MalGEN: A Generative Agent Framework for Modeling Malicious Software in Cybersecurity

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Abstract— The dual use nature of Large Language Models (LLMs) presents a growing challenge in cybersecurity. While LLM enhances automation and reasoning for defenders, they also introduce new risks, particularly their potential to be misused for generating evasive, AI crafted malware. Despite this emerging threat, the research community currently lacks controlled and extensible tools that can simulate such behavior for testing and defense preparation. We present MalGEN, a multi agent framework that simulates coordinated adversarial behavior to generate diverse, activity driven malware samples. The agents work collaboratively to emulate attacker workflows, including payload planning, capability selection, and evasion strategies, within a controlled environment built for ethical and defensive research. Using MalGEN, we synthesized ten novel malware samples and evaluated them against leading antivirus and behavioral detection engines. Several samples exhibited stealthy and evasive characteristics that bypassed current defenses, validating MalGEN's ability to model sophisticated and new threats. By transforming the threat of LLM misuse into an opportunity for proactive defense, MalGEN offers a valuable framework for evaluating and strengthening cybersecurity systems. The framework addresses data scarcity, enables rigorous testing, and supports the development of resilient and future ready detection strategies.

Index Terms—Malware generation, synthetic data, machine learning, malware detection, GenAI, Multi-agent, Malicious code generation, cybersecurity

I. INTRODUCTION

The escalating complexity of the cybersecurity landscape has placed defenders under constant pressure to adapt to rapidly evolving threats [13], [38]. Traditional detection systems based on static signatures, predefined rules, or historical patterns are increasingly inadequate against adversaries who adopt dynamic and creative attack strategies. As threats continue to grow in sophistication, there is an urgent need for intelligent, adaptive, and anticipatory defense mechanisms that can proactively counter both known and emerging attack vectors [22].

In response to this need, Large Language Models (LLMs) have emerged as powerful tools capable of transforming cybersecurity workflows [7], [28]. Their ability to generate code, interpret complex documentation, simulate reasoning, and process natural language queries opens new possibilities across threat intelligence extraction, vulnerability analysis, and automated response [11], [23], [25], [30], [31], [33]. However,

these same capabilities also introduce unprecedented risks. The dual-use nature of LLMs means they can be repurposed to automate the creation of highly evasive, AI-generated threat that can bypass conventional detection strategies [16], [18].

While this risk is increasingly acknowledged, research into LLM-generated malicious software, also known as malware, is still in its infancy. Most current studies are either theoretical in nature or involve only basic demonstrations [15], [17]. Existing malware generation approaches often rely on handcrafted samples or static datasets, which fail to capture the behavioral diversity and adaptive logic characteristic of modern threats. Furthermore, current detection systems are often not equipped to recognize malware generated via autonomous agents or language models, resulting in a widening gap between the offensive potential of generative models and the readiness of defensive solutions [12].

This dual capability, however, can be transformed from a risk into a strategic advantage. Just as attackers might exploit LLMs to automate malware creation, defenders can proactively simulate this behavior in a safe environment to strengthen their systems [2]. Simulating adversarial behavior is a core tenet of red teaming, where security professionals evaluate the robustness of their defenses by mimicking realistic attack scenarios [27], [32]. Yet, the research community lacks open, extensible frameworks for generating realistic, context-aware, LLM-driven malware in a controlled and ethical manner. This limitation slows progress in developing resilient and adaptive security systems.

To address this gap, we introduce MalGEN, a novel malware generation framework designed for defensive cybersecurity research. MalGEN is based on a multi-agent architecture in which autonomous LLM-powered agents collaborate to simulate coordinated adversarial workflows. Each agent is responsible for a specific stage in the attack chain, such as planning capabilities, generating payloads, or implementing evasion techniques. These agents work together toward a shared objective: the generation of diverse, malicious, activitydriven malware samples aligned with realistic threat scenarios.

MalGEN adopts an agentic approach that goes beyond passive code generation to model adversarial reasoning. It synthesizes malware that reflects real-world tactics, techniques, and procedures (TTPs), with alignment to established threat frameworks such as MITRE ATT&CK [27]. Instead of reusing existing malware signatures or assembling preexisting code fragments, MalGEN generates new novel binaries from scratch that are tailored to behavioral objectives. This enables the creation of malware samples that are unique, stealthy, operationally realistic, and mission-aligned malware artifacts.

To validate MalGEN, we generated ten synthetic malware samples and evaluated them against leading antivirus and behavioral detection engines. Several of the samples were able to evade modern detection tools, which suggests they exhibit deceptive and evasive characteristics. To ensure that these samples represent true malicious behavior, we analyzed their underlying Tactics, Techniques, and Procedures (TTPs). The TTPs associated with each sample correspond to known malicious activity and confirm the threat relevance of the generated samples.

This capability serves several defensive goals. MalGEN helps overcome data scarcity bottlenecks by generating synthetic yet realistic datasets. It enables robust testing of detection systems against novel unseen threats and supports the design of red team exercises through the creation of adversarial samples with controlled behavioral profiles. The framework empowers researchers, blue teams, security operations teams, and analysts with a practical and ethical tool for testing and improving detection capabilities in preparation for future AIpowered threats.

Importantly, MalGEN is explicitly designed with ethical safeguards. All malware generation occurs in secure, isolated environments; the samples are non-propagating and intended exclusively for academic and defensive research purposes. By safely simulating the offensive potential of LLMs, MalGEN provides the cybersecurity community with a much-needed capability to anticipate, test, and prepare for the next generation of AI-enabled threats.

