite.

This multi-stage, context-aware prompting was crucial for assessing whether models could go beyond surface-level static checks and demonstrate adaptive reasoning under more realistic, project-scale scenarios.

Evaluation Criteria

Detection performance was rated using a graded visual scheme:

- ○ **Empty Circle** — No detection of the bug
- □ **Quarter Circle** — Minimal or speculative hint
- △ **Half Circle** — Partial detection
- Ⓛ **Three-Quarter Circle** — Near-complete detection
- ● **Full Circle** — Complete detection of the bug

IV. QUALITY OF BUG DETECTION

Table I lists the compilers and libraries used for the evaluation. We used the standard GCC and Python version.

A. Easy C++ Bugs

This section evaluates the ability of LLMs to identify basic C++ programming bugs, representative of issues commonly introduced by novice programmers during early coursework. These bugs were selected to reflect pedagogical examples typically used in *introductory computer science curricula at universities and colleges*, where students learn fundamental programming constructs such as pointer management, reference passing, and basic memory operations. These examples

form a baseline for assessing LLMs’ capability to statically reason about localized, self-contained code snippets.

We examined seven such C++ snippets (denoted as **E1** to **E7**) and submitted them to ChatGPT-4, Claude 3, and LLaMA 4 under consistent prompt conditions. Each model was asked to identify any compile-time, runtime, logical, or vulnerability-related bugs in isolation and, if possible, suggest a corrective action. All code snippets were additionally compiled and executed locally to validate their error conditions and match LLM responses with observed behavior.

a) **E1: Unbounded Allocation via std::rand()**: This snippet triggers a potential std::bad_alloc error by using an unbounded call to std::rand() to reserve a vector size, possibly exceeding available memory. All LLMs correctly identified this risk and recommended bounding the random value using modulo or conditional checks to limit memory allocation, a clear affirmation of their understanding of unsafe dynamic allocation patterns.

b) **E2: Pass-by-Value Semantics and Side Effects**: In this snippet, a template function intended to square a value is passed by value, leading to no effect on the original variable. All models accurately flagged the semantic bug—namely, that pass-by-value prevents mutation of the calling context—and recommended using references to preserve side effects.

c) **E3: Double Deletion Across Scopes**: This example involves deleting the same dynamically allocated memory in both a helper function and in main(), resulting in undefined behavior due to double deletion. All three LLMs correctly identified the ownership confusion and suggested smart pointer usage, such as std::unique_ptr, to resolve the issue.

d) **E4: Use-After-Free Before Function Call**: In this case, memory is deallocated before being passed to a function that attempts to iterate over the now-invalid pointer. All models correctly flagged this use-after-free bug, suggesting the pointer be freed after the loop completes.

e) **E5: Misuse of std::move and Vector Invalidity**: This snippet misuses std::move() to transfer ownership of a std::vector into a function, after which its size is queried. The models identified that the moved-from vector’s state is unspecified post-transfer and suggested redesigning the call or avoiding post-move usage.

f) **E6: Null Pointer Dereference**: This example attempts to dereference an uninitialized pointer (`cppcodenullptr`) in a loop, leading to undefined behavior. All LLMs identified the segmentation fault risk and noted the pointer lacked memory allocation before accessing an example of proper detection of null-pointer safety.

g) **E7: Buffer Overflow via Unbounded String Copy**: A classic buffer overflow scenario, this snippet copies input from `argv[1]` into a fixed-size buffer without bounds checking. Claude and LLaMA correctly identified the overflow risk. ChatGPT flagged the problematic line but gave only partial elaboration.

In summary, for these foundational bugs, all LLMs demonstrated strong diagnostic capabilities, routinely identifying the nature, location, and remedy of errors. Their recommendations

aligned with *modern C++ best practices*, showing fluency in using smart pointers and proper memory ownership semantics. These findings suggest that LLMs are well-suited for beginner-level static analysis tasks and could potentially augment educational tooling in programming pedagogy. Table II summarizes the results.

