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

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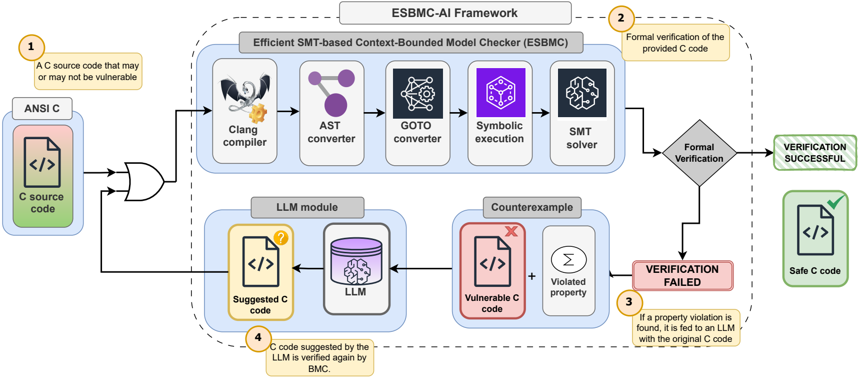
Challenges in automatic code repair (ACR) using LLMs

Automatic Code Repair Framework



Research questions to be answered..

- **RQ1**: Can we enhance the ACR capabilities of current LLMs by combining them with an external FV tool?

- **RQ2**: Which vulnerabilities are the most challenging to repair successfully for LLMs?

- **RQ3**: How reliable is the generated patch, and how likely is it that the new code remains compilable and does not disrupt the original program workflow?

Motivation: Fixed code based on external FV tool

Vulnerable C code example

```c
1 int main() {
2     int x=77;
3     int y=x*x*x;
4     int z=y*y;
5     unsigned int r= z/1000;
6     return 0;}
```

Using BMC, we can easily detect the arithmetic overflow: **PROPERTY VIOLATION: line 4 function main arithmetic overflow on mul !overflow("*", y, y)**.

Corrected C program suggested by the LLM

```c
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;
    return 0;}
```

Bug detection and repair methods

TABLE I: Comparison of related software bug detection and repair approaches.

Framework details					Repair		
Name	**Year**	**Open Source**	**Dataset**	**Language**	**Granularity**	**Compiles**	**Method**
Bhayat et al. [57]	2021	✗	SV-COMP [89]	C/C++	N/A	N/A	N/A
OpenGBF [58]	2022	✓	SV-COMP [89]	C/C++	N/A	N/A	N/A
ESBMC-Solidity [59]	2022	✓	Own[2]	Solidity	N/A	N/A	N/A
FuseBMC [60]	2022	✓	Test-Comp [90]	C/C++	N/A	N/A	N/A
COMPCODER [84]	2022	✗	AdVTest [91], CodeSearchNet [92]	Python	Program	✓	Compiler Feedback based code completion
Jigsaw [72]	2022	✗	PandasEval1, PandasEval2 [72][2]	Python	Snippets	✗	Program Synthesis
Conversational ACR [83]	2023	✗	QuixBugs [74]	Java, Python	Function	✗	Prompt-based repair
ChatRepair [88]	2023	✗	Defects4J [93], QuixBugs [74]	Java, Python	Patch	✗	Learns from previously failed tests
Pearce et al. [23]	2023	✓	ExtractFix [94]	C, Python	Program	✓	Security tests-based
RING [87]	2023	✗	BIFI [95], Bavishi et al. [96], TFix [97]	Excel, C, PowerFx, PS, Python, JS	Program	✓	Compiler message
Huang et al. [65]	2023	✓	Defects4J [93], CPatMiner [17]	Java, C/C++, Python	Patch	✗	Model trained on buggy code - fix pair
FuzzGPT [98]	2024	✗	Own [98] (unavailable)	Python	-	✗	LLM-based Fuzzing
RepairAgent [78]	2024	✗	Defects4J [93]	Java	Program	✓	Invoking suitable tools
SecRepair [79]	2024	✗	InstructVul [79] (unavailable)	C/C++	Program	✓	Fine-tuned instruction training
Self-Edit [77]	2024	✓	APPS [99], HumanEval [18]	Python	Program	✓	Compile/Runtime with tests
LLM-CompDroid [77]	2024	✗	ConfFix [100]	XML	Configuration	✗	Prompt-based
ContrastRepair [101]	2024	✗	Defects4J [93], HumanEval [18], QuixBugs [74]	Java, Python	Program	✓	Contrastive test-pair
CigaR [102]	2024	✓	Defects4J [93], HumanEval [18]	Java	Patches	✗	Prompt optimization
ESBMC-AI	**2025**	✓	FormAI [29], [103]	C/C++	Program	✓	Formal verification based feedback

Bounded Model Checking (BMC)

Bounded Model Checking

We define a state transition system $M = (S, R, s_1)$ with states S, transitions $R \subseteq S \times S$, and initial states s_1. A state s includes a program counter pc and variable values, with s_1 starting at the CFG's initial location. Transitions $T = (s_i, s_{i+1})$ are logical formulas reflecting program constraints.