This research makes the following contributions:

- We introduce MalGEN, a novel, agentic malware generation framework that leverages multi-agent collaboration to simulate realistic adversarial workflows and generate activity-driven, behaviorally diverse malware samples.
- We demonstrate how the offensive capabilities of LLMs can be ethically harnessed in a controlled, sandboxed environment to support red teaming, adversarial robustness testing, and benchmarking of detection systems.
- 3) We show that MalGEN-generated samples exhibit functional and evasive behaviors aligned with MITRE ATT&CK tactics, and validate this through experiments where multiple samples successfully bypass state-of-theart antivirus engines.

The remainder of the paper is structured as follows: Section II reviews the existing literature related to adversarial behavior generation using LLMs. Section III provides the necessary background to help readers understand the concepts used in the proposed framework. Section IV outlines the motivation behind this work. Section V presents a detailed explanation of each component of the MalGEN framework. Section VI

describes the experiments conducted to validate the framework, the key findings, and observations. Section VII discusses limitation and potential future directions. Finally, Section IX concludes the paper.

II. RELATED WORK

The emergence of LLMs has prompted increasing concern over their potential misuse in malware generation. While several recent studies have demonstrated that even instructiontuned or commercial LLMs can be manipulated to produce malicious payloads, most existing work remains focused on individual code generation demonstrations. There is a lack of frameworks that model adversarial workflows in a structured, modular, and ethically controlled manner for red-teaming or defensive simulation.

Early efforts such as Pa et al. [29] and Alotaibi et al. [3] examine how prompt engineering can elicit malicious outputs from LLMs. Pa et al. show how ChatGPT can be coerced into generating reverse shells, keyloggers, and persistence mechanisms using varied prompts. Alotaibi et al. further explore the manipulation of prompt phrasing and context to circumvent alignment barriers. However, both works limit their focus to prompt-level behavior and static code snippets without considering adversarial planning or execution context.

Moving beyond simple prompt-response studies, Adamec et al. [1] assess LLM capabilities across different malware lifecycle stages such as delivery, exploitation, and commandand-control. Similarly, Beckerich et al. [5] introduce RatGPT, showing that online LLMs can generate Remote Access Trojans (RATs) with multiple malicious components including persistence, keylogging, and exfiltration. Despite these advances, both works treat malware generation as a flat task and lack modular control, logging, or behavioral labeling.

Other research has explored pipeline-based generation. Li et al. [24] propose an automated mass malware factory that embeds LLMs into a high-throughput generation system. The system demonstrates the ability to synthesize payload variants at scale, but lacks behaviorally grounded control, multi-stage logic, or traceability. Yamin et al. [39] take a hybrid approach by combining outputs from censored and uncensored LLMs to generate functional ransomware samples.

Devadiga et al. [14] introduce GLEAM, a framework that fuses GANs with LLMs to generate evasive malware samples. While GLEAM presents a creative use of generative models for obfuscation, it does not support intent-driven generation or behavioral tagging, and lacks transparency needed for defensive testing. In contrast, MalGEN generates malware that is aligned with specific adversarial goals (e.g., persistence, privilege escalation) and logs relevant behavioral metadata.

Systematic benchmarking studies such as Shandilya et al. [34] and Botacin [6] provide evaluations of LLM outputs across diverse malicious prompts. These works score models based on their compliance with dangerous instructions or alignment breakdowns, offering broad visibility into model behavior under red-teaming conditions. However, they stop short of contributing reusable simulation frameworks or behaviordriven evaluation pipelines.

Conceptual investigations such as Madani et al. [26] raise concerns about the future of AI-powered metamorphic malware, where LLMs evolve code structures dynamically. While these discussions are valuable, they lack implementation. More practice-oriented studies include Ionescu [19], who stress-test code-generating LLMs through structured adversarial prompts, and Iturbe et al. [20], who map generated code to MITRE ATT&CK techniques. Nonetheless, neither work attempts to generate complete malware sample in a behaviorally aligned, multi-step fashion.

In contrast to these studies, MalGEN introduces a modular, multi-agent framework for simulating realistic adversarial workflows. Each autonomous agent in MalGEN contributes to a specific stage of the malware generation process, such as planning, payload construction, or stealth optimization. MalGEN outputs are aligned with high-level threat objectives and tagged with API traces, behavioral labels, and MITRE ATT&CK mappings. This structure enables red teams and security researchers to test detection systems against behaviorally grounded, ethically generated malware in a reproducible and controlled environment. By emphasizing modularity, traceability, and simulation utility, MalGEN fills a critical gap in the current literature and offers a research-safe approach to exploring the offensive potential of LLMs for defensive gain.

III. BACKGROUND

This section outlines key concepts that support Mal-GEN's design: the dual-use nature of LLMs in cybersecurity, agent-based malware simulation for realism and modularity, behavior-driven analysis using MITRE ATT&CK alignment, and the emerging role of generative AI in ethical red teaming.

A. Large Language Models and Their Role in Cybersecurity

Large Language Models (LLMs), such as GPT-4, LLaMA, and PaLM, have demonstrated remarkable proficiency across a wide range of natural language understanding and generation tasks. Their ability to generate code, interpret structured and unstructured inputs, and simulate decision-making has opened up transformative possibilities for cybersecurity applications. In defensive contexts, LLMs have been employed for tasks such as incident triage, threat intelligence summarization, attack simulation, and vulnerability explanation [10], [40]. These capabilities are reshaping traditional workflows by enhancing automation, augmenting analyst decision-making, and improving accessibility to security knowledge.

