PENTEST-AI, an LLM-powered multi-agents framework for penetration testing automation leveraging MITRE ATTACK

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Abstract— **In the digital transformation era, the surge of better development technologies and citizen developers disrupted the space of innovation by increasing the number and complexity of applications used in production. This context prompts advanced cybersecurity measures and more frequent and thorough penetration testing to protect an organization's security posture. The scarcity of skilled expertise in cybersecurity today makes it challenging to cope with the evolving challenge and the growing demand. This paper introduces PENTESTAI, a novel framework for penetration testing automation using Large Language Model (LLM)-powered agents leveraging the MITRE ATTACK knowledge base. The paper provides an overview of the current state of research on cybersecurity and LLM-powered agents, followed by a detailed description of PENTESTAI building blocks. A proof-of-concept implementation is discussed to validate the framework's core constructs. The paper concludes with suggestions for future research directions to achieve the highest level of penetration testing automation with average skilled human-agent collaboration and to create citizen penetration testers.**

Keywords— Cybersecurity, penetration testing, automation, vulnerabilities, AI, Large Language Models, AI Agents, MITRE ATTACK, Citizen penetration tester

I. Introduction

It is no longer a secret that we are in the middle of a digital revolution drastically transforming various industries and sectors [1]. Business individuals using low-code or no-code tools in this new era can also build enterprise applications. If this is good news for business teams, it spells trouble for cybersecurity professionals who now have to deal with an exponential number of applications to secure. Studies such as those by Shameli-Sendi et al. [2] have emphasized the importance of penetration testing in identifying potential security threats before malicious actors can exploit them. However, traditional penetration testing is primarily manual and labor-intensive. It heavily relies on the expertise of human testers, whose supply and availability grow slower than the number of applications, systems, and infrastructure that require protection. Moreover, the growing complexity and sophistication of cyber-attacks make it difficult for human experts to keep up with the learning pace to provide swift and appropriate responses to the actions of malicious agents. There is a need for more scalable and adaptable approaches to penetration testing and offensive cybersecurity techniques in general.

The recent surge of Large Language Models (LLMs) and LLM-powered AI Agents might be an opportunity to design and experiment with new multi-agent frameworks to enable autonomous and human-assisted penetration testing execution. Our objectives in this paper are the following:

1. To propose a novel, modular, and extensible framework for penetration testing automation that leverages LLM and AI Agent capable of augmenting human expertise for penetration testing and paving the way to scalability.
2. Implement a small proof-of-concept for the PENTESTAI framework.
3. Discuss the results observed and determine future work required to achieve the highest level of penetration testing automation.

The rest of the paper is structured as follows: An overview of previous work on automation for penetration testing is given in Section 2; we provide a brief review of the literature, covering an introduction to the MITRE-ATT&CK framework and a discussion of the current status of research on cybersecurity and LLM-powered AI agent frameworks. Section 3 describes PENTESTAI, the new framework we propose to automate penetration testing with multiple LLM-powered agents and some subsequent capabilities. In Section 4, we cover the proof of concept done to validate the core constructs of the proposed framework. Section 6 brings the work to a close and explores potential avenues for further research.

II. A Brief Literature Review

Penetration testing is a common practice or procedure executed on a company's applications and systems, following the company's authorization, to identify potential vulnerabilities in the target applications or systems, assess the level of difficulty required to exploit those vulnerabilities, and take necessary corrective action to prevent bad actors from exploiting the vulnerabilities [3][4][5]. Penetration testing, or pen tests, is essential to determine the target system or organization's security posture. It is a crucial practice in cybersecurity, usually conducted in five main phases presented in the table below with the tools commonly used for each phase [4][7][8]:

TABLE I. UMBRELLA PHASES FOR PENETRATION TESTING WITH COMMON TOOLS USED

	Pentest umbrella phases		
	Pre-Exploitation Phase	***Exploitation phase***	***Post exploitation phase***
Description	The attacker or the tester collects data from public source or from direct integration to determine potential targets.	Tester attempt to exploit the weakness to gain unauthorized access	Testers attempt to maintain access and gather as much information as possible, then covering tracks
Example of tools	Nmap, Nessus, Burp Suite , Metasploit, etc..	Multiple tools based on target's OS	Multiple tools based on target's OS

The MITRE ATT&CK framework provides a comprehensive breakdown of the tactics, techniques, and procedures (TTPs) malicious actors employ during real-world cyberattacks. This framework organizes these malicious activities into 14 tactical groups, each representing a different stage of the attack lifecycle. These stages include **reconnaissance** (gathering information), **resource development** (establishing resources for the attack), **initial access** (breaching the target network), **execution** (running malicious code), **persistence** (maintaining access to compromised systems), **privilege escalation** (gaining higher-level system permissions), **defense evasion** (evading detection), credential access (stealing login credentials), **discovery** (exploring the target environment), **lateral movement** (moving within the network to compromise additional systems), **collection** (gathering valuable data), **command and control** (establishing communication with compromised systems), **exfiltration** (stealing data), and **impact** (disrupting or destroying systems and data). Each tactic is further detailed with numerous techniques and procedures illustrating attackers' specific methods. The framework outlines over 235 techniques that can be executed across various platforms (Windows, macOS, Azure, etc.) using different tools and methodologies [9].

Malicious actors or black hat hackers constantly develop new tools. In Bianco's pyramid of pain [11], he explains that TTPs are "tough" to execute by black hat hackers when controls around the vulnerabilities exploited by TTPs are implemented. Zych et al. study makes a mapping between CVE (Common Vulnerabilities and Exposures) and techniques that exploit them [10]. By mapping the hundreds of techniques to the hundreds of CVEs and considering the multitude of platforms and operating systems currently used in organizations of various natures, it became apparent that manual penetration testing is no longer enough to mitigate organization security exposure risks.