B. Security Vulnerability Detection in C++ Snippets

This section evaluates how large language models (LLMs) perform in detecting and reasoning about security-relevant flaws in C++ code. The selected code samples (denoted as **S1 to S7**, originally Snippets #10–#16) are sourced from the SEED Labs framework³, encompassing real-world inspired vulnerabilities such as unsafe input handling, race conditions, resource exhaustion, and insecure file manipulation. These examples are designed to simulate scenarios where poor coding practices could lead to severe security risks, particularly when operating in privileged or system-level contexts.

a) **S1: Format String Vulnerabilities and Buffer Overflow:** This snippet presents a combination of unbounded string input into format functions and unchecked memory writes. All three LLMs successfully identified the core vulnerabilities. Notably, ChatGPT-4 and Claude 3 extended their analysis to include the potential for shell command injection, thus acknowledging *chained exploitation vectors* in unsafe I/O pipelines. LLaMA 4, while detecting the buffer overflow, did not surface the compound risk posed by uncontrolled format strings—a partial gap in holistic reasoning about compound attack surfaces.

b) **S2: Race Condition in Temporary File Handling:** This example tests the model’s recognition of time-of-check to time-of-use (TOCTOU) vulnerabilities, particularly those exploitable in Set-UID contexts. All LLMs demonstrated an understanding of the fundamental race condition. ChatGPT further noted the potential for symbolic link attacks—a critical path in privilege escalation. While Claude and LLaMA correctly recommended safer file creation primitives, they generalized the issue as file overwriting without linking it explicitly to Set-UID or privilege boundaries. Nonetheless, the responses collectively adhered to *secure coding principles*.

c) **S3: Environment Variable Manipulation and Shell Execution :** This snippet involves unsafe reliance on environment variables and the execution of external commands. ChatGPT-4 and Claude 3 accurately identified issues such as environment poisoning, unvalidated input propagation, and shell injection. Additionally, they noted the lack of proper file descriptor sanitization. LLaMA 4 surfaced the risk of shell execution but failed to comment on unclosed file descriptors, an omission that diminishes detection completeness from a *secure resource management* standpoint.

d) **S4: Null Pointer Dereferencing:** All LLMs successfully detected this memory safety violation. The responses reflected a shared baseline proficiency in identifying dereferencing of potentially uninitialized or null pointers, reaffirming

the maturity of LLMs in static analysis for fundamental safety errors.

e) **S5: Zip Bomb and Resource Exhaustion via Archive Extraction:** This snippet explores decompression behavior without bounds checks, simulating conditions for a denial-of-service (DoS) through zip bombs. Claude 3 alone recognized the issue in its full severity, explicitly citing *resource exhaustion* and lack of decompression limits. In contrast, ChatGPT-4 and LLaMA 4 required more probing to link the snippet to DoS-style threats, indicating a lower sensitivity to *non-obvious latent vulnerabilities*.

f) **S6: Out-of-Bounds Access and Memory Leaks:** Here, the models were uniformly capable of identifying both an out-of-bounds write and failure to free dynamically allocated memory. Suggested remediations included array bounds checking and correct use of ‘delete’, showing convergence in the detection of classical low-level programming mistakes.

g) **S7: Insecure Temporary File Creation:** This snippet checks whether the models can detect insecure practices in creating temporary files. All three LLMs noted the predictability of filenames and the absence of atomic creation mechanisms. Each recommended the use of secure system calls like `mkstemp()`, demonstrating a solid grasp of *safe file handling procedures* and suggesting appropriate secure alternatives.

Summary. While all LLMs demonstrated the ability to detect major security vulnerabilities, ChatGPT-4 and Claude 3 consistently delivered more contextually rich and accurate analyses. They often captured both the primary issue and potential exploitation chains. LLaMA 4, although capable in foundational detection, occasionally missed subtler but crucial aspects such as file descriptor management or privilege context—critical in real-world systems security. These findings underscore important variance in how current-generation LLMs reason about *system-level behavior and security implications* in code. The results are summarized in Table III.

V. DETECTION OF ADVANCED C/C++ BUGS IN REAL-WORLD CODEBASES

To assess LLM capabilities in more complex, real-world scenarios, this section investigates advanced C and C++ bugs sourced from production-level open-source repositories, specifically the OpenSSL project, as cataloged in the Suresoft-GLaDOS bug database. These examples (denoted as **A1 to An**) embody challenging categories including cryptographic misconfigurations, platform-specific numerical precision issues, pointer misuse, and low-level error state ambiguities. Unlike pedagogical examples, these bugs require *contextual reasoning, awareness of API contracts, and precise understanding of compiler behavior and runtime semantics*.

