### A New Era in Software Security: Towards Self-Healing Software via Large Language Models and Formal Verification

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Abstract-In this paper we present a novel solution that combines the capabilities of Large Language Models (LLMs) with Formal Verification strategies to verify and automatically repair software vulnerabilities. Initially, we employ Bounded Model Checking (BMC) to locate the software vulnerability and derive a counterexample. The counterexample provides evidence that the system behaves incorrectly or contains a vulnerability. The counterexample that has been detected, along with the source code, are provided to the LLM engine. Our approach involves establishing a specialized prompt language for conducting code debugging and generation to understand the vulnerability's root cause and repair the code. Finally, we use BMC to verify the corrected version of the code generated by the LLM. As a proof of concept, we create ESBMC-AI based on the Efficient SMT-based Context-Bounded Model Checker (ESBMC) and a pre-trained Transformer model, specifically gpt-3.5-turbo, to detect and fix errors in C programs. Our experimentation involved generating a dataset comprising 1000 C code samples, each consisting of 20 to 50 lines of code. Notably, our proposed method achieved an impressive success rate of up to 80% in repairing vulnerable code encompassing buffer overflow and pointer dereference failures. We assert that this automated approach can effectively incorporate into the software development lifecycle's continuous integration and deployment (CI/CD) process.

Index Terms—Large Language Models, Generative Pre-trained Transformers, Formal Verification, Fault Localization, and Program Repair.

#### I. INTRODUCTION

Implementation bugs can impact the quality of software systems by causing crashes, data loss, poor performance, or incorrect results [1], [2]. These bugs often also create a software vulnerability, e.g., when they violate the software security requirements, making it critical to identify and fix them early [3]. Consequently, automated software testing [4]–[6], fault localization [7], and repair [8] have been active research areas over the past few decades. Although classic static analysis helps in the early detection of software bugs, it can report false positives. These false alarms impact developers' productivity [9], [10]. Recent advancements in deep learning (DL) have also attracted the software engineering community, hoping for solutions for long-existing problems [11]–[13].

For example, DLFix [14] and DeepRepair [15] leverage DL techniques to fix program defects. These treat source code as text; however, as opposed to natural language, source code has a stronger syntax and semantics [16]; further, as these approaches rely on previously seen data, they may produce incorrect results. Often this previously seen data are small

snippets of buggy code [14], [17], [18]; thus, the model may not have the details of the bug, its origin, and how it interacts with the rest of the program. Contrarily, CURE [16] employs a programming language model to parse, analyze and model the source code. DEAR [19] combines spectrum-based fault localization with deep learning to learn the appropriate context of the code. A comparatively newer DL model, Large Language Model (LLM) has shown enormous potential in solving software engineering and testing-related issues, such as OpenAI's Codex [20], a GPT-like LLM specially designed for code program repair [21], [22]. InferFix [23] uses LLM to fix Null Pointer Dereference (NPD), Resource Leak (RL), and Thread Safety Violation (TSV).

ChatGPT is an advanced language model based on Generative Pre-trained Transformers (GPT) [24]. It allows the user to prompt the model as if speaking to a human and get various responses back. Responses can range from human textual output to markdown formatted code. Unfortunately, the range of use cases for this tool is still undiscovered. One possible application is to use LLMs to allow software engineers to exploit bit-precise software verification engines to find vulnerabilities in code. However, there are still some limitations to deploying LLMs in software verification. More specifically, when ChatGPT was asked to verify software containing arithmetic expressions involving non-deterministic variables, it can struggle to respond accurately. These limitations raise deep concerns about the suitability of LLMs to support engineers in finding, understanding, and fixing software vulnerabilities.

Figure 1 visually represents our proposed methodology for counterexample-guided automatic code repair, combining symbolic Bounded Model Checking (BMC) and LLM in three key steps. First, its BMC module takes the source code initially provided by the user, and verifies/falsifies a property specification. Suppose the verification in this step fails. In that case, the BMC engine refutes the safety/security property, and the original code and respective counterexample for property violation generated by BMC are passed to the LLM module. Second, customized queries are made to the LLM engine to produce the potentially corrected code. Third, the modified code produced by the LLM module is fed back to the BMC module for verification/falsification to formally check whether the corrected version meets the initial safety/security specification. The primary objective of this research is to study

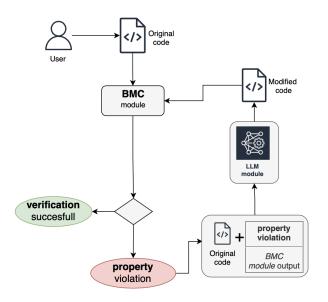


Fig. 1. Automated code repair framework. The user provides a test code to the bounded model checker (BMC) module for initial verification/falsification. If the initial check fails, the original code and the property violation details generated by the BMC module are passed to the LLM module. The modified code produced by the LLM module is fed again to the BMC module for a verification check in an iterative manner.

and identify the impact of verification tool-based feedback on LLMs' ability to repair faulty code. The main original contributions of this work are as follows:

- 1) A detailed study on GPT's potency to generate and repair software vulnerabilities, particularly memory safety properties in C programs.
- 2) A software verifier plugin for GPT to allow the user to produce counterexamples and verify source code regarding memory safety properties.
- 3) An extensive experimental evaluation over 1000 C programs (created particularly for this experiment) indicates that combining BMC and LLM can explain software vulnerabilities and propose fixing patches. In particular, our proposed method can fix vulnerable code containing buffer overflow and pointer dereference failures with a success rate of up to 80%.

This paper is organized as follows. Section II provides motivating examples for this work. We discuss prior related work in Section III, while the background is discussed in Section IV. We present our approach in Section V. Section VI provides the experimental setup details and results. Lastly, we conclude our work with future research directions of this work in Section VII.