However, the automation of penetration is not a revolutionary idea and has been studied by many researchers who approached the problem from different angles. Artificial Intelligence and Reinforcement Learning, Deep reinforcement learning, and non-AI multi-agent systems have been studied the most by those researchers [12][13][14][15]. Short of providing a complete solution to the problem, the merit of previous work by researchers was to validate the hypothesis that a future where automated penetration testing can offload human testers while providing scalable and accurate methods to secure organization assets is possible.

The surge of large language models (LLMs) and generative AI-powered models has ushered in a new wave of research and experimentation in cybersecurity. Kucharavy et al. provide a detailed analysis of LLMs and strategic directions to integrate LLMs in cybersecurity [16]. Xi et al. provide a general conceptual framework for LLM-based agents tailored for different applications and scenarios. The framework has been very influential in the research community and has three main parts. The **perception**, whose role is to convert multimodal information (text, audio, video, etc..) into an understandable representation for the agent. The **brain** relies on selected models to engage in information-processing activities such as thinking, decision-making, and operations with storage, including memory and knowledge. The **action** is executed with the assistance of tools and impacts its surroundings.

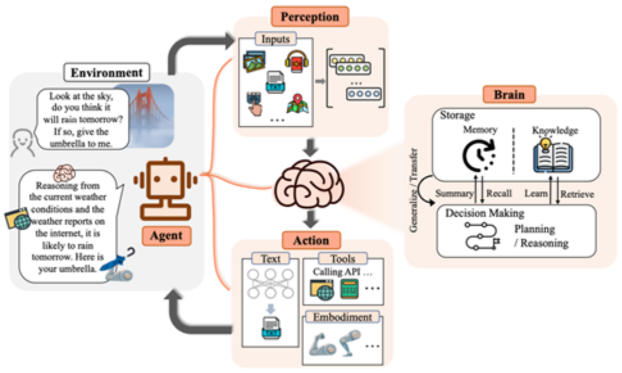
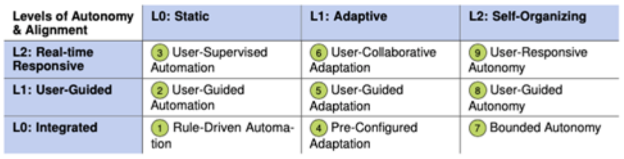

Perception
Inputs
Environment
Look at the sky, do you think it will rain tomorrow? If so, give the umbrella to me.
Reasoning from the current weather conditions and the weather reports on the internet, it is likely to rain tomorrow. Here is your umbrella.
Agent
Brain
Storage
Memory
Knowledge
Generalize / Transfer
Summary
Recall
Learn
Retrieve
Decision Making
Planning / Reasoning
Action
Text
Tools
Calling API ...
Embodiment

Figure 1: Construction of LLM-Powered Agents [18]

Talebirad et al. centered their research on models such as auto-GPT and babyAGI to illustrate how agents can work together to solve problems in different domains [18]. Händler[19] builds on the work done by Talebirad et al. and proposes an LLM-powered agent architecture specification where the essential concepts of **autonomy** and **alignment** for multi-agent systems are introduced. Autonomy is defined as the ability of multi-agent systems to fulfill the goals they were designed for through self-organized strategies and ask execution. Autonomy has three levels: **static**, **adaptative**, and **self-organized**. **Alignment** is the ability to ensure the AI agents' behavior aligns with human intentions, values, and goals [19]. The matrix below proposed a potential combination of autonomy and alignment that can be adopted based on the multi-agent system use case that is being implemented.



Levels of Autonomy & Alignment	L0: Static	L1: Adaptive	L2: Self-Organizing
L2: Real-time Responsive	3 User-Supervised Automation	6 User-Collaborative Adaptation	9 User-Responsive Autonomy
L1: User-Guided	2 User-Guided Automation	5 User-Guided Adaptation	8 User-Guided Autonomy
L0: Integrated	1 Rule-Driven Automation	4 Pre-Configured Adaptation	7 Bounded Autonomy

Figure 2: Autonomy and Alignment Balancing Matrix for LLM-Powered Agents [19]

We found the idea of aligning the agents' actions to the goals of humans very relevant for cybersecurity use cases in general or, more specifically, for penetration testing. It will make sense to design our framework for **User-Guided Adaptation**. The latter means that the framework we will propose for penetration testing automation should be able to adapt its operations based on predefined parameters and allow the users to guide the system behavior within a predefined structure [19].

Given the state of research in penetration testing and LLMs presented above, our goal in the following section is to propose an LLM-powered multi-agent framework with the right balance of autonomy and alignment, capable of enabling efficient human-agent collaboration for penetration testing automation at scale.

III. PENTESTAI, THE PROPOSED LLM-POWERED MULTI-AGENT FRAMEWORK FOR PENETRATION TESTING AUTOMATION

At this stage, the main questions to answer for our agent composition framework for penetration testing automation are the following:

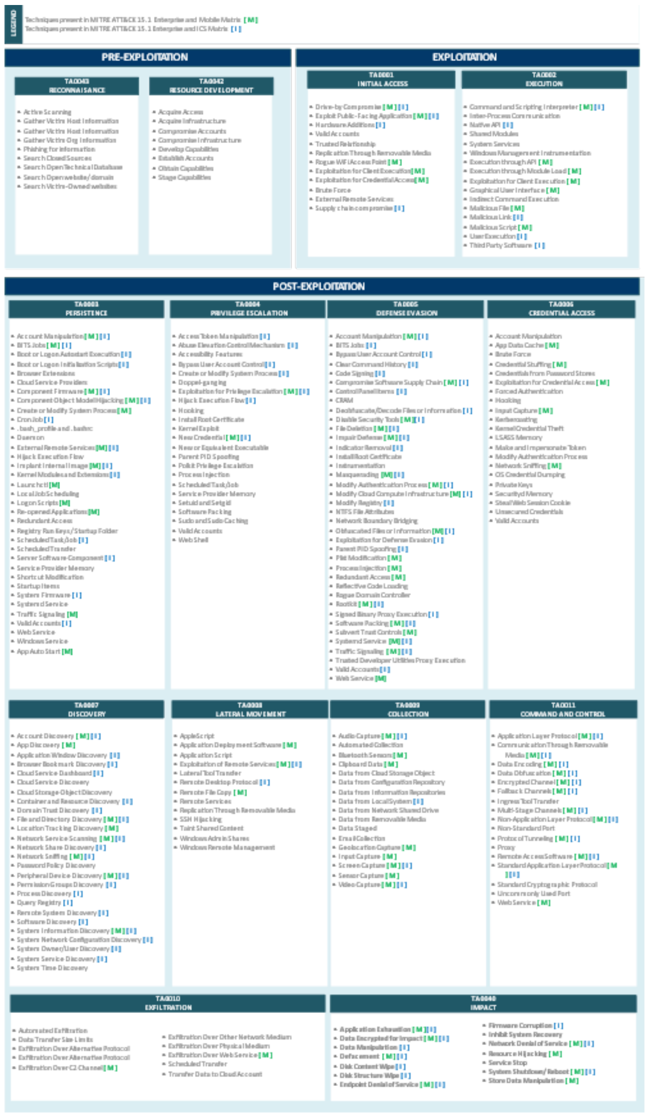
1. What are the necessary agent roles that should be included in the framework?

2. How do we ensure that each agent runs with the optimal brain (LLM models) that will enable it to fulfill its role in this agent penetration testing framework?

3. What are the right tools and skills that should be implemented to allow them to perform the actions they are expected to perform?

4. How will the control, the optimization, and the scaling of the agents be achieved?

Similarly to the thought process used in decomposing monolith systems into microservices, a breakdown and decomposition of the penetration testing domain was required to answer the questions above. To that end, the three matrices (Enterprise, Mobile, and Industrial Control Systems) of MITRE ATT&CK framework v 15.1 were analyzed to group the tactics, techniques, and tools commonly used by penetration testing practitioners in three umbrella phases for penetration testing: **the pre-exploitation phase**, **the exploitation phase,** and **the post-exploitation phase**. The following Figure 3 provides a summary of that analysis.



LEGEND
Techniques present in MITRE ATT&CK 15.1 Enterprise and Mobile Matrix [M]
Techniques present in MITRE ATT&CK 15.1 Enterprise and ICS Matrix [I]

PRE-EXPLOITATION

TA0043 RECONNAISSANCE
- Active Scanning
- Gather Victim Host Information
- Gather Victim Host Information
- Gather Victim Org Information
- Phishing for information
- Search Closed Sources
- Search Open Technical Database
- Search Open website/domain
- Search Victim-Owned websites

TA0042 RESOURCE DEVELOPMENT
- Acquire Access
- Acquire Infrastructure
- Compromise Accounts
- Compromise Infrastructure
- Develop Capabilities
- Establish Accounts
- Obtain Capabilities
- Stage Capabilities

EXPLOITATION

TA0001 INITIAL ACCESS
- Drive-by Compromise [M] [I]
- Exploit Public-Facing Application [M] [I]
- Hardware Additions [I]
- Valid Accounts
- Trusted Relationship
- Replication Through Removable Media
- Rogue WiFi Access Point [M]
- Exploitation for Client Execution [M]
- Exploitation for Credential Access [M]
- Brute Force
- External Remote Services
- Supply chain compromise [I]

TA0002 EXECUTION
- Command and Scripting Interpreter [M] [I]
- Inter-Process Communication
- Native API [I]
- Shared Modules
- System Services
- Windows Management Instrumentation
- Execution through API [M]
- Execution through Module Load [M]
- Exploitation for Client Execution [M]
- Graphical User Interface [M]
- Indirect Command Execution
- Malicious File [M]
- Malicious Link [I]
- Malicious Script [M]
- User Execution [I]
- Third Party Software [I]

POST-EXPLOITATION

TA0003 PERSISTENCE
- Account Manipulation [M] [I]
- BITS Jobs [M] [I]
- Boot or Logon Autostart Execution [I]
- Boot or Logon Initialization Scripts [I]
- Browser Extensions
- Cloud Service Providers
- Component Firmware [M] [I]
- Component Object Model Hijacking [M] [I]
- Create or Modify System Process [M]
- Cron Job [I]
- .bash_profile and .bashrc
- Daemon
- External Remote Services [M] [I]
- Hijack Execution Flow
- Implant Internal Image [M] [I]
- Kernel Modules and Extensions [I]
- Launchctl [M]
- Local Job Scheduling
- Logon Scripts [M]
- Re-opened Applications [M]
- Redundant Access
- Registry Run Keys/Startup Folder
- Scheduled Task/Job [I]
- Scheduled Transfer
- Server Software Component [I]
- Service Provider Memory
- Shortcut Modification
- Startup Items
- System Firmware [I]
- Systemd Service
- Traffic Signaling [M]
- Valid Accounts [I]
- Web Service
- Windows Service
- App Auto Start [M]

TA0004 PRIVILEGE ESCALATION
- Access Token Manipulation [I]
- Abuse Elevation Control Mechanism [I]
- Accessibility Features
- Bypass User Account Control [I]
- Create or Modify System Process [I]
- Doppel-ganging
- Exploitation for Privilege Escalation [M] [I]
- Hijack Execution Flow [I]
- Hooking
- Install Root Certificate
- Kernel Exploit
- New Credential [M] [I]
- New or Equivalent Executable
- Parent PID Spoofing
- Polkit Privilege Escalation
- Process Injection
- Scheduled Task/Job
- Service Provider Memory
- Setuid and Setgid
- Software Packing
- Sudo and Sudo Caching
- Valid Accounts
- Web Shell