All snippets were tested using the same evaluation protocol applied to earlier categories. The buggy code was extracted directly from historical OpenSSL commits and tested locally. LLMs were prompted with the code context and were asked to identify latent bugs and propose fixes. Models were allowed

³<https://seedsecuritylabs.org/labs.html>

Language C++	LLM		
Bug	GPT	Llama	Claude
E1: Memory allocation error (std :: bad_alloc) on oversized int	●	●	●
E2: Integer Underflow and Truncation	●	●	●
E3: Pass-by-value prevents actual update	●	●	●
E4: Memory freed twice	●	●	●
E5: Accessing deallocated heap via pointer	●	●	●
E6: std :: move leaves vector in unknown state	●	●	●
E7: Buffer overflow risk (no bounds check)	●	●	●

TABLE II: Evaluation of bugs commonly done by C++ novices on the bachelor level.

Description	GPT	Llama	Claude
Snippet number: Description of the issue	GPT	Llama	Claude
S1: Format string vulnerability, Buffer Overflow Vulnerability and leaking memory addresses	●	∅	●
S2: Race-condition vulnerability	∅	∅	∅
S3: Leaked file descriptor, weak privilege dropping, unsafe spawning of a shell, and passing a null environment to execve	●	∅	●
S4: Zip bombs attack, disk exhaustion	∅	∅	●
S5: Out-of-bound and memory leak possibility	●	●	●
S6: Temp file creation using temp() and mstemp() functions	●	●	●

TABLE III: C++ Security Bug Evaluation

multiple prompt rounds if necessary to refine their understanding. In cases where the buggy logic spanned dependencies, key auxiliary lines and API references were included in the prompt to mirror the reasoning a security researcher would perform when reviewing production code.

a) **A1: Array Decay and Dimensional Metadata Loss:** This snippet models a subtle but common pitfall—passing statically sized arrays to functions, triggering implicit decay to pointers. As a result, size information is lost, and any function relying on ‘sizeof’ within the callee context behaves incorrectly. All LLMs recognized the semantic consequence of array-to-pointer decay and its potential to cause logic bugs or out-of-bound access. The models recommended safer interface patterns, such as explicitly passing array size or using ‘std::array’.

b) **A2: Validity Checks in X.509 Chain Verification (OpenSSL):** Sourced from OpenSSL’s certificate handling logic, this snippet involves parsing and validating self-issued intermediate certificates. ChatGPT-4 demonstrated high contextual awareness, flagging the use of “x509_check_cert_time” and “X509_NAME_cmp” as security-critical operations. It also inferred the need for precise issuer matching and error propagation. LLaMA 4 noted general trust anchor concerns but missed specific time validity enforcement. Claude 3 provided intermediate insight, detecting logical complexity but lacking full propagation path analysis.

c) **A3: Missing Null Guard in Cryptographic Assignment (EVP_PKEY_assign):** This bug stems from neglecting to null-check pointer arguments before assignment in cryptographic operations. ChatGPT correctly diagnosed the need for null guarding before invoking ‘EVP_PKEY_assign’, citing the undefined behavior risk. LLaMA surfaced the pointer access issue but offered only partial fixes. Claude aligned closely

with ChatGPT, referencing API-level guarantees and defensive programming idioms common in cryptographic codebases.

d) **A4: Improper Error Flag Usage (ERR_TXT_MALLOCE):** This case explores the misuse of OpenSSL’s internal error reporting flags. Improper initialization of the ‘ERR_TXT_MALLOCE’ flag leads to ambiguous or silently dropped error messages, impacting post-failure diagnostics. ChatGPT and Claude identified the flag mismanagement and recommended defensive resets or more explicit error-state initialization. LLaMA responded with generic error handling suggestions but missed the specificity of the flag’s role in memory ownership tracking.

e) **A5: Floating-Point Precision Loss on Casting ULONG_MAX to Double:** This precision bug arises from casting ‘ULONG_MAX’ to ‘double’, which exceeds the representable range in IEEE-754 double precision, leading to subtle errors in range checks. ChatGPT and Claude both identified the architectural precision loss and noted the potential for misbehavior when ‘ULONG_MAX’ exceeds 2^{53} . Although their suggestions were not exact matches to the patch used upstream, they reflected sound numeric reasoning. LLaMA failed to pinpoint the type conversion as the root cause, indicating challenges in interpreting *hardware-level numeric edge cases*.