At the same time, these generative models raise new security concerns due to their dual-use nature. Studies have shown that LLMs can be misused to generate malicious artifacts such as obfuscated scripts, reverse shells, and even functional ransomware through prompt manipulation or jailbreaking techniques [5], [29]. This dual capability underscores the importance of developing frameworks that explore both sides of the equation: using LLMs for defensive innovation while rigorously stress-testing their offensive misuse potential.

B. Agent-Based Malware Simulation

The concept of using autonomous agents for simulating cyberattacks has been widely adopted in red teaming, cyber range simulations, and automated penetration testing. Agents offer a modular and goal-oriented paradigm, where each component can independently reason, plan, and act based on assigned objectives. This approach allows for the creation of realistic attack chains that reflect adversarial intent and adaptive decision-making, mirroring how real-world threat actors operate.

In the context of malware simulation, agent-based systems provide several advantages over static or rule-based methods. They enable behavioral diversity, allow scenariospecific customization, and support multi-stage attack logic that aligns with operational goals. Prior efforts in agent-based red teaming, such as MITRE CALDERA [4], demonstrate how adversarial agents can autonomously emulate tactics like lateral movement, privilege escalation, and command-andcontrol communication.

MalGEN builds upon this philosophy by integrating Large Language Models (LLMs) into the agent loop. Instead of scripting behavior manually, each agent uses an LLM to dynamically generate attack components, reason about evasion strategies, and adapt code output based on context. This fusion of agent architecture and generative intelligence introduces a new level of realism and complexity in malware simulation, making it ideal for stress-testing detection systems and analyzing potential failure modes.

C. Behavior-Driven Malware and ATT&CK Mapping

Modern cybersecurity defenses are increasingly shifting from signature-based detection to behavior-based analysis. Unlike static detection, which relies on known patterns and byte sequences, behavior-driven methods analyze runtime characteristics such as API calls, file system access, registry modifications, and network behavior to detect anomalies and malicious activity. This approach enables the detection of novel threats that may evade traditional mechanisms through obfuscation or polymorphism.

To standardize the representation of adversarial behavior, the MITRE ATT&CK framework [37] has become widely adopted. ATT&CK organizes threat actor activities into Tactics (e.g., Persistence, Defense Evasion) and Techniques (e.g., T1055 – Process Injection, T1566 – Phishing), providing a shared vocabulary and structure for red teaming, threat intelligence, and detection development. Security tools and analysts increasingly use ATT&CK mapping to benchmark detection coverage, analyze attack surfaces, and train machine learning models for threat classification [21].

MalGEN aligns with this paradigm by generating malware artifacts that are not only functionally valid but also semantically rich in behavioral context. Each generated sample is annotated with the corresponding ATT&CK tactics and techniques it embodies, enabling downstream tasks such as adversarial robustness testing, behavior-aware model training, and MITRE-based telemetry validation. This alignment ensures that the generated malware samples serve as high-fidelity inputs for behavior-driven cybersecurity research.

D. Red Teaming with Generative AI

Red teaming involves simulating adversarial attacks to evaluate the effectiveness of security defenses. Traditionally a manual process, it increasingly incorporates automation, with LLMs enabling the generation of dynamic, context-aware adversarial scenarios. Generative AI presents an opportunity to scale red teaming by producing diverse attack patterns, polymorphic malware, and automated reasoning. However, this also introduces ethical risks. Without safeguards, red teaming frameworks may be misused for offensive purposes.

Recent studies [9], [35] emphasize the need for responsible AI experimentation, calling for transparency, containment, and reproducibility. MalGEN adheres to these principles by operating in isolated environments, logging all generated artifacts, and restricting usage to defensive research.

IV. MOTIVATION

LLMs are reshaping both the offensive and defensive landscape of cybersecurity. Their ability to synthesize functional malware from simple prompts introduces a potent dual-use challenge [5], [29], [39]. However, most existing explorations of this threat either remain theoretical or focus narrowly on static payload generation without modeling the full behavioral workflow of an attacker.

Security researchers, red teams, and developers of detection engines require tools that go beyond basic code synthesis. They need frameworks that can simulate entire adversarial workflows, aligned with tactics, techniques, and procedures (TTPs) commonly seen in advanced threats. Unfortunately, current approaches lack modularity, reproducibility, or the ability to generate diverse, behaviorally annotated datasets [24], [26].

Another pressing issue is that most malware detection systems are trained on legacy datasets that do not reflect the evasion strategies or behavioral nuances of LLMgenerated threats. As detection systems become increasingly AI-powered, they must also be tested against AI-powered adversaries. A controlled framework capable of producing dynamic, functionally rich malware samples is essential for robust, forward-looking defense development.

Moreover, the absence of publicly available, ethically grounded frameworks impedes the ability of academic and industrial researchers to conduct meaningful red teaming. There is a strong need for a tool that supports transparent experimentation, reproducibility, and controlled risk—all while simulating real-world adversarial logic.

To address this gap, we propose MalGEN as a purpose-built solution for simulating malware generation through agentic, adversarial workflows. Unlike existing proof-of-concept tools, MalGEN models the full sequence of attacker decisions—from objective formulation to evasion planning—making it not only a generator of malware samples but also a testbed for AIenhanced cyber defense readiness.