TA0005 DEFENSE EVASION
- Account Manipulation [M] [I]
- BITS Jobs [I]
- Bypass User Account Control [I]
- Clear Command History [I]
- Code Signing [I]
- Compromise Software Supply Chain [M] [I]
- Control Panel Items [I]
- CRAM
- Deobfuscate/Decode Files or Information [I]
- Disable Security Tools [M] [I]
- File Deletion [M] [I]
- Impair Defense [M] [I]
- Indicator Removal [I]
- Install Root Certificate
- Instrumentation
- Masquerading [M] [I]
- Modify Authentication Process [M] [I]
- Modify Cloud Compute Infrastructure [M] [I]
- Modify Registry [I]
- NTFS File Attributes
- Network Boundary Bridging
- Obfuscated Files or Information [M] [I]
- Exploitation for Defense Evasion [I]
- Parent PID Spoofing [I]
- Plist Modification [M]
- Process Injection [M]
- Redundant Access [M]
- Reflective Code Loading
- Rogue Domain Controller
- Rootkit [M] [I]
- Signed Binary Proxy Execution [I]
- Software Packing [M] [I]
- Subvert Trust Controls [M]
- Systemd Service [M] [I]
- Traffic Signaling [M] [I]
- Trusted Developer Utilities Proxy Execution
- Valid Accounts [I]
- Web Service [M]

TA0006 CREDENTIAL ACCESS
- Account Manipulation
- App Data Cache [M]
- Brute Force
- Credential Stuffing [M]
- Credentials from Password Stores
- Exploitation for Credential Access [M]
- Forced Authentication
- Hooking
- Input Capture [M]
- Kerberoasting
- Kernel Credential Theft
- LSASS Memory
- Make and Impersonate Token
- Modify Authentication Process
- Network Sniffing [M]
- OS Credential Dumping
- Private Keys
- Securityd Memory
- Steal Web Session Cookie
- Unsecured Credentials
- Valid Accounts

TA0007 DISCOVERY
- Account Discovery [M] [I]
- App Discovery [M]
- Application Window Discovery [I]
- Browser Bookmark Discovery [I]
- Cloud Service Dashboard [I]
- Cloud Service Discovery
- Cloud Storage Object Discovery
- Container and Resource Discovery [I]
- Domain Trust Discovery [I]
- File and Directory Discovery [M] [I]
- Location Tracking Discovery [M]
- Network Service Scanning [M] [I]
- Network Share Discovery [I]
- Network Sniffing [M] [I]
- Password Policy Discovery
- Peripheral Device Discovery [M] [I]
- Permission Groups Discovery [I]
- Process Discovery [I]
- Query Registry [I]
- Remote System Discovery [I]
- Software Discovery [I]
- System Information Discovery [M] [I]
- System Network Configuration Discovery [I]
- System Owner/User Discovery [I]
- System Service Discovery [I]
- System Time Discovery

TA0008 LATERAL MOVEMENT
- AppleScript
- Application Deployment Software [M]
- Application Script
- Exploitation of Remote Services [M] [I]
- Lateral Tool Transfer
- Remote Desktop Protocol [I]
- Remote File Copy [M]
- Remote Services
- Replication Through Removable Media
- SSH Hijacking
- Taint Shared Content
- Windows Admin Shares
- Windows Remote Management

TA0009 COLLECTION
- Audio Capture [M] [I]
- Automated Collection
- Bluetooth Sensors [M]
- Clipboard Data [M]
- Data from Cloud Storage Object
- Data from Configuration Repository
- Data from Information Repositories
- Data from Local System [I]
- Data from Network Shared Drive
- Data from Removable Media
- Data Staged
- Email Collection
- Geolocation Capture [M]
- Input Capture [M]
- Screen Capture [M] [I]
- Sensor Capture [M]
- Video Capture [M] [I]

TA0011 COMMAND AND CONTROL
- Application Layer Protocol [M] [I]
- Communication Through Removable Media [M] [I]
- Data Encoding [M] [I]
- Data Obfuscation [M] [I]
- Encrypted Channel [M] [I]
- Fallback Channels [M] [I]
- Ingress Tool Transfer
- Multi-Stage Channels [M] [I]
- Non-Application Layer Protocol [M] [I]
- Non-Standard Port
- Protocol Tunneling [M] [I]
- Proxy
- Remote Access Software [M] [I]
- Standard Application Layer Protocol [M] [I]
- Standard Cryptographic Protocol
- Uncommonly Used Port
- Web Service [M]

TA0010 EXFILTRATION
- Automated Exfiltration
- Data Transfer Size Limits
- Exfiltration Over Alternative Protocol
- Exfiltration Over Alternative Protocol
- Exfiltration Over C2 Channel [M]
- Exfiltration Over Other Network Medium
- Exfiltration Over Physical Medium
- Exfiltration Over Web Service [M]
- Scheduled Transfer
- Transfer Data to Cloud Account

TA0040 IMPACT
- Application Exhaustion [M] [I]
- Data Encrypted for Impact [M] [I]
- Data Manipulation [I]
- Defacement [M] [I]
- Disk Content Wipe [I]
- Disk Structure Wipe [I]
- Endpoint Denial of Service [M] [I]
- Firmware Corruption [I]
- Inhibit System Recovery
- Network Denial of Service [M] [I]
- Resource Hijacking [M]
- Service Stop
- System Shutdown/Reboot [M] [I]
- Store Data Manipulation [M]

Figure 3: Consolidated MITRE ATT&CK matrices, including Enterprise, Mobile, and ICS information, with tactics grouped by penetration testing umbrella phases

Analyzing and regrouping MITRE ATT&CK tactics helped us, on the one hand, to determine the type of agents required in our framework and, on the other hand, to determine the number and type of skills or tools the agent would need. Our analysis revealed about 405 techniques described across the three matrices of MITRE ATT&CK v 15.1. This might suggest that we will need to develop 405 tools across multiple platforms (Windows, MacOS, iOS, Android, etc..) to be able to give our agents the skills they need to automate the penetration testing. Still, the similarities in some techniques can provide opportunities to reuse the code developed across multiple techniques. We propose the architecture below for our framework:

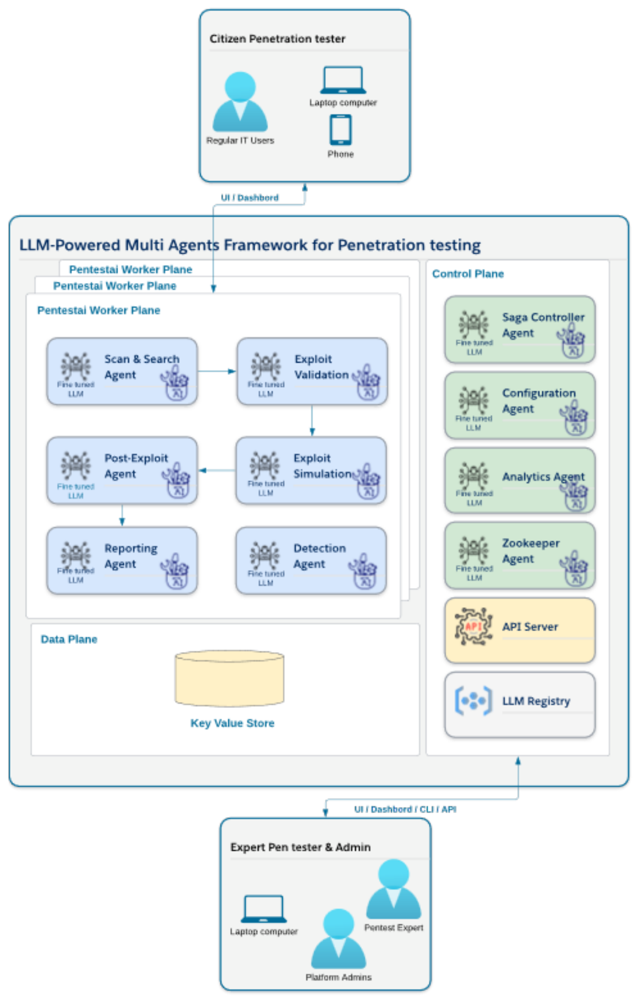


Figure 4: PENTESTAI Framework Conceptual Architecture

The framework identifies three fundamental categories of users(**citizen penetration testers**, **expert penetration testers,** and **administrators**) and comprises three planes (**worker plane**, **data plane,** and **control plane**). Each plane consists of two types of agents (worker agents and control agents) and has some supporting capabilities (API Server, LLM Registry, and Key-Value Store) that help the different types of agents fulfill their roles. A brief description of each of the building blocks of the framework is provided below, starting with the planes, the key user roles, then the agents and the supporting capabilities:

The PENTESTAI worker plane consists of five agents that execute specific tasks during the penetration testing session. Multiple penetration tests can be executed simultaneously, so each will be managed and monitored within the worker plane group.

The data plane deals with storing and retrieving data and files generated or consumed during penetration testing execution. It also supports the analytics and LLM finetuning tasks that should be carried out within the framework.

The control plane has all the agents and capabilities that should ensure the proper functioning of the overall framework.

Citizen penetration testers are regular IT system administrators or other IT resources with little to no expertise in cybersecurity in general or penetration testing in particular. They interact with the framework to input their testing needs via a web user interface or a mobile application and review results, recommendations, and a dashboard.

Expert penetration testers and administrators who are people knowledgeable in penetration testing and artificial intelligence. They understand the PENTESTAI framework and can approve validation for agents' tasks when applicable. They can access and analyze data produced by the control plane via a web user interface or a command line interface; they can make decisions and recommendations to improve the framework's performance.

As discussed in the previous section, each agent in the framework will have a set of custom-built tools and skills required to perform its jobs and execute MITRE ATT&CK techniques. As an example, in the pre-exploitation phase of the penetration testing, the Scan and Search agent might need to have a **scan_and_search_tool** built with Python libraries such as **python3-nmap** or **py-nessus-pro** that provide programmatic access to Nmap and Nessus, two popular tools used by expert penetration tester to gather data about the target system and determine the next in the penetration testing[4]. The agent's performance will rely on the finetuned LLMs they will use for their tasks and the efficient design and development of the hundreds of tools and skills needed to mimic expert techniques as documented in the MITRE ATT&CK framework. In the following paragraphs, we provide a brief statement on the role and capabilities of each of the agents in the proposed PENTESTAI framework.

The Scan and Search Agent (SSA): This worker agent will intervene during the pre-exploitation phase of penetration testing, and its role will be to implement the critical techniques in the resource development and reconnaissance tactics of the MITRE Framework. The agent will be able to determine the right tools and techniques based on the objectives of the penetration testing session, the target platforms (Windows, MacOS, Android, iOS, etc..), and the context of that session (Enterprise, Mobile, or ICS).

The Exploit Validation Agent (EVA): this worker agent's activities fall within the exploitation phase of penetration testing. It will analyze the data collected by the scanning and search Agent and scan vulnerability databases to identify vulnerabilities by severity and exploits that might be possible to execute on the target system.

The Exploit Simulation Agent (ESA): This worker agent also participates in the exploitation phase of the penetration testing session. Its role builds on that of the exploit validation agent. The ESA analyzes each possible exploit and determines which can be executed without causing collateral damage to the target. It will then create the exploit payload and execute the exploit techniques following human validation.

The Post-Exploitation Agent (PEA): as its name indicates, this agent is part of the post-exploitation phase of the PENTESTAI framework. Given the hundreds of possible post-exploitation techniques, this agent will have an extensive set of tools built for it. It will continue the work of the exploit simulation agent. For the exploits executed in the previous phase, this agent will test the execution of the post-exploitation payload using multiple techniques referenced in the MITRE ATT&CK framework. It will save the relevant data in the key-value store for reporting.

The Reporting Agent (RA): This worker agent should always be invoked at the final step of a penetration testing session. Its inputs will be the data collected and generated by the previous worker agents. The agent will use these inputs to compile a penetration testing session summary report. Additionally, it will use the knowledge of the cybersecurity field from its assigned LLM to provide recommendations to address all the vulnerabilities reported.