f) **A6: Spiral Matrix Pattern (Edge Inclusion):** Although distinct from the OpenSSL corpus, this snippet was included as an edge case to test LLM spatial and logical reasoning. The code attempts to generate an $n \times n$ spiral matrix, but the output is incorrect due to flawed index management and loop control. None of the models provided a correct fix upon first pass. ChatGPT came closest by suggesting loop boundary refactorings. Claude and LLaMA required multiple hints and failed to detect off-by-one indexing and directional

flow control as core issues. This test underscores a current limitation in LLMs when reasoning about *algorithmic layout and pattern synthesis*, even when syntactic bugs are absent.

Summary. When confronted with production-grade bugs from OpenSSL, both ChatGPT and Claude exhibited strong contextual understanding and were able to map specific function behaviors to security semantics. They often produced relevant mitigation, demonstrating maturity in handling pointer hygiene, error propagation, and defensive API use. LLaMA, while technically competent in basic detection, lagged in synthesizing implications that cross abstraction layers—such as cryptographic correctness, state-management and API contract violations. Overall, this evaluation affirms the increasing viability of LLMs as tools for *assisting in secure code reviews and automated vulnerability analysis* across modern C and C++ codebases. Table IV summarizes the results.

VI. DETECTION OF ADVANCED PYTHON BUGS IN REAL-WORLD LIBRARIES

This section evaluates how well large language models (LLMs)—ChatGPT, Claude, and LLaMA—detect and reason about nuanced bugs in Python code originating from widely used real-world libraries such as NumPy and Pandas. The code examples (denoted A7 through A12) were curated from the PyBugHive repository, which catalogs manually validated bugs along with corresponding test cases and patch commits. These bugs span a range of issues including semantic mismatches, type inconsistencies, and logic faults in high-level data processing workflows. Each code snippet was validated locally and accompanied by minimal contextual augmentation when required to simulate realistic diagnostic conditions. Table V lists the information for the studied bugs.

a) **A7: Incorrect Fortran Character Expansion (NumPy):** Sourced from `capi_maps.py`, this bug concerns the mishandling of a single Fortran character being expanded incorrectly into an array structure. ChatGPT and LLaMA partially identified the flaw, each noting unusual data behavior but requiring further context to isolate the transformation logic. Claude, however, diverged toward unrelated control path explanations and missed the root cause.

b) **A8: TypeError when given a `pathlib.Path` instead of a string (Pandas):** The bug in Pandas from the `read_html()` function raising a `TypeError` when passed a `pathlib.Path` object, as it expected a string or file-like input. The fix involved wrapping the `io` argument with `stringify_path()`, ensuring compatibility with Path types.

In identifying this issue, ChatGPT-4 clearly recognized the root cause and the appropriate resolution. Claude and LLaMA performed similarly; they understood there was a type mismatch but didn't fully trace it to the missing path string conversion, making their analysis less complete compared to GPT.

c) **A9: `DataFrame.groupby()` misinterpreted a tuple key on a MultiIndex as multiple keys:** Both GPT-4 and Claude effectively identified the root cause —

`DataFrame.groupby()` was treating a tuple key as multiple group keys instead of a single key when used with a `MultiIndex`. This subtle misinterpretation led to incorrect grouping results. Both models accurately traced the logic to the `_get_grouper` function and recognized the added conditional check for `is_axis_multiindex` in the patch.

In contrast, LLaMA struggled to pinpoint the nuance of the bug. While it recognized the method involved and the general idea of grouping behavior, it failed to differentiate between tuple-as-key vs. tuple-as-list-of-keys, which is critical to understanding the issue. Its responses were either vague or missed the specific edge case that caused the bug.

d) **A10: `pd.concat` Mishandling MultiIndex with None Level Names (Pandas):** This snippet presented a `MultiIndex` construction failure in Pandas when concatenating objects that include `None` as level names. All three LLMs surfaced the `MultiIndex` construction error and suggested layered structural fixes. However, none accurately proposed the actual minimal solution—refining the iterator evaluation logic—highlighting the challenge LLMs face in mapping high-level errors to minimal diffs in complex libraries.