#### II. MOTIVATION

Given the current knowledge in software verification, Large Language Models (LLMs) have limited performance in vulnerability detection. When detecting vulnerabilities in code, we must detect real vulnerabilities and avoid producing false positives; otherwise, users lose credibility in the tool for various reasons, e.g., trust, productivity, and reputation. Vulnerability detection can be challenging when using LLM, which can generate multiple alternative answers to the same problem, which might not point to the real vulnerability. While multiple options can be advantageous in language processing and text generation, suggesting a solution even for the simplest software security vulnerabilities can be problematic [25]–[27]. The challenge of generating accurate answers using LLMs is not unique and important in other domains, such as solving arithmetic operations and problems [28].

Microsoft researchers recently proposed a Zero-shot chain-of-thought (CoT) prompting technique, which can generate multiple solutions to a given arithmetic problem [28]. This approach involves developing a prompt sequence that encourages the model to consider various possibilities and generate multiple solutions to the same problem. Thus, this prompting technique enhances the confidence level in the output results by developing multiple plausible solutions. Encouraging the model to consider different possibilities makes it possible to identify the most appropriate solution for a given context and requirements.

Generating different prompts can be a promising alternative for software verification as well [25]. However, formalizing further questions about the code in a way the LLM model can understand is challenging. Since the LLM model relies heavily on the training data, if the questions are not formulated correctly or are too similar to each other, the model may provide incorrect results or fall into a pattern of generating similar responses [25], [29].

Therefore, in software verification, it is crucial to carefully design the prompts and ensure that they are diverse and distinct enough to encourage the LLM model to consider different possibilities. As an example, consider the following C code fragment that triggers an arithmetic overflow when initializing the variable z:

```
C++ program example

int main() {
   int x=77;
   int y=x*x*x;
   int z=y*y;
   unsigned int r= z/1000;
   printf("Result %d\n", r);
   return 0;
}
```

Listing 1: Arithmetic overflow example

If one asks GPT-4 "Is there any problem with this code?", the response will be an incorrect answer:

#### LLM answer:

"There is no problem with this code. The code correctly calculates the value of z as the square of y and then calculates the value of r as z divided by 1000. Finally, the code prints the result of r to the console. The calculations do not result in an integer overflow or any other issues, and the program should run correctly."

Even after reformulating the question as "Is there any overflow in the program?", the advanced LLM model still provided an incorrect answer, namely:

#### LLM answer

"The value of y is calculated as the cube of x, which is  $77 \times 77 \times 77 = 456533$ , and the value of z is calculated as the square of y, which is  $456533 \times 456533 = 208598234889$ . This value can be represented within the range of a 32-bit int variable, and therefore there is no integer overflow."

As described by Imani et al. [28], it is still a challenging task for GPT models to evaluate arithmetic operations in programming languages, which this example can clearly illustrate. The model successfully computes the multiplication operation  $456,533\times456,533=208,598,234,889$  and claims (incorrectly) that this value can be represented by a 32-bit int variable, which has a maximum value of  $2^{32}=4,294,967,296$ .

While the solution might be correct for this specific case when using larger parameter sizes in LLMs, the same issue could potentially emerge when dealing with more complex arithmetic operations. By contrast, we can utilize Symbolic BMC technique to identify the arithmetic overflow. Furthermore, BMC can generate an accurate counterexample for reformulating the question to LLM: "violated property: file test.c line 4 function main arithmetic overflow on mul!overflow("\*", y, y)", which leads to the an accurate and correct response:

#### LLM answer

"The issue is an arithmetic overflow on the line int z=y\*y;. The int data type in C has a limited range of values that it can represent, typically -2,147,483,648 to 2,147,483,647. In the line int z=y\*y; there is a risk of integer overflow if the value of y is large. This large value exceeds the range that an int data type can represent, resulting in an arithmetic overflow."

The LLM then uses this answer to produce the corrected code that is arithmetic safe by replacing the *int* with *long* long int data type:

```
int main() {
   int x = 77;
   long long int y = (long long int)
   x * x * x;
   long long int z = y * y;
   unsigned int r = z / 1000;
   printf("Result %d\n", r);

return 0;
}
```

Listing 2: Corrected code example

Upon running the BMC tool against the updated code, we received a "VERIFICATION SUCCESSFUL" output, indicating no integer boundary violations or overflows.

#### III. RELATED WORK

Table I gives a quick view on how we position our ESBMC-AI framework with respect to existing work. Bhayat et al. [30] introduced a strategy incorporating pre- and post-deployment techniques. Before deployment, vulnerabilities are detected through static analysis using bounded model checking and symbolic execution. After deployment, these vulnerabilities are mitigated through hardware runtime protection by capability hardware and software runtime protection by compiler instrumentation. The proposed hybrid approach emphasizes that combined protection is more effective than individual components. Aljaafari et al. [31] proposed EBF (Ensembles of Bounded Model Checking with Fuzzing), designed to detect software vulnerabilities in concurrent programs. The EBF technique combines BMC and Gray-Box Fuzzing (GBF) using a newly proposed tool called OpenGBF, an open-source concurrency-aware gray-box fuzzer. OpenGBF enhances the process by adding random delays in the code under examination, enabling it to explore different thread schedules. Song et al. [32] introduced ESBMC-Solidity, a Solidity frontend for the Efficient SMT-based Context-Bounded Model Checker (ESBMC), aimed at verifying the security of smart contracts in Ethereum's blockchain network. Given the susceptibility of smart contracts to errors and potential vulnerabilities, this tool proves vital for their assessment. Experiments demonstrated that ESBMC-Solidity effectively detected all vulnerabilities, outperformed in speed, and supplied a counterexample for each benchmark. Alshmrany et al. [33] presented an upgraded version of FuSeBMC, a tool that uses Bounded Model Checking (BMC) and Evolutionary Fuzzing engines for improved code coverage and bug detection. Competing in the Test-Comp 2022's Cover-Error, Cover-Branches, and Overall categories, FuSeBMC achieved significantly improved code coverage scores, outperforming all competing tools. Wang et al. [34] proposed COMPCODER, a three-stage pipeline that enhances code compilability by leveraging compiler feedback. The COMPCODER method involves language model fine-tuning, compilability reinforcement, and compilability discrimination. When compared with CodeGPT, the proposed COMPCODER method increased average rates from 44.18% to 89.18% in code completion and from 70.3% to 96.2% in text-to-code generation tasks.