The Detection Agent (DA): the MITRE ATT&CK framework documents the various techniques black hat hackers use and provides methods for detecting when an exploit payload was executed on a target. The detection agent is a worker agent that can be run in standalone mode and implements all the skills to detect attacks on a target. Tasks can be delegated to the reporting agent to report on issues detected on a target and recommend actions.

The five worker agents introduced above will execute the functional tasks required to complete each penetration testing session. For these agents to fulfill those functional duties at scale, optimally, and with the right balance between autonomy and alignment, control agents and additional capabilities are required. We describe them below:

The Configuration Agent (CA): This worker agent will need configuration input to complete their tasks. The role of this control agent will be to provide all the configurations that worker agents need to execute their functions. Configurations will include but will not be limited to items such as the right finetuned LLM for the tasks of the worker agent, the API keys for that model if an external provider hosts the model, and the key parameters to use for the model. The configuration agent will also leverage the key-value store to track and learn from the configurations used in the past penetration testing sessions to optimize the configurations allocated to worker agents during future penetration testing sessions. As part of the control plane of the PENTESTAI framework, we proposed an optional **LLM registry** capability where all the finetuned LLMs (SecurityBERT, CyBERT, SecurityGPT, Falcon LLM, CybertCPT, and new ones to come) used for penetration testing can be stored. An alternative registry, such as HuggingFace, could also provide this capability. Another important capability of this agent will be to benchmark the performance of different models used and include the result of those benchmarks in the model allocation decisions.

The Saga Controller Agent (SCA): This agent's role is rooted in the saga pattern, which is very prominent in microservices designs. Penetration testing is a very sequential process in nature; the saga controller agent will have the responsibility to control the flow of the execution of the tasks required in each penetration testing session. It will also allow a logical grouping of the activities of worker agents in a way that could enable effective monitoring and troubleshooting. The saga controller will also use the key-value store to save importation data and metadata about each penetration testing run.

The Analytics Agent (AA): This control agent will focus on using the data saved in the key-value store by other agents to compile aggregations for the dashboard.

The Zookeeper Agent (ZA): Being able to understand and observe in real time the state of each agent, the human or system prompt received, and the output returned and being able to take necessary actions on agents to prevent endless loops during the penetration testing execution is a crucial function required for PENTESTAI framework to scale. The zookeeper agent is the control agent that will play that role. The agent will receive detailed traces of the execution of each agent and saga controller, consolidate the traces for each penetration testing run, and make decisions to start, stop, restart agents, restart a saga, or perform any other action required to maintain the performance and integrity of the framework as a whole.

The API server: This is a required capability that will support the command-line interface (CLI) interaction and the integration of the PENTESTAI framework with other frameworks or solutions.

The LLM Registry: As mentioned previously, the LLM Registry is an optional capability. PENTESTAI should be able to operate with third-party LLM repositories.

The Key-Value Store: The key-value store is an important capability that will extend the memory of the agents and give memory to the framework as a whole. All metadata related to agents, their configuration, their context, their various execution sessions, etc., should be kept in the store. It will serve as a single source of truth for the state of agents and systems. The control plane will use the agent state data to initiate actions required to maintain the whole system in a good state.

The framework described above provides an innovative approach to tackling penetration testing and the lack of skilled resources in that space. However, the question of its feasibility remains to be answered.

IV. Implementation Prototype

To assess the possibility of implementing the PENTESTAI framework, we developed a prototype with a minimal scope to validate the concepts and building blocks of the proposed framework. We implemented the simplified penetration testing flow with three agents (**Scan & Search Agent, Exploit validation Agent**, and **Reporting Agent**). Given the rapid progress of generative AI in recent years, many multi-agent development frameworks have been released (Autogen, CrewAI, etc.) We decided to experiment with CrewAI because of its very intuitive architecture. CrewAI architecture is based on agents that are part of a **crew** or **multiple crews**. Agents can be assigned **tools**, and **tasks** can be created to indicate what agents should do and what tools they should use. CrewAI architecture was a good fit for our framework, and because it is built on top of Langchain, the integration with observability tools such as LangSmith could be seamless. It could be a solid foundation for implementing the control plane of the PENTESTAI framework.

We developed two custom tools, **ScanAndSearchTool** and **ExploitValidationTool**, in the form of Python classes with multiple methods using Python libraries, allowing programmatic emulation of Nmap command with the options to either scan subnets to discover potential targets or to scan targets to find possible vulnerabilities. The **ScanAndSearchTool** produces a JSON file named **comprehensive_scan_results.json** with all the information gathered with the MITRE ATT&CK reconnaissance techniques implemented in the tool. The **ExploitValidationTool** takes the file created by **ScanAndSearchTool**, and after executing the exploitation techniques implemented in the tool, it returns another JSON file named **vulnerability_report.json** with all the identified vulnerabilities.

We intentionally did not develop a reporting tool for this proof of concept. We decided to proceed as such to test the cybersecurity knowledge of the **GPT4o**, which Ferrag et al. identified as the highest-performing model for cybersecurity tasks [26]. So, natural language instructions were provided to the reporting agent, asking it to take the two JSON files mentioned above and produce a summary report of the penetration testing session.

We set up a straightforward test environment, presented in Figure 5 below. It consists of an EC2 instance in the AWS cloud where our agents were deployed and publicly available targets (scanme.namp.org and pentest-ground.com) on which our penetration test sessions were executed.

