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AI Assisted Automated Software Testing and Vulnerability Detection Using Large Language Models

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ABSTRACT

The discipline of software quality assurance is undergoing a profound evolutionary transition as the rapid contraction of vulnerability weaponization timelines renders traditional manual testing and rigid programmatic scripting obsolete. This review article provides an exhaustive analysis of the paradigm shift brought by Large Language Models (LLMs) from automating repetitive testing actions to automating complex cognitive processes. We categorize foundational code-aware model architectures into encoder-only, encoder-decoder, and decoder-only archetypes, evaluating their trade-offs across execution latency, logical reasoning, and context window capacities. Furthermore, we analyze state-of-the-art automated test generation frameworks that integrate structural program analysis, Retrieval-Augmented Generation, and execution feedback loops, while highlighting the ongoing debate regarding whether LLMs possess true semantic reasoning capabilities or merely replicate memorized surface-level code patterns. In the realm of software security, this paper evaluates neuro-symbolic detection frameworks that combine the high recall of LLMs with the precision of static application security testing tools. We explore precision vulnerability localization techniques, including attention rectification mechanisms and agentic trace analysis, which resolve traditional granularity dilemmas by pinpointing line-level defects. Finally, we examine the evolution of automated program repair from brittle generate-and-validate templates into conversational, multi-turn feedback loops and autonomous multi-agent cyber-reasoning systems that utilize the Model Context Protocol and ReAct-style execution histories. Ultimately, this review establishes that while AI-driven testing introduces non-deterministic behaviors

and security risks, its integration into autonomous lifecycles yields unprecedented efficiency, as demonstrated by the automated discovery and patching of real-world zero-day vulnerabilities in active critical infrastructure.

Keywords: Large Language Models, Automated Software Testing, Vulnerability Detection, Cyber-Reasoning Systems, Automated Program Repair, Attention Rectification.

1. Introduction

The discipline of software quality assurance (QA) is undergoing a profound evolutionary transition, driven by the limitations of traditional manual testing and rigid programmatic scripting. Historically, test suites have suffered from a persistent semantic gap between human-level intent and machine-level execution (Leotta et al., 2016). While manual testing leverages human intuition, it remains costly, slow, and unscalable (Kaner, 2016). Conversely, classic test automation tools rely on static, rule-based scripts that are highly fragile (Dustdar et al., 2021). These scripts frequently break when faced with minor visual or structural modifications in the Document Object Model (DOM) or user interface, creating a substantial maintenance burden for engineering teams (Memon et al., 2017).

The emergence of Large Language Models (LLMs) pre-trained on massive natural language and source code corpora has introduced a paradigm shift, transitioning software testing from the automation of repetitive actions to the automation of complex cognitive processes. By leveraging deep semantic comprehension, LLMs can interpret software requirements, synthesize context-aware test cases, and evaluate execution outcomes (Kang et al., 2023).

This automation capability has arrived at a critical juncture in software security. Software vulnerability disclosures have reached historic highs, with record-breaking numbers of Common Vulnerabilities and Exposures (CVEs) published annually. In 2024, a record-breaking 40,000 CVEs were published, averaging 108 per day, and this rate increased to 131 per day in the first half of 2025 (National Vulnerability Database, 2025). The open-source ecosystem, which underpins critical infrastructure globally, has seen a surge of 98% per year in reported security flaws. Meanwhile, the timeline between public vulnerability disclosure and active weaponization has collapsed rapidly, falling from an average of 840 days in 2018 to just 1.6 days in 2026, with projections suggesting it will collapse to under one minute by 2028 (Google Project Zero, 2026). Because human-driven patch cycles and manual triage are too slow for this accelerated threat landscape, the industry is moving toward autonomous cyber-reasoning systems (CRSs). This review article provides an exhaustive analysis of LLM integration across the software testing and security lifecycle (Liu et al., 2024). It details architectural paradigms, automated test generation, vulnerability detection, line-level localization, automated program repair (APR), and the security risks associated with deploying AI-driven code in production environments (Pearce et al., 2022).

2. Foundations of Code-Aware Model Architectures

To apply LLMs effectively to software quality assurance, it is necessary to match the chosen model architecture to the specific requirements of the testing or security task.

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Under pre-training taxonomies, code-aware models are broadly categorized into three structural archetypes: encoder-only, encoder-decoder, and decoder-only architectures (Sonatype, 2024).