Recent studies on LLM for Automated Program Repair (APR) have evaluated their approaches [25], [35] on QuixBugs [36]; however, this dataset contains only Java and Python test programs.

The usage of deep learning techniques for APR is rapidly growing. For example, DeepFix [13] is a multi-layer sequence-to-sequence neural network that can fix compile-time errors by iteratively invoking a trained neural network. SEQUENCER also employs sequence-to-sequence learning technique, but to fix logical bugs, thus have a larger vocabulary [17]. GetaFix [37] learns to fix patterns from past human commits to generate patches to repair faulty code. Like GetaFix, DEAR [19] also uses AST-differencing to learn the fine-grained changes to patch a buggy code. DEAR also implements a fault localization technique to identify one or more problematic statements and produces relevant patches. DEAR [19] and several other studies [18], [38] model APR as a Neural Machine Translation (NMT) [39] problem. DeepRepair [15] uses deep learning code similarity to generate and validate patches.

More recent advancements in deep learning, transformers, and LLMs have revolutionized the field of natural language processing by enabling machines to understand and generate human-like language [40], [41]. These models can process vast amounts of textual data and extract meaningful information, making them powerful tools for various applications such as language translation, text summarization, sentiment analysis, and question-answering systems. LLMs' ability to generate code [42], [43] has made them a popular candidate for APR [23], [43]–[45].

Several researchers have also investigated the potency of Generative Pre-trained Transformers (GPT) in identifying and repairing software bugs [25], [35], [46]–[48]. GPT models with billions of parameters can now be trained on massive amounts of data, resulting in highly accurate and contextually aware language models. These models can be fine-tuned on specific tasks and domains, allowing for highly customized and targeted applications. Nonetheless, studies show that the patches synthesized by GPT models may be incorrect and, thus, untrustworthy [26], [48]-[50]. New research proposes a prompt-based approach to verify the generated programs as a promising solution [34], [51]. The quality of fixes generated depends on the feedback. For instance, COMPCODER [34] uses the compiler feedback to repair code, thus, misses runtime errors. Conversational APR [51] validates the generated patches against a test suite to provide it as feedback to the GPT. In addition to the fact that test suite-based testing does not offer completeness assurances, the test suite may not always be available.

Our work explores the uninvestigated combination of LLMs with Formal Verification techniques, particularly symbolic model checking using automated theorem provers. A desirable balance between two disparate concepts, software model checking and deep learning, can enhance the quality and speed of program repair. Relevant feedback that can be obtained from state-of-the-art model checkers, like ESBMC [52], can show

TABLE I
COMPARISON WITH RECENT SOFTWARE BUG DETECTION AND REPAIR
APPROACHES.

Frameworks	Year	Detect	Repair	BMC	LLM
Bhayat et al. [30]	2021	<b>√</b>	Х	<b>√</b>	Х
Aljaafari et al. [31]	2022	<b>√</b>	Х	<b>√</b>	Х
Song et al. [32]	2022	<b>√</b>	Х	<b>√</b>	Х
Alshmrany et al. [33]	2022	<b>√</b>	Х	<b>√</b>	Х
COMPCODER [34]	2022	<b>√</b>	<b>√</b>	Х	<b>√</b>
Jigsaw [45]	2022	<b>√</b>	<b>√</b>	Х	<b>√</b>
Lajkó et al. [47]	2022	<b>√</b>	<b>√</b>	Х	<b>√</b>
Conversational APR [51]	2023	<b>√</b>	<b>√</b>	Х	<b>√</b>
Sobania et al. [35]	2023	<b>√</b>	<b>√</b>	Х	<b>√</b>
Pearce et al. [48]	2023	<b>√</b>	<b>√</b>	Х	<b>√</b>
FuzzGPT [53]	2023	<b>√</b>	Х	Х	<b>√</b>
Our work	2023	<b>V</b>	<b>√</b>	$\checkmark$	<b>√</b>

✓: Supported, X: Not Supported.

massive improvements in the patches suggested by GPTs.

In the next section, we present the essential background to understand our approach, introducing the basic notations and techniques of BMC and discussing LLMs and related background.

#### IV. PRELIMINARIES

Bounded Model Checking (BMC) and Large Language Models (LLMs) are complementary techniques used in software engineering and artificial intelligence, respectively, and they are not directly connected. Given the current knowledge of automated reasoning and software verification, both methods have yet to be used to solve similar problems, such as software bug detection and debugging. Here, we use BMC to verify programs and provide diagnostic counterexamples via text to LLM. In contrast, LLM is used to understand the textual trace that leads to the program bug and thus tentatively produce code to fix the identified vulnerability.

#### A. Bounded Model Checking (BMC)

BMC is used as one primary component of our proposed counterexample-guided repair framework. State-of-theart BMC engines support various industrial programming languages [54]–[57]. BMC represents the program as a state transition system extracted from the control-flow graph (CFG) [58]. Note that this CFG is built as part of a translation process from program text to Static Single Assignment (SSA) form. SSA is the "language" that the state-of-the-art SAT/SMT solvers understand, i.e., SSA expressions are converted to an SMT formula [54]. A node in the CFG represents either a (non-) deterministic assignment or a conditional statement, while an edge in the CFG represents a possible change in the program's control location.

We define a state transition system, denoted by M, as a triple  $(S,R,s_1)$  where S represents the set of states,  $R\subseteq S\times S$  represents the set of transitions and  $s_1\subseteq S$  represents the set of initial states. A state  $s\in S$  consists of the value of the program counter pc and the values of all program variables. An initial state  $s_1$  assigns the initial program location of the CFG to pc. We identify each transition  $T=(s_i,s_{i+1})\in R$  between two states  $s_i$  and  $s_{i+1}$  with a logical formula  $T(s_i,s_{i+1})$ . This

captures the constraints on the corresponding values of the program counter and the program variables.