For BMC, $\phi(s)$ encodes safety/security, and $\psi(s)$ encodes termination states, with $\phi(s) \wedge \psi(s)$ being unsatisfiable. The BMC formula is:

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

It represents M's executions of length k, where $BMC(k)$ is satisfiable if ϕ is violated within k steps, yielding a counterexample.

Vulnerability Classification using ESBMC 7.6.1

Define Σ as the set of all C samples, $\Sigma = \{c_1, c_2, \ldots, c_{50,000}\}$.

3 Main Categories

- $\mathcal{VS} \subseteq \Sigma$: *the set of samples for which* **verification was successful** *(no vulnerabilities have been detected within the bound k);*
- $\mathcal{VF} \subseteq \Sigma$: *the set of samples for which the* **verification status failed** *(known counterexamples);*
- $\mathcal{VU} \subseteq \Sigma$: *the set of samples for which the* **verification process is unknown**

Subcategories for $\mathcal{VF}$

Table: Top Vulnerabilities ($>$ 1%) in the 50000 dataset

Cat	Violation Type	Count (%)
	Vulnerability distribution	
$\mathcal{DF}$	Dereference failure: NULL pointer	14,700 (23.49%)
$\mathcal{BO}$	Buffer overflow on `scanf`	13,518 (21.60%)
$\mathcal{DF}$	Dereference failure: forgotten memory	7,681 (12.27%)
$\mathcal{DF}$	Dereference failure: invalid pointer	5,487 (8.77%)
$\mathcal{DF}$	Dereference failure: array bounds violated	4,020 (6.42%)
$\mathcal{AO}$	Arithmetic overflow on add	2,761 (4.41%)
$\mathcal{AO}$	Arithmetic overflow on sub	2,349 (3.75%)
$\mathcal{DF}$	Array bounds violated: upper bound	1,893 (3.02%)
$\mathcal{DF}$	Array bounds violated: lower bound	1,521 (2.43%)
$\mathcal{AO}$	Arithmetic overflow on mul	1,145 (1.83%)
$\mathcal{DF}$	DF: invalidated dynamic object	977 (1.56%)
$\mathcal{BO}$	Buffer overflow on `fscanf`	961 (1.54%)
$\mathcal{AO}$	Arithmetic overflow on FP ieee_mul	943 (1.51%)
$\mathcal{DF}$	Division by zero	631 (1.01%)

Misleading Vulnerable C code (LLM hallucination)

This code **does not implement** the MD5 algorithm in C:

Vulnerable C code

```c
#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;}
```

Verification output

```
Counterexample:

State 5 file gpt661.c line 4 func MD5
----------------------------------------
Violated property:
 file gpt661.c line 5 function MD5
  arithmetic overflow on mul
  !overflow("*", a << 5 ^ b
  corresponding to << b, a - b)

VERIFICATION FAILED
```

Code fixation results (GPT-4o) - human validated

Original Programs				Patched Programs				
Vulnerability Type	Sample size	Avg LOC	Avg CC	$\mathcal{VS}$	$\mathcal{VF}$	$\mathcal{VU}$	Avg CC	Accuracy
Array bounds violation (upper bound)	182	79.56	6.72	174	4	4	8.35	95.60%
Buffer overflow on fscanf (I/O error)	241	74.95	4.61	220	13	8	5.62	91.29%
Buffer overflow on scanf	175	78.92	6.91	160	8	7	8.30	90.40%
Division by zero	133	73.52	3.77	115	8	10	4.42	86.47%
Dereference Failure: NULL pointer	229	78.05	5.44	184	40	5	7.70	80.35%
Arithmetic overflow on add	73	74.9	4.45	52	16	5	5.17	70.27%
Dereference Failure: forgotten memory	187	79.70	5.53	91	83	13	6.49	48.66%
Array bounds violation (lower bound)	117	81.69	5.74	48	65	4	6.59	41.03%

Thank you for your attention!

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