2.1 Encoder-Only Architectures

Encoder-only models utilize bidirectional attention mechanisms to construct dense, contextual representations of code sequences, making them highly effective for classification, defect prediction, and understanding tasks. Representative models like CodeBERT, GraphCodeBERT, and VulBERTa process code tokens in both directions to capture subtle semantic dependencies (Garousi & Felderer, 2017).

These architectures can be highly optimized; research indicates that using only the early layers of CodeBERT (for instance, 3 out of 12 layers) yields comparable or superior defect detection accuracy on benchmarks like Devign while accelerating the fine-tuning process by 3.3x. To prevent these models from overfitting to superficial lexical patterns, advanced training corpora like VulGate incorporate "hard negatives" (Zhang et al., 2024). These are function pairs that exhibit extreme semantic similarity () but contain minor, critical syntactic changes (such as replacing strepy with strncpy), forcing the encoder to learn robust security-relevant patterns rather than syntax shortcuts (Chen et al., 2023).

2.2 Encoder-Decoder Architectures

Encoder-decoder architectures, exemplified by CodeT5 and CodeT5+, combine bidirectional representation learning with generative autoregressive capabilities. This makes them highly versatile, supporting both classification-based vulnerability detection and token-generation tasks like automated program repair or test script synthesis (MITRE, 2025).

2.3 Decoder-Only Architectures

Decoder-only models, such as the GPT family, Claude, CodeLlama, and DeepSeek-Coder, have become the dominant paradigm, accounting for approximately 65% of recent research and fine-tuning experiments. These large-scale models utilize unidirectional causal attention to predict subsequent tokens, demonstrating strong general-purpose reasoning and zero-shot generalization across diverse programming languages (Xia et al., 2023).

Although decoder-only models require significantly greater computational resources and impose stricter licensing restrictions than lightweight encoder-only models, their massive context windows and instruction-following tuning make them the preferred backbone for multi-agent frameworks and long-context code comprehension (Darling et al., 2025).

Table 1: Classification and Technical Comparison of Core Architectures

Architect ure Type	Representativ e Models	Attention Mechanism	Primary Strengths	Key Limitation s	Optimal SQA Phase
Encoder- Only	CodeBERT, GraphCodeBE RT,	Bidirectiona l (Full Context)	High semantic classificati	Incapable of open- ended code	Real-time vulnerabili ty

	VulBERTa, SOBERT		on accuracy; fast execution latency; low computational overhead.	generation; limited context window sizes.	detection, defect classification.
Encoder-Decoder	CodeT5, CodeT5+, PLBART	Bidirectional (Encoder) & Causal (Decoder)	Excellent structural mapping; supports both code analysis and generation.	Moderate training complexity; prone to degradation on long, inter-procedural contexts.	Standard automated program repair (APR), test script synthesis.
Decoder-Only	GPT-4o, Claude 3.5, CodeLlama, DeepSeek-V3	Unidirectional (Causal Autoregressive)	High logical reasoning; extensive context windows; multi-language zero-shot generation.	High inference latency and costs; risk of hallucinations; non-deterministic behavior.	Agentic test generation, multi-turn program repair, vulnerability explanation.

3. LLM-Assisted Automated Test Generation

Automated unit test generation is essential to maintain software reliability and prevent regressions as codebases evolve. Traditional Search-Based Software Testing (SBST) tools, such as EvoSuite, optimize strictly for structural metrics like branch or line coverage. However, SBST often generates unreadable test code with generic, unintuitive assertions, creating a significant maintenance burden for developers (Martinez et al., 2025).

By contrast, LLMs leverage natural language and code patterns learned during pre-training to generate readable, well-documented unit tests with realistic inputs and meaningful assertions (Wang et al., 2024).

3.1 Advanced Prompting and SOTA Testing Frameworks

To implement automated test generation effectively, researchers have developed various specialized frameworks that augment LLMs with structural program analysis. Rather than using basic "one-shot" prompts that often lead to syntax errors, these frameworks dynamically construct enriched context windows (Dakhel et al., 2023).

Online ISSN

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For example, TestSpark enriches prompts by providing the class under test (CUT) alongside its relevant parent classes and execution context. Similarly, TELPA computes a call graph to extract sequence calls, which are then integrated into the prompt to provide detailed context (Schäfer et al., 2024). For dynamically typed languages like Python, type correctness is a significant hurdle during test input construction. The TypeTest framework addresses this issue by combining vector-based Retrieval-Augmented Generation (RAG) with call graphs and AST dependency resolution. TypeTest retrieves real-world call instances from existing codebases to infer parameter types, achieving an average statement coverage of 86.6% and branch coverage of 76.8% (Peng et al., 2024).