We also define properties under verification in BMC:  $\phi(s)$  is the logical formula encoding states satisfying a safety/security property, and  $\psi(s)$  is the logical formula encoding states satisfying the completeness threshold, i.e., states corresponding to the program terminating.  $\psi(s)$  will contain unwindings no deeper than the maximum number of loop iterations in the program. Note that, in our notation, termination and error are mutually exclusive:  $\phi(s) \wedge \psi(s)$  is by construction unsatisfiable; s is a deadlock state if  $T(s_i, s_{i+1}) \vee \phi(s)$  is unsatisfiable. The associated BMC problem is formulated by constructing the following logical formula:

BMC(k) = 
$$I(s_1) \land \bigwedge_{i=1}^{k-1} T(s_i, s_{i+1}) \land \bigvee_{i=1}^{k} \neg \phi(s_i).$$
 (1)

Here, I the set of initial states of M and  $T(s_n,s_{n+1})$  is the transition relation of M between time steps i and i+1. Hence,  $I(s_1) \wedge \bigwedge_{i=1}^{k-1} T(s_i,s_{i+1})$  represents the executions of M of length k and BMC(k) can be satisfied if and only if for some  $i \leq k$  there exists a reachable state at time step i in which  $\phi$  is violated. Suppose BMC(k) is satisfiable. In that case,  $\phi$  is violated, and the SMT solver provides a satisfying assignment from which we can extract the values of the program variables to construct a counterexample.

We define a counterexample (or trace) for a violated property  $\phi$  as a finite sequence of states  $s_1,\ldots,s_k$  with  $s_1,\ldots,s_k\in S$ , and  $T(s_i,s_{i+1})$  for  $0\leq i< k$ . This sequence informs our LLM engine on reproducing the software vulnerability since it tells how to go from the program entry point to the property violation. Now, suppose that BMC(k) is unsatisfiable. We could conclude that no error state is reachable in k steps or less. In this case, we use this information to conclude that no software vulnerability exists in the program up to the bound k.

#### B. Large Language Models (LLMs)

LLMs are deep learning systems typically based on a type of architecture called transformers. LLMs are indeed capable of processing and understanding and generating human-like natural language. Typically, the network's input is a sequence of tokens, which could be words, subwords, or even characters. These tokens are transformed into a high-dimensional vector space through a process known as embedding. The embedded tokens are then passed through multiple network layers, each applying non-linear transformations. These transformations are governed by a set of learnable parameters or weights, which are adjusted during training to optimize the model's performance. The output of these LLMs is often a probability distribution over possible next tokens, such as the next word in a sentence. The model chooses the token with the highest probability as its output. These models have been applied in various natural language processing tasks, including but not limited to language translation, question answering, and text generation.

Tom et al. [59] introduced GPT-3, the third iteration of the Generative Pretrained Transformer model developed by OpenAI. This paper's primary focus is on the few-shot learning capability of language models. The authors demonstrate that language models start exhibiting remarkable few-shot performance when scaled up, essentially learning from a limited number of examples. Lampinen et al. [60] investigated how AI systems interpret, understand, and apply knowledge from explanations provided in various contexts. Specifically, this is an important contribution to AI, particularly in language understanding and knowledge acquisition by machine learning models.

Training or fine-tuning a transformer-based LLM (e.g., GPT4 [61], BERT [62], T5 [63]) involves providing it with a large amount of data in the form of input-output pairs. In this task, our inputs are the preprocessed counterexamples from BMC, and the outputs are human-readable interpretations of those counterexamples. When training LLM, the model uses a mechanism called "Scaled Dot-Product Attention" and "Multi-Head Attention". The attention mechanism allows the model to focus on different parts of the input sequence when producing the output sequence. This is especially useful when translating between complex BMC outputs and human language. In this sub-section, we will present the preliminaries of the transformers model [64] adopted in our work.

Mathematically, the scaled dot-product attention is calculated as:

$$\operatorname{Attention}(Q, K, V) = \operatorname{softmax}\left(\frac{QK^T}{\sqrt{d_k}}\right)V, \tag{2}$$

where Q, K, and V are queries, keys, and values respectively, and  $d_k$  is the dimension of the queries and keys. This attention function is used in parallel or in "heads", thereby enabling the model to focus on different features in the input.

The objective of the training process is to find the model parameters that minimize the loss function, which measures the discrepancy between the model's predictions and the actual output. This is done through backpropagation and a variant of stochastic gradient descent.

$$\theta = \theta - \eta \nabla_{\theta} L(Y, \hat{Y}(\theta, X)), \tag{3}$$

where  $\theta$  represents the model's parameters,  $\eta$  is the learning rate, X is the input, Y is the actual output,  $\hat{Y}(\theta, X)$  is the model's predicted output, and  $\nabla_{\theta} L(Y, \hat{Y}(\theta, X))$  is the gradient of the loss function concerning the parameters  $\theta$ .

The training continues until the model's performance on a validation set stops improving or after a certain number of epochs. With transformer models, an epoch is one complete pass through the entire training dataset. After every epoch, we calculate the validation loss to check the model's performance on unseen data. Mathematically, if we denote the validation loss as  $L_{val}$ , the training process can be summarized as follows:

$$\min_{\theta} L_{val}(Y_{val}, \hat{Y}_{val}(\theta, X_{val})), \tag{4}$$

where  $X_{val}$  and  $Y_{val}$  are the input and the actual output of the validation set, and  $\hat{Y}_{val}(\theta, X_{val})$  is the model's predicted output for the validation set.

The transformer model also utilizes a position-wise feedforward network, which is applied to each position separately and identically. This includes two linear transformations with a ReLU activation in between, as represented by the following equation:

$$FFN(x) = \max(0, xW_1 + b_1)W_2 + b_2, \tag{5}$$

where x is the input,  $W_1$  and  $W_2$  are weight matrices, and  $b_1$  and  $b_2$  are bias vectors.

The model's output is produced by a final linear transformation followed by a softmax function, which generates the probability distribution over the target vocabulary for each position:

$$P(Y|X) = \operatorname{softmax}(Y(\theta, X) \cdot W_o), \tag{6}$$

where  $W_o$  is the weight matrix of the output linear transformation, and P(Y|X) represents the probability of the target output sequence Y given the input sequence X under the model's parameters  $\theta$ .