V. MALGEN

MalGEN is a modular, multi-agent framework designed to simulate realistic malware behaviors in a controlled and ethical manner using LLMs. It operates by decomposing high-level malicious intents into a sequence of sub-tasks, generating code for each task via LLMs, and assembling the code into fully functional malware-like artifacts. Each stage of this pipeline is handled by a dedicated agent, enabling scalability, transparency, and traceability throughout the malware generation process.

Unlike traditional malware datasets or isolated code snippets, MalGEN emphasizes activity-driven generation, producing samples that reflect realistic attacker workflows and behavioral objectives such as reconnaissance, persistence, or data exfiltration. This makes MalGEN particularly suitable for stress-testing detection systems, training behavior-aware models, and conducting red-teaming experiments grounded in adversarial realism.

A. Agent-Based Architecture

MalGEN is architected as a modular, multi-agent system where each agent autonomously handles a specific stage in the malware generation pipeline. This decomposition facilitates interpretable automation, enables task-level debugging, and allows future extensions such as adding new code generation models, validation layers, or language targets. Moreover, it mirrors the multi-stage nature of real-world attack chains, making MalGEN suitable for generating behaviorally realistic malware-like artifacts.

Figure 1 provides an architectural overview of MalGEN, outlining the sequential flow between agents. Starting from a high-level activity description, the system progresses through planning, code generation, integration, and packaging, with each agent handling a specific transformation step. The key agents in the system include:

1) Task Planner Agent: The Task Planner Agent acts as the initial interpreter of the user's intent. It receives a high-level description of the desired malicious behavior, for example, "collect system information and exfiltrate it to a remote server," and breaks it down into a structured sequence of atomic sub-tasks. The decomposition output is formatted as a structured list (e.g., JSON or dictionary of task types and descriptions) to ensure compatibility with downstream agents in the pipeline.

Task Planner Agent

Decomposes high-level user queries into a structured sequence of atomic sub-tasks. This enables modular, interpretable planning for downstream code generation.

These sub-tasks represent concrete operations necessary to fulfill the overarching activity, such as:



Fig. 1. MalGEN architecture showing modular agent interactions across the malware generation pipeline.

- Capturing OS and environment details,
- Listing active processes and network configuration,
- Initiating outbound communication to transmit data.

To achieve this, the Task Planner rely on prompt-driven LLM to perform hierarchical task decomposition. This modularization ensures that downstream agents can operate independently on each sub-task, improving clarity, reproducibility, and fault isolation in the generation process.

2) Developer Agent: The LLM-powered Developer Agent receives the sub-tasks generated by the Task Planner and translates each one into executable code. This agent formulates context-specific prompts that describe the sub-task in natural language and passes them to a compact, instruction-tuned code generation model.

Developer Agent

Uses LLMs to generate modular Python code snippets for each sub-task, ensuring clarity and functional correctness.

For example, for a task like "list all running processes," the prompt might be:

"Generate a Python script that lists all running processes on a Linux system using the psutil library."

The resulting code snippets are designed to be:

- Lightweight: Avoid unnecessary complexity or bulk.
- Modular: One script per sub-task for composability.
- Transparent: Maintain clarity for audit and debugging.

Optionally, generation parameters such as sampling temperature or top-k values can be adjusted to introduce controlled randomness. This allows the creation of multiple diverse variants for the same sub-task, which is important when simulating polymorphic or evasive malware.

By decoupling code generation for each sub-task, Mal-GEN ensures behavioral diversity across samples, as different prompts or randomness settings can produce unique variations for the same intent.

3) Code Integration Agent: The Code Integration Agent is responsible for assembling the modular code snippets into a

coherent, single script. As multiple sub-tasks are implemented independently, integration is critical to resolve interdependencies and produce a unified malware-like artifact.

Code Integration Agent

Merges modular code snippets into a logically coherent, syntactically valid script representing the entire malicious behavior.

The Integration Agent may perform:

- Import resolution: Avoids redundant imports and resolves conflicts.
- Naming standardization: Unifies variable names, function identifiers, and object references across snippets.
- Execution ordering: Aligns the flow of actions to preserve intended sequence and logic.
- **Data flow alignment**: Ensures outputs of one module can feed into the next where needed (e.g., collected data passed to the exfiltration step).

The output is a syntactically valid, semantically coherent Python script that reflects the complete behavioral objective specified by the original input. This agent also ensures compatibility with the executable packaging step that follows. A lightweight validation step also ensures that the composed script is free from syntax errors and respects runtime constraints, helping avoid failures during execution or packaging.

4) Executable Builder: The Executable Builder transforms the integrated Python script into a standalone, platform-ready executable. This is achieved using open-source packaging tools like PyInstaller or cx_Freeze, which bundle the script with all necessary dependencies and runtime components.

Executable Builder

Converts finalized code into execution-ready artifacts suitable for testing in sandboxed environments.

Benefits of executable generation include:

Agent	Role	Illustrative Input/Output
Task Planner	Decomposes user activity into sub-tasks	Input: "Exfiltrate system info" Output: (i) Get OS info, (ii) Get IP, (iii) Send to server
Developer Agent	Uses LLM to generate mod- ular code	Input: Sub-task like "Get OS info" Output: Python script using platform module
Code Integration Agent	Merges modular code into a complete script	Input: Multiple Python snippets Output: Unified malware-like script
Executable Builder	Converts final script to stan- dalone executable	Input: Python script Output: Platform-ready '.exe' file

 TABLE I

 Summary of MalGEN Agent Roles with Illustrative Examples

- **Platform portability**: Artifacts can be tested on systems without a pre-configured Python environment.
- **Deployment realism**: Enables end-to-end simulation in sandboxed or red team environments.
- **Integration with test harnesses**: Easier evaluation in detection pipelines or behavioral sandboxes.