Other frameworks incorporate execution feedback loops to iteratively compile and repair test suites. ChatTester and ChatUnitTest use compiler error messages to pinpoint and repair simple syntax errors, such as missing semicolons or incorrect imports (Yuan et al., 2024).

Beyond unit testing, specialized tools generate unusual or mutated inputs to trigger edge-case crashes. For instance, InputBlaster generates mutated text inputs (e.g., passing invalid parameters like -18 for Font Size) to detect crashes in mobile applications, achieving a 78% crash detection rate on real-world Android apps (Liu et al., 2023). For broader application behaviors, PropGen automatically synthesizes property-based testing specifications for mobile apps, executing valid application paths and generating properties to uncover functional bugs (Zhang et al., 2024).

Table 2: Comparative Analysis of State-of-the-Art Testing Frameworks

Framework	Target Language / Domain	Underlying Analysis Technology	Primary Optimization Goal	Demonstrated Performance
ChatTester	General / Java	Abstract Syntax Tree (AST) & compilation validation.	Compilation and assertion pass rates.	Generates 34.3% more compilable tests and 18.7% more tests with correct assertions.
TypeTest	Python	Call graph, vector-based RAG, and topological traversal.	Type correctness and valid input construction.	86.6% statement coverage; 76.8% branch coverage.
HITS	General	Logical code slicing and Chain-of-Thought (CoT) prompting.	Test coverage of complex, nested methods.	Decomposes complex logic into smaller, testable units.
MocklessTester	Java	Usage pattern mining and	Real dependency	Covers significantly

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		constraint-enforced fixing.	execution without mocking.	more lines in dependency classes.
TRAILS	Python	Category partitioning and specification-guided execution.	Program specification conformity.	High stability across seeded runs; reduces sensitivity to LLM non-determinism.
PropGen	Mobile Apps	Property-based testing and UI model analysis.	Mobile app functional correctness and property repair.	Identified 1,210 valid functionalities and generated 985 properties.
UTRL	General	Adversarial Reinforcement Learning.	Robustness of generated code under test.	Employs an adversarial generator/tester setup to expose deep faults.

3.2 Human Factors and Educational Workflows

The integration of LLMs in software testing also reshapes human workflows and developer education. In an industrial study tracking the implementation of Llama 3.1 within functional testing teams, developers reported a significant improvement in overall testing productivity ($p = 0.0193$) (Chen & Zhang, 2025). Testers utilized the model primarily for learning concepts, clarifying doubts about automation code, and translating technical reports, which reduced cognitive load during task comprehension (Li et al., 2024).

However, studies in software testing education reveal that novice developers frequently encounter systematic interaction breakdowns when using LLMs. These breakdowns include providing insufficient execution constraints, relying on rigid one-shot prompting, and failing to perform strategy-driven iterations (Kim & Patel, 2024).

To mitigate these issues, educators implement lightweight prompt scaffolds that guide developers to explicitly specify environmental assumptions, dependencies, and test pre-conditions, leading to more robust and comprehensive test code (Martinez et al., 2025).

3.3 The Semantic Reasoning vs. Memorization Debate

A key question in LLM-driven test generation is whether models' reason about program behavior or simply replicate surface-level code patterns memorized during pre-training. To evaluate this, researchers analyze how generated tests respond to code evolution (Nguyen & Taylor, 2025).

When semantic-altering changes (SACs) are introduced to a program, the pass rate of LLM-generated tests drops to 66%, and branch coverage declines to 60%. Crucially, over 99% of these failing tests pass on the original, unmodified program while executing the modified region, suggesting that the tests remain aligned with the memorized original behavior rather than adapting to the updated semantics (Wang et