### V. TOWARDS SELF-HEALING SOFTWARE VIA LLMS AND FORMAL VERIFICATION

We chose the Efficient SMT-based Context-Bounded Model Checker (ESBMC) [52] and GPT-3.5 [65] model to implement our approach towards building self-healing software via LLMs and formal verification methods illustrated in Figure 1. In particular, we chose ESBMC since it is an efficient software verifier that can solve the highest amount of verification tasks within 10 seconds time-limit according to SV-COMP 2023. In this section, we describe ESBMC-AI, which is an AI-powered platform that uses counterexamples produced by ESBMC in conjunction with LLMs to enable natural language interactions between the user and ESBMC. We describe the ESBMC-AI architecture and its underlying methods and algorithms.

#### A. Architecture

Figure 2 illustrates the detailed interactions inside ESBMC-AI, which has currently two modes of operations: *User Chat Mode* and *Solution Generation Mode*.

a) User Chat Mode: In this mode, the AI model answers basic natural language prompt questions to the user queries. As in Listing 3, in this mode the user sends the prompt to the AI model and returns a response. While a large variety of tasks is sufficient for this mode, such as asking questions about vulnerability detection, questions that require multiple steps are not. For example, asking the AI model to fix the code that ESBMC reports as problematic will cause the User Chat Mode to respond with code it claims resolves the issues. However, from our empirical evaluation, possibly due to AI model limitations (e.g., as showcased in the example Listing 12), most of the suggested code is incorrect. Even if the corrected code is verified using a precise verification engine like ESBMC, there is still a possibility that the verification may fail.

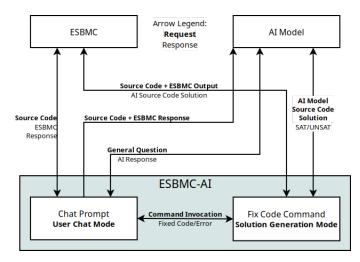


Fig. 2. Design of ESBMC-AI, each system interacts separately with the AI model and contains its own message history, system message, and initial message to accomplish its requirements. While some details are omitted, the diagram shows the essential interactions between each system.

#### User Mode Chat Prompt

- How can I correct this code?
- What is the problematic line of code?
- Can you explain why the vulnerability occurs in more depth?

Listing 3: A list of prompts that could be asked to the ESBMC-AI user chat mode prompt.

b) Solution Generation Mode: The other Solution Generation Mode of ESBMC-AI is triggered using a custom text command such as fix-code. Once this mode is invoked, the AI model will be given different instructions by changing the system and initial messages and using a separate message stack, as seen in Figure 2, which shows the interactions between the Fix Code command, and all other components of ESBMC-AI system. The solution generation AI model restricts its responses to generating only the corrected source code as output, excluding any natural language acknowledgements or explanations in the response. This is achieved by using system messages and an initial prompt to guide the model's behavior. This is to provide a consistent output format to automatically extract the source code and verify it with the underlying software verification engine. Although this worked most of the time consistently, there were rare instances where the AI model added small strings of acknowledgment text (e.g., "Absolutely!", " Certainly!", "Sure!"). However, these messages could easily be cleaned between calls to ESBMC using string processing techniques.

#### B. Implementation

The pseudocode in listing 5 defines the basic operations of the user chat mode. Initially, the chat is created in lines 3-7, an object that tracks the message history in an array and can send messages to the AI model. The system message,

<sup>&</sup>lt;sup>1</sup>https://sv-comp.sosy-lab.org/2023/results/results-verified/quantilePlot-Overall.svg

```
Wrong Code Generation Example

#include <stdio.h>
#include <stdlib.h>
int main() {

int x=77;

int y=x*x*x;

int z= y*y;

unsigned int r= z/1000;

printf("Result %d\n", r);

return 0;

}
```

Listing 4: Example of gpt-3.5-turbo generating a wrong solution. The incorrect code used in this example is from Listing II.

```
Pseudocode: User Mode Chat
   esbmc_output = esbmc(source_code)
   chat = create_user_mode_chat(
       load_system_message(),
       source_code,
       esbmc_output,
6
   response = chat(load_initial_prompt())
   print_chat_response(response)
11
   prompt: str = ""
12
   while prompt != "/exit":
13
       prompt = user_input()
14
       if prompt == "/fix-code":
15
            solution = fix_code()
16
           print_solution(solution)
17
       else:
18
            response = chat (prompt)
19
            print_chat_response(response)
20
```

Listing 5: Pseudocode that explains the user chat mode. This is the base functionality of ESBMC-AI.

the source code of the file, and the output from ESBMC are provided in the chat. The chat is initially invoked with the initial prompt message, and then the response is shown to the user in lines 9 and 10, respectively. Right after, in line 13, a while loop will facilitate the user chat interactions. The user input is collected in line 14. Line 15 checks the user input to determine whether it is a command. If the user is calling /fix-code, then the solution generator mode is invoked in line 16, and in line 17, the solution is printed using print\_solution (solution) if a solution is returned. If the message is not a special command, then the AI model is given the prompt, and the response is shown to the user in lines 19 and 20.

```
Pseudocode: Solution Generator Mode
   # Runs when fix_code is invoked.
   chat = new_solution_generator(
       source code,
       esbmc_output,
       load_system_message(),
       load_initial_prompt(),
   max_attempts: int = 10
   for idx in range (max attempts):
10
11
       code = chat.generate()
       ok, output = esbmc_verify(code)
12
       if ok:
13
14
            return code
       else:
15
            chat (output)
16
            print("Failed... Retrying")
17
18
   print("Failed to generate solution")
   return None
```

Listing 6: Pseudocode that explains the functionality of the solution generator mode, invoked when the /fix-code command is called.