This step finalizes the malware-like artifact and prepares it for safe storage and analysis, completing the MalGEN generation loop. All executables are handled within controlled environments, ensuring they are only used for ethical research purposes such as red teaming, sandbox analysis, or stresstesting of detection pipelines.

To provide a concise overview of the agent responsibilities, Table I summarizes the roles and outputs of each agent in the MalGEN framework.

B. Design Choices

The development of MalGEN involved a series of intentional design decisions aimed at balancing generation quality, operational control, ethical safeguards, and extensibility. These choices make the framework efficient for defensive research while maintaining transparency and modularity.

- Compact LLMs for Code Generation: MalGEN leverages compact, instruction-tuned language models such as Qwen2.5 Coder-3B for generating code snippets. These models strike a balance between code quality and execution control, minimizing the risk of overly complex or harmful outputs and making the generation process interpretable and reproducible.
- **Python as Target Language:** Python is used as the default output language due to its ease of auditing, high-level semantics, and sandbox-friendly nature. Python supports a wide range of system-level behaviors (e.g., file I/O, subprocess, networking) without requiring low-level execution privileges, reducing the chance of unintentional damage.
- Agent-Based Modular Architecture: Each stage of the malware generation pipeline is encapsulated as a distinct agent responsible for planning, development, integration, or packaging. This modular architecture enhances maintainability, fault isolation, and future extensibility,

such as plugging in newer LLMs or extending to multilanguage outputs.

• **Prompt Engineering with Context Awareness:** Prompts used for code generation are tailored per sub-task and include contextual constraints (e.g., use psutil for process enumeration). This mitigates prompt injection risks and guides the LLMs to produce safe and relevant code aligned with the simulation goals.

These design choices reflect a commitment to building responsible AI systems for cybersecurity experimentation, enabling researchers to simulate attacker workflows without enabling real-world abuse.

C. MalGEN Workflow

The operation of MalGEN follows a structured, multistage workflow that transforms a high-level malicious behavior description into a fully functional, executable malware-like artifact. This agentic pipeline ensures that each stage of generation is interpretable, auditable, and modular, supporting safe experimentation and robust extension. As depicted earlier in Figure 1, the workflow proceeds through the following phases:

- 1) **Input Stage:** The process begins with a user-provided query specifying the desired malicious behavior in natural language (e.g., "gather system information and exfiltrate it to a remote server"). This abstract intent guides the entire generation process.
- 2) **Planning Stage:** The Task Planner Agent interprets the input and decomposes it into a sequence of atomic sub-tasks. Each sub-task represents a well-defined unit of behavior (e.g., "capture IP configuration" or "create socket connection").
- 3) **Code Generation Stage:** For each sub-task, the Developer Agent formulates a task-specific prompt and invokes a compact LLM (e.g., Qwen2.5 Coder) to synthesize a modular Python script. These scripts are kept lightweight, interpretable, and self-contained.
- 4) **Integration Stage:** The Code Integration Agent merges all modular scripts into a unified, syntactically and semantically coherent Python program. This includes resolving imports, harmonizing variable names, ordering execution blocks, and preserving data dependencies.

TABLE II Behavioral Analysis of Malware Samples: Mapped MITRE TTPs (excerpt; full table in Appendix A)

Hash	TTPs Present in Malware
9048dd0e447bb9abc7b1ecf5f055ca892d8e 1275f4acd02ded35e94b9268d9ad	 Execution (TA0002): Scripting (T1064), Shared Modules (T1129) Persistence (TA0003): Create or Modify System Process (T1543), Systemd Service (T1543.002) Defense Evasion (TA0005): Obfuscated Files or Information (T1027), Masquerading (T1036), Scripting (T1064), Indicator Removal (T1070), File Deletion (T1070.004), File and Directory Permissions Modification (T1222), Hide Artifacts (T1564), Hidden Files and Directories (T1564.001) Privilege Escalation (TA0004): Abuse Elevation Control Mechanism (T1548), Setuid and Setgid (T1548.001) Discovery (TA0007): System Information Discovery (T1082), Software Discovery (T1518), Security Software Discovery (T1518.001) Command and Control (TA0011): Ingress Tool Transfer (T1105), Application Layer Protocol: Web Protocols (T1071.001)
2190ce1cfc98bc3a81cefa8a607a74246afbb 94b6ceb760a53b35d9d79ff51ac	 Execution (TA0002) : Scripting (T1064), Shared Modules (T1129) Persistence (TA0003) : Create or Modify System Process (T1543), Systemd Service (T1543.002) Defense Evasion (TA0005) : Obfuscated Files or Information (T1027), Masquerading (T1036), Scripting (T1064), Indicator Removal (T1070), File Deletion (T1070.004), File and Directory Permissions Modification (T1222) Privilege Escalation (TA0004) : Create or Modify System Process (T1543), Systemd Service (T1543.002) Discovery (TA0007) : System Information Discovery (T1082), File and Directory Discovery (T1083)
(Additional rows omitted for brevity)	

- 5) **Executable Building Stage:** The integrated script is passed to the Executable Builder, which packages it into a standalone binary using tools such as PyInstaller. This output can then be deployed in controlled testbeds or sandboxes for evaluation.
- 6) **Outcome:** The result is an execution-ready, malwarelike artifact that simulates a complete malicious behavior chain. These artifacts can be used for benchmarking detection systems, simulating adversarial scenarios, or training defensive models in safe, ethical environments.