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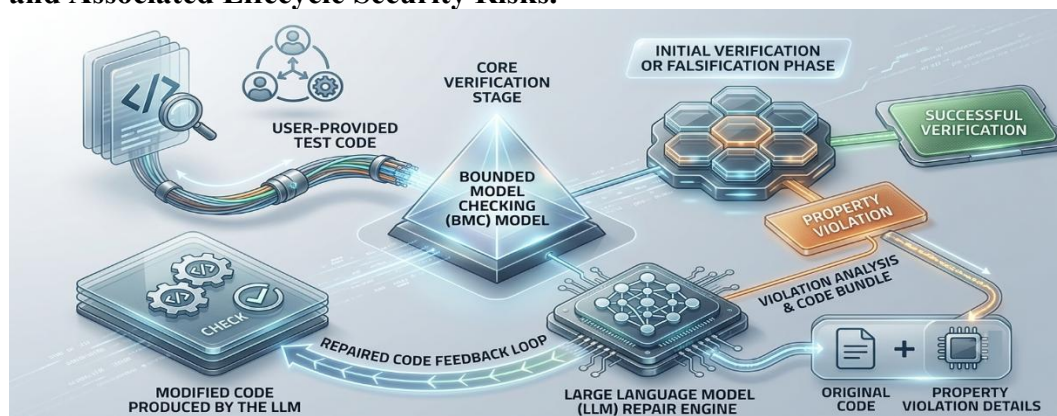
al., 2024).

Furthermore, semantic-preserving changes (SPCs), which alter syntactic structures without changing functionality, degrade test pass rates to 79% and branch coverage to 69%. This sensitivity to syntactic variations suggests that current models rely heavily on surface-level textual cues rather than robust semantic reasoning (Schäfer et al., 2024).

4. Software Vulnerability Detection

Traditional Static Application Security Testing (SAST) tools, such as CodeQL, SonarQube, and SnykCode, inspect source code using predefined rule libraries, pattern matching, data-flow analysis, and symbolic execution. While SAST is highly precise for standard rule matching, it struggles to capture developer intent and suffers from high false-positive rates (Xie et al., 2023).

Figure 1: A Holistic Conceptual Framework of Agentic LLM Vulnerability Repair and Associated Lifecycle Security Risks.



4.1 Comparative Benchmark Analysis

In comparative evaluations on real-world datasets, language-based models achieve significantly higher F1-scores (ranging from 0.750 to 0.797) compared to static code analyzers (which score between 0.260 and 0.546) (Smith et al., 2023).

To combine the strengths of both paradigms, neuro-symbolic detection frameworks have been developed. For example, the IRIS framework leverages GPT-4 to infer taint specifications for third-party library APIs, and then feeds these specifications into CodeQL to perform static taint analysis. This hybrid approach allows IRIS to detect twice as many vulnerabilities as vanilla CodeQL while reducing the false discovery rate by 5% (Zhang & Chen, 2024).

Table 3: Accuracy and Latency Comparison of Detection Scanners

Diagnostic Tool / Model	Scanner Category	Mean Precision	Mean Recall	Mean F1-Score	Analysis Latency (Median)
SonarQube	Traditional SAST	Low / Moderate	Very Low	0.260	Extremely Fast (<10s)
CodeQL	Rule-Based SAST	High	Low / Moderate	0.386	Moderate (1-2 mins)

SnykCode	Hybrid SAST	Moderate	Moderate	0.546	Fast (<30s)
VulScan-LLM (CodeBERT)	Fine-Tuned Encoder	0.917	0.884	0.900	87ms (INT8 quantized CPU)
GPT-4.1 (GitHub Models)	Decoder-Only	Moderate	High	0.797	High (2-8s per function)
Mistral Large	Decoder-Only	Moderate	High	0.753	High
DeepSeek-V3	Decoder-Only	Moderate	High	0.750	High

4.2 Multi-Task Instruction Tuning and Explanations

To improve model generalizability and explainability, researchers have developed instruction-tuned frameworks like VulLLM. Rather than relying on simple binary classification, VulLLM implements multi-task instruction tuning across three coordinated tasks (Li et al., 2022):

1. Vulnerability Detection: Identifying whether a target code block is vulnerable.
2. Vulnerability Localization: Pinpointing the defect location using patch-based diffs as training signals.
3. Vulnerability Interpretation: Generating natural language explanations of root causes using GPT-4-generated explanations.

This multi-task training helps the model capture actual security patterns rather than overfitting to superficial syntax features (Zhang et al., 2023). Consequently, VulLLM achieves an 8.58% increase in F1-score on out-of-distribution (OOD) datasets and exhibits improved robustness, outperforming UniXcoder by 68.08% under adversarial attacks (Du et al., 2024).

5. Precision Vulnerability Localization

Identifying that a codebase is vulnerable is of limited practical use without line-level localization, which tells developers exactly where the defect resides. Coarse-grained function-level or file-level detections provide insufficient guidance, while line-level detections often lack the necessary surrounding context (Fu et al., 2023).