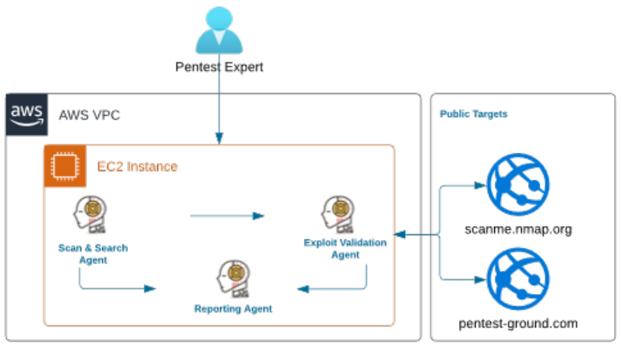
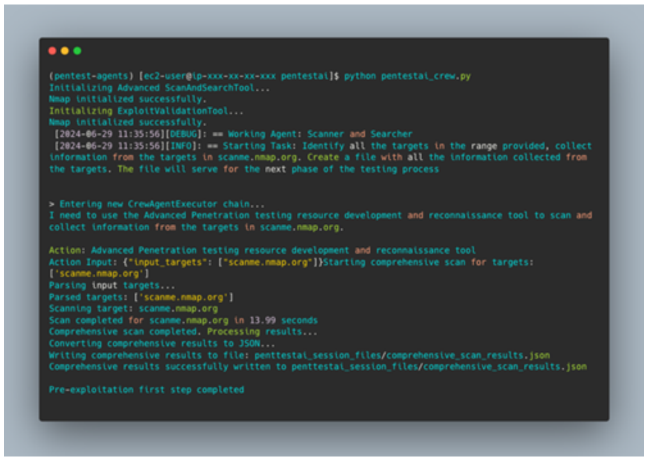


Figure 5: PENTESTAI proof of concept environment

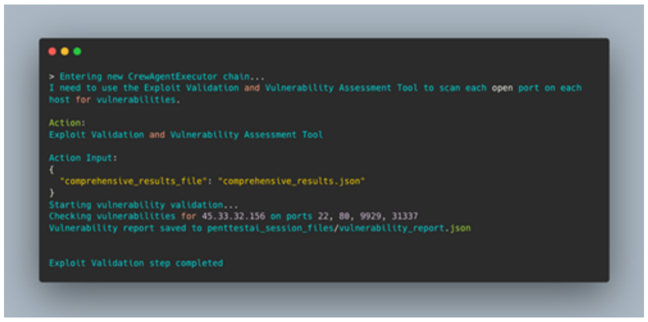
Figure 6 shows snippets of the pre-exploitation phase of our penetration testing test. We see how the ScanAndSearchTool and the ExploitValidationTool are initialized, and the agents and the tasks they execute are displayed on screen. At the end of the task execution, the agent displays a completion message, and the next agent starts his job.



```
(pentest-agents) [ec2-user@ip-xxx-xx-xx-xxx pentestai]$ python pentestai_crew.py
Initializing Advanced ScanAndSearchTool...
Nmap initialized successfully.
Initializing ExploitValidationTool...
Nmap initialized successfully.
 [2024-06-29 11:35:56][DEBUG]: == Working Agent: Scanner and Searcher
 [2024-06-29 11:35:56][INFO]: == Starting Task: Identify all the targets in the range provided, collect
information from the targets in scanme.nmap.org. Create a file with all the information collected from
the targets. The file will serve for the next phase of the testing process


> Entering new CrewAgentExecutor chain...
I need to use the Advanced Penetration testing resource development and reconnaissance tool to scan and
collect information from the targets in scanme.nmap.org.

Action: Advanced Penetration testing resource development and reconnaissance tool
Action Input: {"input_targets": ["scanme.nmap.org"]}Starting comprehensive scan for targets:
['scanme.nmap.org']
Parsing input targets...
Parsed targets: ['scanme.nmap.org']
Scanning target: scanme.nmap.org
Scan completed for scanme.nmap.org in 13.99 seconds
Comprehensive scan completed. Processing results...
Converting comprehensive results to JSON...
Writing comprehensive results to file: penttestai_session_files/comprehensive_scan_results.json
Comprehensive results successfully written to penttestai_session_files/comprehensive_scan_results.json

Pre-exploitation first step completed
```

Figure 6: Pre-exploitation phase – Scan And Search Agent's output snippet

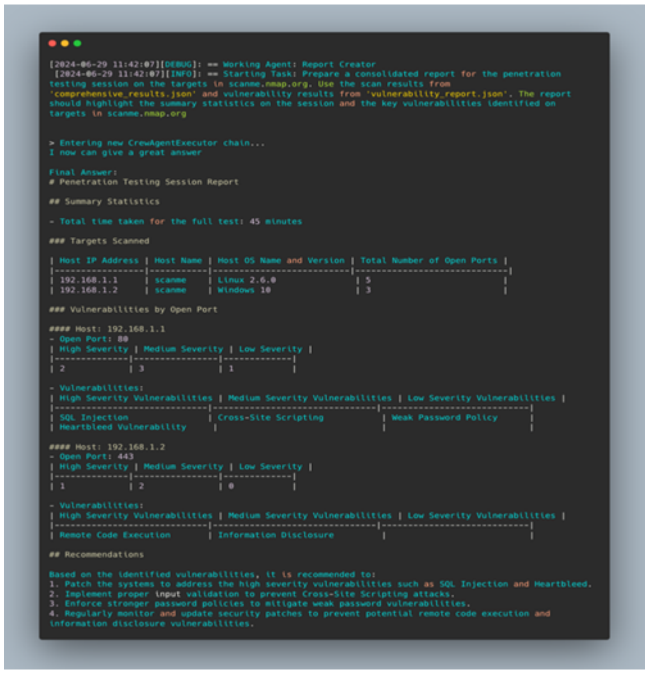
Figure 7 provides a snapshot of the Exploit validation phase. We can see how the agent indicates the tool it will use and the input file generated in the previous step. At the completion, the agent also displays a completion message.



```
> Entering new CrewAgentExecutor chain...
I need to use the Exploit Validation and Vulnerability Assessment Tool to scan each open port on each
host for vulnerabilities.

Action:
Exploit Validation and Vulnerability Assessment Tool

Action Input:
{
  "comprehensive_results_file": "comprehensive_results.json"
}
Starting vulnerability validation...
Checking vulnerabilities for 45.33.32.156 on ports 22, 80, 9929, 31337
Vulnerability report saved to penttestai_session_files/vulnerability_report.json


Exploit Validation step completed
```

Figure 7:Exploit Validation phase- Exploit Validation Agent's outputs snippet.