This workflow ensures that MalGEN maintains a clean separation of concerns while enabling end-to-end malware synthesis from user intent to executable. Its modularity also opens the door for fine-grained analysis and dynamic extensions across code models, programming languages, and threat behaviors.

VI. EVALUATION AND INSIGHTS

To assess the functional realism and behavioral diversity of generated malware samples, we conducted a series of controlled experiments using MalGEN. This section presents our evaluation setup, key observations, and reflective insights into the framework's effectiveness, limitations, and future potential.

A. Experimental Setup

To evaluate MalGEN, we designed experiments that focus on two core aspects: (i) the functionality and realism of generated artifacts, and (ii) their detection evasion capability and TTP alignment. The evaluation was conducted in a controlled environment to ensure operational safety and prevent unintended propagation. 1) Sample Generation: We curated a set of 10 highlevel malicious behavior prompts, covering activities such as data exfiltration, privilege escalation, credential dumping, persistence, and network reconnaissance. These were chosen to simulate real-world threat scenarios mapped to different MITRE ATT&CK tactics. MalGEN generated a malware-like sample for each prompt using its full pipeline — from task planning to executable building.

2) Execution Environment: All generated samples were submitted to VirusTotal for analysis, where static and dynamic insights were collected through its integrated scanning engines. The platform provided information on runtime behavior, system interactions, network activity, and generated Indicators of Compromise (IOCs) observed during the automated analysis.

3) Detection Analysis: Building on the earlier submission of samples to VirusTotal, we analyzed the results to evaluate the evasiveness of the generated executables. The platform's integration with over 60+ antivirus engines enabled us to quantify static detection rates. Additionally, dynamic behavior reports from the platform provided insights into any flagged malicious actions, offering a measure of behavioral detection efficacy.

4) *TTP Mapping:* We obtained TTPs directly from Virus-Total's behavioral analysis, as reported by state-of-the-art dynamic analysis tools. These tools map observed activities to MITRE ATT&CK techniques, allowing us to compare the intended behavior from the input prompt with the TTPs manifested during execution.

B. Quantitative Results and Observations

The malware-like artifacts generated by MalGEN were evaluated based on (i) the number and variety of MITRE

ATT&CK TTPs manifested during execution, and (ii) their detection rates across commercial antivirus engines. Table II presents a glimpse of sample-wise breakdown of observed TTPs extracted via dynamic analysis, aligned with corresponding MITRE tactics.

We also summarizes the overall behavioral and detection characteristics of the generated malware corpus in Table III and Fig. 2. The results highlight several key observations:

- Behavioral Realism: Table III shows the behavioral complexity and diversity of MalGEN-generated samples. On average, each sample demonstrated 11.3 distinct TTPs across 4.3 MITRE ATT&CK tactics, with individual samples ranging from 5 to 18 TTPs. Collectively, the corpus covered 20 distinct ATT&CK techniques spanning 6 different tactics, indicating broad coverage across the attack lifecycle. These results underscore MalGEN's ability to generate behaviorally rich, multi-stage malware samples that realistically simulate adversarial workflows observed in real-world threat campaigns.
- Static Detection Evasion: As shown in Figure 2, 50% of the generated binaries were not detected by any antivirus engines on VirusTotal at the time of upload, indicating a low static signature footprint. The remaining 50% were flagged based on heuristic rules, suggesting partial recognition of suspicious characteristics despite the absence of known signatures.
- Malware Family Mislabeling: Figure 2 also shows the family classification results for MalGEN-generated samples. Four out of ten samples were correctly labeled with malware families aligned with their intended behavior (e.g., *Keylogger* and *Backdoor*). However, one ransomware sample exhibiting T1486-like behavior (*Data Encrypted for Impact*) was misclassified as a generic *Trojan*, highlighting how static classifiers can miss specialized functionalities when the code does not resemble known ransomware patterns.

These metrics collectively underscore MalGEN's ability to generate behaviorally rich and evasive malware samples that mimic real-world adversarial workflows. From multi-tactic execution traces to static evasion and partial family recognition, the results demonstrate both the potential and limitations of current detection mechanisms when confronted with AIgenerated threats. This evaluation provides a foundation for future red-teaming efforts and highlights areas where detection strategies may require adaptation to handle generative threats.

C. Qualitative Output Illustration

To illustrate MalGEN's ability to generate functionally diverse and behaviorally aligned malware artifacts, we present three representative examples covering distinct adversarial objectives. Each example consists of an input intent, the decomposed sub-tasks produced by MalGEN, the behavioral traits of the generated code, and the corresponding MITRE ATT&CK techniques.