The pseudocode in listing 6 describes the functionality of the solution generator mode. Much like the user chat mode that this mode is invoked from, a new chat is created, which, as previously stated, is an object that tracks the message history in an array and can send messages to the AI model, even though in this case the user does not directly control the chat. The solution generator system message and initial prompt are passed directly this time, along with the source code and ESBMC's output, as seen in lines 2-7. When the method chat.generate() is invoked, in line 11, the AI model will be asked to create a solution using the initial prompt. After generating the solution, it is verified with ESBMC in line 12. If the generated solution is correct, it is returned to the user mode chat in line 13, where it is displayed. If it is incorrect, then a new solution is generated, and the process repeats until the attempts to generate a solution have reached max\_attempts, and the mode exits without a solution. On each failed attempt, the output of ESBMC is added to the message stack; this has been shown to significantly increase the accuracy of the AI model when generating code, as the ESBMC counterexamples guide the LLM to converge towards a valid solution.

The AI model's responses would include a textual paragraph acknowledging the instructions given to it, and then the code, which would feature 3 back-ticks before and after the source code's inclusion. The text processing conducted to detect the three back-ticks is illustrated along with an example in Listing 7.

#### Extracting Source Code From Responses

The following is an example of how the AI model may respond:

```
Certainly, here is the corrected code:
2
   #include <stdio.h>
   int main() {
       printf("Hello, World!\n");
       return 0;
 The following is how the code is extracted:
       # Back-ticks from start
       s = solution.index(""") + 3
       # Reverse string and get index
       # of back-ticks from end.
       rs = code[::-1].index("``")
       # Convert string and result back
       # to the initial string.
       e = len(code) - 3 - rs
       # Extract code.
       code = code[s:e]
11
  except ValueError:
12
13
       pass
```

Listing 7: Example of how the source code returned by the AI model was extracted by the *Solution Generation Mode*. The 3 backticks are used to denote code sequences in Markdown format, which is how the AI model formats code.

#### C. System Message

When designing the behavior and allowed actions of the LLM, it is crucial to ensure that the system message is well-defined, as an ill-defined system message may induce responses from the LLM that are not desired. This is even more important in scenarios where the output needs to adhere to a specific form. Such as solution generation mode, where the output is expected to be source code only. In such scenarios, string processing may be required, as previously explained in Listing 7 where natural language text is added into the response by the LLM and is required to be removed using simple string processing.

The importance of a well-defined system message is exemplified in cases where the AI model is instructed to produce source code solutions with security features included inside. Such as, NULL checks etc. The following criteria were found to produce good AI model behavior:

- The explanation needs to be succinct, and each sentence needs to be formed as if giving direct instructions. The sentences that connect words are not necessary.
- Start the system message with instructions on the AI model's purpose.
- The instructions should be in absolute terms. It is advised

sentences begin with "You shall..." or "You shall not...". This narrows down the possible responses of the AI model to the defined domain. Providing instructions in non-absolute terms, such as "You may..." will mean that in some scenarios, the responses will deviate from the domain defined in the system message.

- The system message should not be too long. In the case of ESBMC-AI, the system message is around 500 tokens in size. Making it too long could cause it not to follow all the rules defined.
- End the system message with a request for the AI model to reply with "OK" if it understands the instructions given. This tends to increase the compliance of the AI model with the given system message.

#### VI. EXPERIMENTAL EVALUATION

This section presents our experimental results achieved using the ESBMC-AI system. Along with this, we are also providing an in-depth statistical analysis to display the rate of success that we have managed to achieve in code generation and fixing. This analysis provides a comprehensive insight into the effectiveness of our approach and the potential improvements that can be explored in the future. Our evaluation answers the following research questions.

- RQ1: (code generation) Are the state-of-the-art GPT models capable of producing compilable, semantically correct programs?
- RQ2: (program repair) Can external feedback improve the bug detection and patching ability of the GPT models?

a) Setup and Objectives: During the experiments, we generated 1,000 C code samples, each consisting of between 20 to 50 lines of code. The generation of the C code samples was executed on an AMD Ryzen Threadripper PRO 3995WX, a processor with 32 CPU cores. We effectively accelerated the sample generation speed by utilizing numerous API keys in parallel. All experiments related to code corrections were carried out on a single 2017 MacBook Pro equipped with 16 GB RAM.

The rest part of this section is organized as follows. We first generate random C programs using the LLM (Section VI-A). We then apply BMC to check how many of these programs fail the verification (Section VI-B). Subsequently, we apply ESBMC-AI to fix such failed programs (Section VI-C). We will also discuss the threats to the validity of our experiments (Section VI-D).

#### A. Code generation by LLM

In the motivation section (cf. Section II), we presented an example of how an LLM model was used to suggest a code fix in the vulnerable code. The immediate follow-up question arises: "Is the code suggested by LLM compilable, semantically correct programs?". A compilable code is a basis for the effective and efficient code fix in ESBMC-AI. To answer this question, we used the gpt-3.5-turbo model to produce a collection of 1,000 samples of C code, with the temperature parameter configured to 1.0. We then validated these with the Clang and GCC compilers to confirm correctness. We used the following guidelines to create the samples: 1) the

code should contain a minimum of 10 lines, not exceeding 50 lines, including at least two functions, and 2) incorporate elements such as strings, arrays, bit operations, and string manipulations. The exact prompt that has been employed for the GPT language model is as follows:

#### Code generation prompt

Generate a minimum of 10 and a maximum of 50 lines of C code. Use at least two functions. Use strings, arrays, bit manipulations, and string manipulations inside the code. Be creative! Always include every necessary header. Only give me the code without any explanation. No comment in the code.

Listing 8: Code generation prompt.

As a result, among all the samples generated, a remarkable success rate of 93.1% was achieved in a successful compilation. There were 29 instances where the code was missing headers, such as math.h, ctype.h, or stdlib.h. Additionally, there were 11 samples lacking certain functions, such as string reserve strrev(). After addressing these problems, the compilation success rate for the generated code increased to 97.1%.