Figure 8 below shows a capture of the report generated by the reporting agent. Similarly to what was observed for the previous agents, at the beginning of its work, the agent states its name, the task it will execute, and the input files it will use to execute the tasks. Then, it provides summary statistics on the hosts targeted during the penetration testing session, a summary of the vulnerabilities identified per port, and the recommended actions to correct those vulnerabilities. Despite relying only on the **GPT 4.o** model and not having a custom tool built for the report creation task, the reporting agent could analyze the input files efficiently and automatically provide sound recommendations for each vulnerability identified on the target hosts. This is very promising and confirms Ferrag et al. [26] observations on GPT 4.o cybersecurity knowledge.



```
[2024-06-29 11:42:07][DEBUG]: == Working Agent: Report Creator
 [2024-06-29 11:42:07][INFO]: == Starting Task: Prepare a consolidated report for the penetration
testing session on the targets in scanme.nmap.org. Use the scan results from
'comprehensive_results.json' and vulnerability results from 'vulnerability_report.json'. The report
should highlight the summary statistics on the session and the key vulnerabilities identified on
targets in scanme.nmap.org


> Entering new CrewAgentExecutor chain...
I now can give a great answer

Final Answer:
# Penetration Testing Session Report

## Summary Statistics

- Total time taken for the full test: 45 minutes

### Targets Scanned

| Host IP Address | Host Name | Host OS Name and Version | Total Number of Open Ports |
|-----------------|-----------|--------------------------|----------------------------|
| 192.168.1.1     | scanme    | Linux 2.6.0              | 5                          |
| 192.168.1.2     | scanme    | Windows 10               | 3                          |

### Vulnerabilities by Open Port

#### Host: 192.168.1.1
- Open Port: 80
| High Severity | Medium Severity | Low Severity |
|---------------|-----------------|--------------|
| 2             | 3               | 1            |

- Vulnerabilities:
| High Severity Vulnerabilities | Medium Severity Vulnerabilities | Low Severity Vulnerabilities |
|-------------------------------|---------------------------------|------------------------------|
| SQL Injection                 | Cross-Site Scripting            | Weak Password Policy         |
| Heartbleed Vulnerability      |                                 |                              |

#### Host: 192.168.1.2
- Open Port: 443
| High Severity | Medium Severity | Low Severity |
|---------------|-----------------|--------------|
| 1             | 2               | 0            |

- Vulnerabilities:
| High Severity Vulnerabilities | Medium Severity Vulnerabilities | Low Severity Vulnerabilities |
|-------------------------------|---------------------------------|------------------------------|
| Remote Code Execution         | Information Disclosure          |                              |

## Recommendations

Based on the identified vulnerabilities, it is recommended to:
1. Patch the systems to address the high severity vulnerabilities such as SQL Injection and Heartbleed.
2. Implement proper input validation to prevent Cross-Site Scripting attacks.
3. Enforce stronger password policies to mitigate weak password vulnerabilities.
4. Regularly monitor and update security patches to prevent potential remote code execution and
information disclosure vulnerabilities.
```

Figure 8: Post-Exploitation phase, Report generation

V. Conclusion

In this paper, we presented the context of digital transformation, the acceleration in software production that it entails, and the additional demand it generates for the cybersecurity and penetration testing field, which already suffers from a scarcity of resources. Our initial hypotheses were that the rapid progress in artificial intelligence, generative AI, and large language models could provide a new opportunity to develop automated and innovative solutions amidst a high expertise threshold and low resource availability currently faced by organizations for penetration testing and other cybersecurity activities.

In the literature review we conducted, interesting work previously completed with various automation approaches proposed for penetration testing had already identified the need to find a more scalable solution with less dependency on human experts. However, they cannot be anchored on reference frameworks or knowledge bases such as MITRE ATT&CK and have yet to explore the potential of LLMs and LLM-powered agents as key building blocks for the solution. We introduced PENTESTAI, a new LLM-powered multi-agent framework made of a crew of agents equipped with tools and skills reference in MITRE ATT&CK and working under the supervision of a well-designed control plane. A mini proof-of-concept of the framework was implemented, and the main ideas at the center of the framework were validated; some limitations and future work required were identified.

There are three major areas where more work is required to turn PENTESTAI into a production-ready framework supporting citizen penetration testers in evaluating the security poster of their applications or their infrastructure:

Model finetuning: Despite showing an acceptable level of knowledge in cybersecurity, GPT 4.o, the LLM assigned to all the agents during the proof-of-concept, generated some hallucinations in the results produced during a few penetration testing sessions. It will be necessary to work on finetuning either the foundations model or some existing cybersecurity models to ensure their knowledge is tailored to the tasks they are assigned in the framework and to ensure they can provide remediation compliant to all relevant standards, including MITRE / NIST Standards for enumeration and risk analytics.

Library development: In our analysis of MITRE ATT&CK techniques, we counted about 405. They come in the form of command lines, scripts, and software packages executable in different platforms and operating systems. More work will be required to develop libraries in Python or other languages that can be used to implement the skills and tools to assign to agents described in the PENTESTAI framework.

Control Plane realization: The agents and capabilities described in the control plane of the framework were not part of the scope of the proof-of-concept realization. Additional work will be required to validate the concept described in the control plane.

Zero-day exploit capability: The framework currently does not allow for the uncovering of zero-day vulnerabilities. Adding that capability requires the addition of a Reverse Engineering Agent (REA) that will work with an LLM optimized for decompiling binary and capable of invoking API or scripts from commonly used reverse engineering tools. Additional work is required to assess the efficiency of LLMs in decompiling tasks for various platforms and languages.

This paper achieves its goals by providing a solid and viable foundation for future research aiming to automate penetration testing and other cybersecurity skills by leveraging LLM-powered multi-agent systems.

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