TABLE III SUMMARY STATISTICS OF MALGEN-GENERATED MALWARE SAMPLES

Metric	Value
Average number of TTPs per sample	11.3
Standard deviation of TTPs per sample	3.5
Minimum / Maximum TTPs per sample	5 / 18
Average number of MITRE tactics covered	4.3
Total distinct ATT&CK tactics observed	6
Total distinct MITRE ATT&CK TTPs observed	20

Summary of Representative Examples

Example 1 – Reconnaissance and Exfiltration

- **Input Intent:** Collect OS and user information and send it to a remote server.
- Generated Sub-Tasks:
 - Gather system info (OS, CPU, RAM)
 - Extract current user identity
 - Transmit data using HTTP POST
- Code Behavior: Utilized platform, psutil, and getpass to collect host/user data, serialized it in JSON, and sent it to a dummy endpoint via requests.post().
- Mapped TTPs: T1082, T1087, T1041

Example 2 – Privilege Escalation and Defense Evasion

- **Input Intent:** Escalate privileges and evade antivirus detection.
- Generated Sub-Tasks:
 - Create a privileged system service
 - Obfuscate file contents and rename script
- **Code Behavior:** Created a service using systemctl, applied base64 encoding for obfuscation, and renamed the script to mimic legitimate binaries.
- Mapped TTPs: T1543.002, T1036, T1027

Example 3 – Multi-Stage Behavior

- **Input Intent:** Install a keylogger, monitor clipboard, and send logs periodically.
- Generated Sub-Tasks:
 - Capture keystrokes and clipboard contents
 - Store logs locally
 - Send logs every 60 seconds to a remote server
- Code Behavior: Leveraged pynput and pyperclip to collect inputs; logs were managed using threading.Timer for periodic network transmission.
- Mapped TTPs: T1056.001, T1115, T1071

The full structured examples are provided below using wide-

format boxes. These highlight MalGEN's prompt-to-behavior fidelity, multi-stage simulation capabilities, and alignment with real-world TTPs.



Fig. 2. Family Distribution Overview: Number of samples with no label, correct label, or mislabeling based on VirusTotal family assignment.

VII. LIMITATIONS AND FUTURE WORK

While MalGEN presents a promising step toward modular and interpretable malware generation using LLMs, several limitations must be acknowledged. First, the framework currently supports only Python for artifact generation. Although this ensures sandbox safety and auditability, it limits realism when emulating malware written in compiled or low-level languages such as C++, PowerShell, or Go. Additionally, Mal-GEN does not validate the execution semantics of generated scripts—meaning there is no built-in mechanism to guarantee that the produced code performs the intended behavior without runtime errors. This can lead to inconsistencies between the abstract intent and concrete behavior, particularly for complex tasks involving inter-module dependencies.

Another constraint lies in the relatively static behavioral patterns of generated samples. While prompt variation and LLM stochasticity introduce some diversity, common libraries and repeated template structures may produce artifacts that are easily detectable by signature-based systems. Furthermore, the current design lacks a behavioral feedback loop; the framework does not refine generation based on runtime outputs, detection reports, or sandbox analysis, which limits its ability to simulate adaptive or evasive behavior. Finally, MalGEN intentionally avoids generation of highly destructive malware behaviors such as ransomware, self-replicating code, or exploit-based privilege escalation. While this boundary is ethically necessary, it constrains its realism for certain adversarial simulation scenarios.

Looking ahead, several extensions are planned to enhance the capabilities of MalGEN. First, we intend to incorporate support for additional programming languages such as C#, PowerShell, and shell scripting to broaden the scope of simulated threat scenarios. A behavior validation module will also be integrated to statically or symbolically verify the safety, correctness, and intent alignment of generated artifacts before packaging. Another major direction is to enable a feedbackdriven refinement loop, where execution results—particularly from sandbox platforms like Cuckoo or Any.Run—inform iterative improvements to prompts or code generation strategies.

Furthermore, we aim to develop adversarial red-teaming scenarios where MalGEN adapts to evade LLM-based detection systems, enabling robust evaluation of defensive tools under polymorphic and evasive threats. The system will also be coupled with threat attribution frameworks (e.g., AURA) to examine attribution reliability under behaviorally diverse malware samples. Lastly, we plan to curate and publicly release a benchmark dataset of MalGEN-generated artifacts, annotated with MITRE ATT&CK TTPs, to facilitate reproducible evaluation of malware detection, classification, and attribution models. These extensions will collectively strengthen MalGEN as a research-grade tool for understanding and mitigating AIenabled cyber threats.

VIII. ETHICAL SAFEGUARDS

MalGEN is designed with strict ethical boundaries to ensure its application is limited to defensive cybersecurity research and responsible academic exploration. The framework does not aim to facilitate malicious intent, but rather to anticipate future AI-driven threats and prepare robust countermeasures.

To enforce these safeguards, MalGEN is governed by the following principles:

- Controlled Input and Execution: MalGEN operates only on predefined malicious behavior descriptions provided in a controlled environment. These inputs are abstracted to ensure they do not directly enable exploitspecific generation.
- Safe Language Scope: All generated artifacts are constrained to Python, a language that is interpretable, sandbox-friendly, and widely used in cybersecurity labs for benign testing.
- Built-in Validation Layer (Future Work): Planned future versions of MalGEN will include a validation agent that filters output against a curated denylist of destructive behaviors (e.g., encryption without key release, filesystem wipes, self-replication).

These safeguards align MalGEN with the broader movement of responsible AI research, similar to risk-mitigating protocols outlined in works such as [8], [35], [36]. By making AI-driven malware generation interpretable, auditable, and limited in scope, MalGEN enables researchers and defenders to prepare for adversaries who may abuse such technologies.

IX. CONCLUSION

This paper presented MalGEN, a modular, LLM-driven framework for the controlled generation of malware-like artifacts from natural language descriptions. By decomposing the generation process into task-specific agents, MalGEN produces behaviorally realistic samples aligned with MITRE ATT&CK techniques, aiding the study of adversarial capabilities of generative models. VirusTotal-based evaluation revealed that many generated samples evade static detection while exhibiting clear malicious behavior dynamically, highlighting weaknesses in traditional defenses. MalGEN not only supports reproducible benchmarking and red-teaming but also promotes safe experimentation through strict ethical controls as detailed in Section VIII. Looking ahead, future extensions may incorporate sandbox feedback, language diversity, and automated validation to deepen the framework's utility in both research and responsible security testing.