e) **A11: Type Inconsistency in Return of `na_values` (Pandas):** This example captures a subtle return-type contract violation in Pandas, where an empty `na_values` input returns a list rather than a set. All models successfully identified the inconsistency and suggested type alignment, demonstrating reliable reasoning within Python's dynamic typing model and contract expectations.

f) **A12: Timezone-Aware Datetime Conversion to Float (Pandas):** This bug concerns improper conversion of timezone-aware datetime objects into floats during numerical transformations. LLaMA provided the closest diagnosis by identifying the context and suggesting a viable correction. ChatGPT and Claude each recognized surrounding semantic mismatches but failed to localize the precise logic misuse or its functional implications.

Summary. Across these real-world Python bugs, ChatGPT and Claude demonstrated comparatively higher diagnostic coverage and more consistent alignment with root causes, especially when prompted with supporting context. LLaMA was frequently able to flag symptoms but struggled with localization or precise patch synthesis. These results reinforce current LLMs' promise in aiding high-level software diagnostics while also revealing their limitations in mirroring *minimal diffs and subtle API contract enforcements* required in production-level patches. Table VI summarizes the results.

VII. PERFORMANCE AND EVALUATION

One metric to estimate the cost of software development is the **Constructive Cost Model** (COCOMO) [20]. The original COCOMO model was developed in the late 1970s and COCOMO II was developed in 1995 and published in the 2000 [21] to address modern software development. The tool `scc`⁴ was used to run the COCOMO analysis on all studied

⁴<https://github.com/boyter/scc>

Description	GPT	Llama	Claude
Snippet number: Description of the issue	GPT	Llama	Claude
A1 #17: Array decay and out of bounds	●	●	●
A2 #8: NxN spiral matrix	○	○	○
A3 #18: Self-issued intermediate certs and only returns issuers that are valid and time-checked	∅	∅	∅
A4 #19: Add a NULL check to EVP-PKEY-assign	∅	∅	∅
A5 #20: Ambiguous error state representations when error flag is ERR-TXT-MALLOCE	∅	∅	∅
A6 #21: Rounding errors in range check	∅	○	∅

TABLE IV: C++ Advanced Bug Evaluation (Snippets A1–A6)

Bug on GitHub	Bug ID in Dataset	Snippet	Library and Version Fixed	Bug Occurrence Version
#15701	15711	#12	Pandas : 0.20.0	0.19.0
#15835	15881	#11	Pandas : 0.20.0	0.19.0
#15787	15787	#10	Pandas : 0.20.0	0.19.2
#22970	22922	#9	Numpy : 1.24.2	1.24.1
#22968	22899	#8	Numpy : 1.24.2	1.23.4

TABLE V: Mapping of Bug Reports to Snippets and Library Versions

Description	GPT	Llama	Claude
A7 Snippet #7: Incorrect expansion of Fortran text vars into arrays	∅	∅	∅
A8 Snippet #8: TypeError when given a pathlib.Path instead of a string	●	∅	∅
A9 Snippet #9: DataFrame.groupby() misinterpreted a tuple key on a MultiIndex	∅	∅	∅
A10 Snippet #10: pd.concat issue with MultiIndexes with None names	∅	∅	∅
A11 Snippet #11: na-values set as a list instead of a Set	●	●	●
A12 Snippet #12: Incorrect tz-aware datetime to float conversion	∅	∅	∅

TABLE VI: Python Advance Bug Evaluation (Snippets 7–12)

code snippets. We used the Estimated Schedule Effort (ESE) with the organic option, which is the amount of labor required to complete the project, measured in person-months; to classify the code development from **easy** to **difficult**.

A. C++ code

Figure 1a shows the effort and quality for the easy C++ bugs in Section IV-A and all models could find and fix the bugs. Figure 1b shows the effort and quality for the security bugs in C++ in Section IV-B. Here, Llama could find two bugs and the remaining bugs were near complete detection. ChatGPT could detect two bugs near completion, and Claude only one bug near detection. Here, Llama could only find and fix the bugs with the lower effort. Figure 1c shows the C++ advanced bugs in Section V. All models could only detect the first bug with the second lowest effort. None could detect the bug with the lowest effort. ChatGPT has the highest rate with \wp . Llama could not detect the last bugs where other models could detect the bug. Claude was comparable to ChatGPT; however, bug A4 has been detected at \square . Where most models have issues, the ESE was between three and five months.