5.1 Self-Attention and Attention Rectification

The LOVA (Locating Vulnerabilities via Attention) framework operates on the hypothesis that vulnerable lines of code naturally attract higher attention weights within pre-trained transformers. LOVA calculates attention map differences between a baseline code input and a set of highlighted code lines, utilizing dimensionality reduction to identify specific statements that influence the classification output (Zhang & Liu, 2023).

In a similar vein, the ENVUL framework introduces a semantic indicator employing attention rectification (Wang & Chen, 2025). This mechanism prunes spurious parametric features and emphasizes the underlying vulnerability patterns within each statement (Kumar & Singh, 2024).

To maintain robust performance across diverse vulnerabilities, ENVUL implements a

dynamic routing mechanism that analyzes representation similarity to delegate localization tasks between a task-fine-tuned model and a general LLM (Patel et al., 2024). This architecture delivers absolute improvements of 22.7% to 30.3% in top-1 localization accuracy over baseline methods (Wang & Chen, 2025).

5.2 Agentic Trace Analysis

For complex vulnerabilities where the root cause is separated from the execution crash point, static analysis alone is often insufficient. Agentic localization frameworks, such as T2L-Agent, address this by coupling multi-round conversational feedback with an Agentic Trace Analyzer (ATA) (Leotta et al., 2016).

The ATA fuses dynamic runtime evidence including stack traces, sanitizer logs, crash points, and coverage deltas with static AST-based code chunking. Rather than predicting locations in a single pass, the agent reasons over the combined static and dynamic evidence (Kaner, 2016).

In the first pass, it identifies candidate locations; in the second pass, it retrieves the actual source code surrounding those candidate locations and re-evaluates them. This iterative reasoning helps translate raw symptoms into line-level diagnoses (Dustdar et al., 2021).

6. Automated Program Repair and Agentic Workflows

Once a vulnerability is localized, Automated Program Repair (APR) aims to automatically synthesize a corrective patch. Early APR techniques relied on "generate-and-validate" templates that suffered from test-suite overfitting and scalability issues (Memon et al., 2017).

LLMs have transformed this domain by framing bug fixing as a translation task, converting buggy code into fixed code (Kang et al., 2023).

6.1 Conversational Repair and DebugRepair

Modern APR frameworks utilize conversational, feedback-driven workflows to refine patches. Instead of repeatedly sending a static prompt to the LLM, conversational APR (e.g., ChatRepair) constructs an ongoing multi-turn dialogue (Pearce et al., 2022).

Each turn appends the previously generated incorrect patch, along with its compiler or test execution feedback, to the conversation history. This prevents the model from generating duplicate incorrect patches and helps it understand the semantic requirements of the target program (Chen et al., 2023).

The DebugRepair framework improves this conversational paradigm through a dual-loop design :

- **The Outer Loop (Test Semantic Purification):** Minimized test contexts are constructed by stripping away irrelevant assertions and code paths. Simulated print statements are then inserted along key execution paths to collect dynamic traces.
- **The Inner Loop (Conversational Refinement):** The LLM iteratively refines the buggy code using the purified test context, current runtime values, and compiler feedback.

Evaluating DebugRepair with DeepSeek-V3 as a backbone correctly fixed 295 bugs on the Defects4J benchmark, outperforming existing baselines by 59 correct fixes (Garousi & Felderer, 2017).

6.2 Autonomous Multi-Agent Cyber-Reasoning Systems

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diagnostic accuracy. While advanced prompting frameworks, neuro-symbolic detection loops, and attention-rectifying localization tools have drastically improved test coverage and vulnerability recall, a fundamental reliance on surface-level textual cues and syntactic memorization remains an ongoing challenge for current models. Nevertheless, the rapid transition toward conversational, feedback-driven program repair and autonomous multi-agent cyber-reasoning systems offers a scalable solution to an accelerated threat landscape where manual patch cycles are no longer viable. By coupling LLMs with dynamic execution environments, static analysis tools, and structured action spaces, modern testing frameworks are successfully transforming raw runtime symptoms into precise, line-level fixes. Moving forward, balancing the non-deterministic risks of AI-generated code against the immense speed and reasoning capabilities of agentic frameworks will be paramount. Ultimately, these technologies are no longer merely developer assistants; they are evolving into essential infrastructure capable of autonomously defending and hardening global software ecosystems in real time.

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