We want to highlight an important observation at this point. The output generated by GCC, such as "gpt-35-turbo370.c:15:39: error: implicit declaration of function 'decimalToBinary' is invalid in C99 [-Werror,-Wimplicit-function-declaration]" was quite helpful. We corrected the code by utilizing the original LLM model and considering these error inputs. When we fed the GCC error outputs back into the LLM, it led to rapid issue resolution, helping us to reach a 99.9% code compilability rate.

Overall, by the results above, we reach high confidence in sending the code fix suggested by the AI engine to the BMC engine for verification in the next step.

#### Answer to RQ1

With the proposed code generation prompt and the GCC error outputs fed back into GPT-3.5, it reached a 99.9% code compilability rate. Overall, these results reach high confidence in sending the code fix suggested by LLM to the BMC engine for verification in the next step.

#### B. Code verification by BMC

After nearly completing code compatibility, our next step was to identify (and fix, if possible) any bugs or errors in the generated samples. Prior research has highlighted that the reliability of code produced by LLMs can be untrustworthy, with errors and vulnerabilities in the code [26], [49], [50]. We assume the model is unaware of these flaws; if it knew about these potential problems or bugs, it would have avoided creating such code samples.

In the initial phase of our analysis, we classified the generated samples into distinct categories. Let  $\Sigma$  be the set of all samples, such that  $\Sigma = \{c_1, c_2, \ldots, c_{1000}\}$ , where each  $c_i$  represents an individual sample. We define four distinct subsets of  $\Sigma$ , each representing a different category of sample:

- S ⊆ Σ: the set of samples for which verification was successful.
- $\mathcal{U}\subseteq\Sigma$ : the set of samples for which the verification status is unknown.
- $\mathcal{B} \subseteq \Sigma$ : the set of samples with buffer overflows based on the C scanf<sup>2</sup> function.
- $\mathcal{O} \subseteq \Sigma$ : the set of samples with other vulnerabilities.

Clearly, we have  $\Sigma = \mathcal{S} \cup \mathcal{U} \cup \mathcal{B} \cup \mathcal{O}$  and  $|\Sigma| = 1000$ . Additionally, we have  $\mathcal{S} \cap \mathcal{U} = \mathcal{S} \cap \mathcal{B} = \mathcal{S} \cap \mathcal{O} = \mathcal{U} \cap \mathcal{B} = \mathcal{U} \cap \mathcal{C} = \mathcal{U} \cap \mathcal{U} \cap \mathcal{C} = \mathcal{U} \cap \mathcal{U} \cap \mathcal{U} \cap \mathcal{U} \cap \mathcal{$ 

The "verification unknown" category (i.e.,  $\mathcal{U}$ ) contains all the samples for which it was not feasible to find a counterexample using BMC since it cannot conclude if there is a vulnerability in the code due to the search depth; here, we set the unwinding bound to 50, which means that BMC can only find the vulnerability if the property violation happens with up to 50 loop iterations. Additionally, if the verification process took an excessively long time (over 10 seconds), we skipped it, and these instances are also included in this category.

After the execution of the ESBMC tool on the generated samples, we obtained 413 instances in the "Buffer Overflows Based on Scanf" category ( $\mathcal{B}$ ), 350 samples in the "Verification Successful" category ( $\mathcal{S}$ ), 123 samples fell under "Other Vulnerabilities" ( $\mathcal{O}$ ), and 114 were categorized as "Verification Unknown" ( $\mathcal{U}$ ). One crucial observation that can be made instantly from the generated samples is that 41.3% contains some buffer overflow. These overflows originate from user inputs through the <code>scanf()</code> function. It becomes evident that GPT-3.5 consistently falls into the same error pattern when handling user input. Specifically, it does not appropriately validate the allocated buffer's limits, consequently resulting in a buffer overflow.

#### C. Code repair by BMC + LLM

Let us start from the following simple C code fragment generated by GPT-3.5 and the corresponding output of the ESBMC tool, in Listing 9. This is a very basic buffer overflow issue, which can be quickly identified by the ESBMC tool. By applying the prompt in Listing 10, we were able to fix the code successfully.

<sup>&</sup>lt;sup>2</sup>https://man7.org/linux/man-pages/man3/scanf.3.html

# C++ program example generated by gpt-3.5-turbo #include <stdio.h> #define MAX\_LEN 10 void to\_uppercase(char str[]); int main() { char word[MAX\_LEN] = {0}; printf("Enter a word: "); scanf("%s", word); printf("%s\n", to\_uppercase(word)); return 0; } ESBMC model verification output

## Building error trace Counterexample: State 4 file r.c line 8 function main thread 0 ----Violated property: file r.c line 8 function main buffer overflow on scanf 0

Listing 9: Property violation: scanf()

#### Code fixing prompt

```
"We have the following vulnerable code:
--{content}--. Fix it based on this:
{counterexample_from_ESBMC}.
Always add header to the code,
Give me the pure code that can
be compiled"
```

Listing 10: Code generation prompt.

The adjustment proposed by the LLM is simple and effective. It proposes altering line number 9 to scanf("\$9s", word);. Upon executing the ESBMC checker once again after the modification, we successfully verified the code fix. This verification indicated that the proposed solution was not only simple but effective as well. To test the effectiveness of this approach, we randomly selected 20 samples from category  $\mathcal{B}$ , applying the same fixing strategy to those code samples. This procedure was successful in 16 out of the 20 cases, further demonstrating the efficiency of this approach in code fixing. This test indicates a promising potential for this automated method to enhance the accuracy and efficiency of future code correction processes.

During our experiment, we identified an additional area of potential interest: the resolution of dereference failure issues. This particular type of issue falls under the broader classification of the  $\mathcal{O}$  (others) category, from which we have randomly chosen 20 samples (see Table II).