B. Python code

Figure 2 showcases the quality and effort for the Python code. Only for snippet A11 could all models find and fix the bug where the effort was high. For snippet A8 only ChatGPT

could find and fix the bug with medium effort. All other snippets were only partially detected.

VIII. DISCUSSION AND CONCLUSION

This study provides a comprehensive evaluation of LLMs—ChatGPT-4, Claude 3, and LLaMA 4—in detecting bugs across a range of programming scenarios, from introductory-level C++ constructs to advanced, real-world vulnerabilities in both C/C++ and Python. Our results reveal a consistent trend; LLMs excel at identifying syntactic and semantic bugs in isolated, well-scoped code snippets, particularly those reflecting beginner-level programming mistakes. All models demonstrated strong alignment with modern C++ practices, correctly identifying issues such as null pointer dereferencing, use-after-free, memory mismanagement, and misuse of std :: move. This supports their potential utility in educational settings, where early-stage feedback on student code could be significantly improved by LLM integration.

However, the models’ performance diverges in more complex scenarios involving security vulnerabilities and production-grade code. While ChatGPT-4 and Claude 3 frequently provided deeper contextual insights—such as recognizing chained exploitation paths, privilege boundaries, or numeric precision loss—LLaMA 4 often produced partial or superficial explanations.

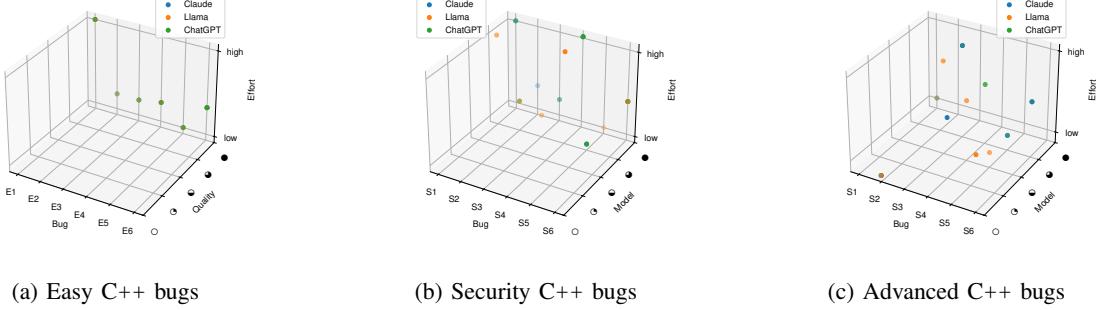


Fig. 1: Effort and Quality of the bug detection for (a) in Section IV-A, (b) in Section V, and (c) in Section V.

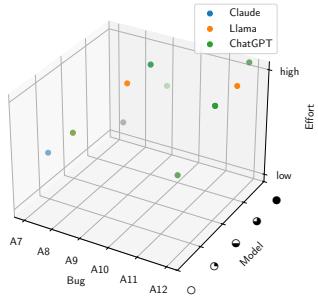


Fig. 2: Advanced Python bugs

In conclusion, LLMs are effective in identifying a broad class of software bugs, particularly those that are syntactic, shallow, or pedagogically motivated. They offer substantial promise in educational tools, static analysis assistance, and as first-pass reviewers in code auditing workflows. However, for more complex tasks, their current capabilities remain limited.

Future Work. We will explore the integration of multi-agent systems to enhance bug detection workflows, enabling task delegation, self-refinement, and collaboration among specialized LLM agents. Additionally, we aim to extend our analysis to a broader range of programming languages beyond C, C++, and Python to assess cross-language generalization and identify language-specific diagnostic strengths and limitations.

Supplementary materials

The generated source code is available on GitHub⁵.

Acknowledgments

This work is partially supported by the US National Science Foundation grant 2431531. This work was supported by the U.S. Department of Energy through the Los Alamos National Laboratory. Los Alamos National Laboratory is operated by Triad National Security, LLC, for the National Nuclear Security Administration of U.S. Department of Energy (Contract No. 89233218CNA000001). LA-UR-25-28306.

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⁵<https://github.com/NoujoudNader/LLM-Bugs-Detection>