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APPENDIX

APPENDIX A: TTP MAPPING OF GENERATED MALWARE

TABLE IV: Malware Hash to TTP Mapping

Hash	TTPs Present in Malware
37d3a0613e89e3a978 542a84593ee1cd59f8c 0e603742b058488e7 3b1eee5d08	 Execution (TA0002) : Scripting (T1064), Shared Modules (T1129) Persistence (TA0003) : Create or Modify System Process (T1543), Systemd Service (T1543.002) Defense Evasion (TA0005) : Obfuscated Files or Information (T1027), Masquerading (T1036), Scripting (T1064), Indicator Removal (T1070), File Deletion (T1070.004), File and Directory Permissions Modification (T1222), Virtualization/Sandbox Evasion (T1497), System Checks (T1497.001) Discovery (TA0007) : System Information Discovery (T1082), File and Directory Discovery (T1083), Software Discovery (T1518), Security Software Discovery (T1518.001), Virtualization/Sandbox Evasion (T1497), System Checks (T1497.001)
bdab969808549a8bc7 2e5debed6534f0fd60c 86e4955240292c652 0e5aa4c2ea	 Execution (TA0002) : Scripting (T1064), Shared Modules (T1129) Persistence (TA0003) : Create or Modify System Process (T1543), Systemd Service (T1543.002) Privilege Escalation (TA0004) : Create or Modify System Process (T1543), Systemd Service (T1543.002) Defense Evasion (TA0005) : Obfuscated Files or Information (T1027), Masquerading (T1036), Scripting (T1064), Indicator Removal (T1070), File Deletion (T1070.004), File and Directory Permissions Modification (T1222) Discovery (TA0007) : System Information Discovery (T1082), File and Directory Discovery (T1083) Command and Control (TA0011): Application Layer Protocol (T1071)
065dd63d75e67dae99 4dc92c1516d7d83197 5f31c4b98af283403 3cabd0e1d36	 Execution (TA0002) : Shared Modules (T1129) Defense Evasion (TA0005) : Obfuscated Files or Information (T1027), Masquerading (T1036), Indicator Removal (T1070), File Deletion (T1070.004), File and Directory Permissions Modification (T1222) Discovery (TA0007) : System Information Discovery (T1082), File and Directory Discovery (T1083) Command and Control (TA0011): Application Layer Protocol (T1071)
48d65214e2bfbbe94 1cbce9279519233b9c 97a25f443c69191507 5d31e36e71a	 Execution (TA0002) : Scripting (T1064), Shared Modules (T1129) Defense Evasion (TA0005) : Obfuscated Files or Information (T1027), Masquerading (T1036), Scripting (T1064), Indicator Removal (T1070), File Deletion (T1070.004), File and Directory Permissions Modification (T1222) Discovery (TA0007) : System Information Discovery (T1082), File and Directory Discovery (T1083)
fb00ba901c9545fae0 66422eb88f5e9de2bf 5206e6ad6daae71f5be 9fb66095f	 Execution (TA0002) : Scripting (T1064), Shared Modules (T1129) Persistence (TA0003) : Create or Modify System Process (T1543), Systemd Service (T1543.002) Privilege Escalation (TA0004) : Create or Modify System Process (T1543), Systemd Service (T1543.002) Defense Evasion (TA0005) : Obfuscated Files or Information (T1027), Masquerading (T1036), Scripting (T1064), Indicator Removal (T1070), File Deletion (T1070.004), File and Directory Permissions Modification (T1222) Discovery (TA0007) : System Information Discovery (T1082), File and Directory Discovery (T1083) Command and Control (TA0011) : Application Layer Protocol (T1071)
3575b2cdd604a973e9 8a326370442768fa3 8dfcd824589e2e3a5b 7d0b7e5f658	 Execution (TA0002) : Shared Modules (T1129) Defense Evasion (TA0005) : Obfuscated Files or Information (T1027), Masquerading (T1036), Indicator Removal (T1070), File Deletion (T1070.004), File and Directory Permissions Modification (T1222), Hide Artifacts (T1564), Hidden Files and Directories (T1564.001) Discovery (TA0007) : System Information Discovery (T1082), File and Directory Discovery (T1083) Command and Control (TA0011): Application Layer Protocol (T1071)
58d7080b134a7b592 3c3cc278481f10cd52f 12edb5ebc6d934f9f6 7d54225891	 Execution (TA0002) : Shared Modules (T1129) Defense Evasion (TA0005) : Obfuscated Files or Information (T1027), Masquerading (T1036), Indicator Removal (T1070), File Deletion (T1070.004), File and Directory Permissions Modification (T1222) Discovery (TA0007) : System Information Discovery (T1082), File and Directory Discovery (T1083), Software Discovery (T1518), Security Software Discovery (T1518.001) Command and Control (TA0011): Application Layer Protocol (T1071)
55a7a4b29c99dbddd4 44722d2dbe0368d5fd 07a52fb4fa0c3b2f90af 6faa1d05	Execution (TA0002) : Shared Modules (T1129) Defense Evasion (TA0005) : Virtualization/Sandbox Evasion (T1497), System Checks (T1497.001) Discovery (TA0007) : System Information Discovery (T1082), File and Directory Discovery (T1083), Virtualization/Sandbox Evasion (T1497), System Checks (T1497.001)