Out of a total of 20 samples examined, we successfully fixed 14 issues using the command esbmc --overflow

TABLE II Dereference failure list

File name	Function name	Line	Error type
gpt850.c	main	35	NULL pointer
gpt449.c	reverseString	47	NULL pointer
gpt504.c	encrypt	40	NULL pointer
gpt461.c	main	21	array bound violated
gpt921.c	reverseString	30	NULL pointer
gpt588.c	reverseString	43	NULL pointer
gpt773.c	main	18	array bound violated
gpt979.c	reverse_string	42	array bounds violated
gpt370.c	stringReversal	49	array bounds violated
gpt957.c	int_to_str	67	NULL pointer
gpt505.c	intToBinaryS	53	NULL pointer
gpt113.c	reverseString	32	array bounds violated
gpt210.c	reverse_string	29	NULL pointer
gpt717.c	reverseString	83	NULL pointer
gp45.c	upperCaseStr	81	NULL pointer
gpt466.c	main	13	array bounds violated
gpt51.c	find_median	54	array bounds violated
gpt995.c	reverse_string	45	NULL pointer
gpt19.c	reverseString	44	array bounds violated

--k-induction --unwind 1, which represents a success rate of 70%. In these specific examples, the maximum number of iterations required was three. Beyond 4-5 iterations, there is a significant likelihood that new errors may be introduced into the program.

At this point, we would like to highlight an interesting phenomenon that we have noticed during our experimentation.

There exist codes in which some parts of the code seems to be vulnerable at first glance, but in reality, they do not. Consider the C code fragment that can be seen in Listing 11.

```
Misleading C example

#include <stdio.h>

unsigned int MD5(int a, int b) {
 return ((a << 5)^(b << b))*(a-b);}

int main() {
 int a = 33;
 int b = a-9;
 const char* password = "Secret!";
 int result=MD5(a,b);
 printf("Result: %d\n", result);
 return 0;</pre>
```

Listing 11: What is the real vulnerability here?

The model provided numerous suggestions to address the issue, such as removing the embedded secret password, stating that the MD5 function is not actually MD5, or even suggesting that MD5 is insecure, and so forth. However, it never identified the real problem: the presence of an arithmetic overflow. Compiling the code results in an overflow, leading to an incorrect result of "Result: -671079136".

However, when we apply the ESBMC engine to our example code, we get the following property violation:

# ESBMC model verification output Building error trace Counterexample: State 5 file gpt661.c line 5 func MD5 thread 0 Violated property: file gpt661.c line 5 function MD5 arithmetic overflow on mul !overflow("\*", a << 5 ^ b << b, a - b) VERIFICATION FAILED Bug found (k = 1)

By providing the output with the property violation to the LLM, we were able to successfully repair the code within two iterations. The suggested code is the following:

```
Misleading C example
   #include <stdio.h>
   #include <stdint.h>
   uint32 t MD5 (int a, int b)
       uint32_t result = ((uint32_t)
        (a << 5) (uint32 t) (b << b))
        * (uint32_t) (a - b);
       return result;
10
11
   int main()
12
   {
13
       int a = 33;
14
       int b = a - 9;
15
       const char* password = "Secret!";
16
       uint32_t result = MD5(a, b);
17
       printf("Result: %u\n", result);
19
       return 0;
20
21
22
```

Listing 12: What is the real vulnerability here?

After compiling the code, we obtained the correct answer, which is "Result: 3623888160".

These examples demonstrate how LLMs can face challenges when accurately calculating arithmetic operations or identifying vulnerable code without external assistance. The proposed method we have explored in this study significantly improves the capability of LLMs using counterexamples provided by software verifiers. The counterexamples provided are valid, not false positive counterexamples, as the BMC tool can prove their existence. By using these tools, we are fully independent

of the used LLM model's ability to handle arithmetic operations. This innovative approach has the potential to improve the software development process.

#### Answer to RQ2

Our proposed method can fix vulnerable code containing buffer overflow and dereference failures with a success rate of up to 80% in a maximum of three iterations.

#### D. Threats to the Validity

The framework heavily relies on the language model's understanding of code semantics, which may not always align perfectly with the program's intended behavior. This can lead to the generation of repairs that, although syntactically valid, do not effectively address the underlying bugs or introduce new issues. Such incorrect repairs can impact the overall accuracy and reliability of the framework's performance evaluation, potentially undermining its effectiveness in real-world scenarios.

The verification process may introduce delays and performance bottlenecks if it is complex or computationally intensive. Lengthy verification procedures can significantly impact the overall efficiency of the framework, particularly when dealing with complex structures like loops or multithreaded programs. Hence, we propose the subsequent practical recommendations for the verification of software using ESBMC-AI:

- Consider analyzing sections of the program, like individual functions, to decrease the execution time of ESBMC.
- 2) Code segments that are relatively small (up to 100 lines of code) are more likely to generate solutions than complex, lengthy software programs.
- 3) Arithmetic overflows involving built-in values are easier for BMC to represent, and they have a higher probability of yielding valid bug fixes, especially when compared to the unpredictability of non-deterministic inputs produced by user input.

The proposed ESBMC-AI framework can detect and fix errors in C programs using BMC and a pre-trained Transformer model (GPT), which in our particular case is the Efficient SMT-based Context-Bounded Model Checker (ESBMC) and (gpt-3.5-turbo).

#### VII. CONCLUSIONS AND FUTURE WORK

This paper presents and evaluates an innovative framework for automatic program repair that leverages the power of LLMs, specifically the GPT coupled with formal verification. Our tool demonstrates significant advancements over existing works in the field by effectively utilizing tailored and domain-specific feedback prompts and feedback from the bounded model checker to achieve enhanced program repair capabilities. First, our approach reached a 99.9% code compilability rate with the proposed code generation prompt. Overall, these results reach high confidence in sending the code fix suggested

by LLM to the BMC engine for verification in the next step. Second, our proposed method can fix vulnerable code containing buffer overflow and dereference failures with a success rate of up to 80%.

Integrating LLMs and formal verification into automatic program repair is a promising future research direction. The power of these models, coupled with appropriate prompts and feedback mechanisms, enables more effective and intelligent code repair. However, addressing potential limitations and challenges is crucial, such as the need for massive computational resources and the potential introduction of unintended vulnerabilities or overfitting specific code patterns. We believe further advancements in this area will continue revolutionizing software development practices by enabling faster and more accurate bug fixes, ultimately enhancing software reliability, productivity, and security.

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