Towards Assessing and Repairing LLM-Generated Code via Model Checking and MaxSAT-Based Fault Localisation

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Outline

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- On Verifying Python via LLM-Based Transpilation to C.

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- LLMs **are widely used, and often blindly**, with developers placing significant trust in their capabilities [Oh et al., 2024].
- However, this growing reliance on LLMs for coding tasks raises a fundamental question:
  - To what extent do LLMs **truly understand code and the underlying semantics of programs**?

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- In other domains, such as mathematical competitions [Petrov et al., 2025], LLMs tend to **provide accurate predictions, but based on flawed reasoning**.

Our work

- Conduct a **manual expert evaluation to assess whether LLMs' code output predictions** are based on logically sound reasoning, flawed reasoning, or mere guesses.

Pedro Orvalho, Marta Kwiatkowska. Are Large Language Models Robust in Understanding Code Against Semantics-Preserving Mutations? arXiv:2505.10443 (2025)

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- Conduct a **manual expert evaluation to assess whether LLMs' code output predictions** are based on logically sound reasoning, flawed reasoning, or mere guesses.

- Evaluate LLMs' **output prediction stability** across five different semantics-preserving code mutations.

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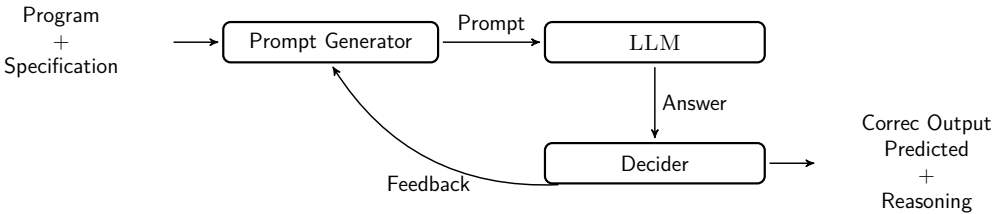
Semantics-Preserving Code Mutations

We introduce **five semantics-preserving code mutations** designed to syntactically modify Python programs without altering their semantics:

- variable renaming;
- comparison expression mirroring;
- swapping if-else statements;
- loop conversion
- partial loop unrolling.

LLM-Based Program Output Prediction



Experimental Setup

- **Evaluation Benchmarks:**
  - LiveCodeBench [Jain et al., 2024] **contains 479 programs** submitted to programming contests across competition platforms, such as LeetCode;
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- For each program mutation, **we generate a separate transformed version of the benchmark**, each program containing at most one mutation;
- We also **check that the semantics of the original program is preserved** in the mutated versions.

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  - **Seven of these models are LLMCs**, i.e., LLMs fine-tuned for coding tasks:
    - IBM's Granite;
    - Google's CodeGemma;
    - Mistral's Mistral;
    - SemCoder;
    - Alibaba's Qwen3-Coder;
    - OpenAI's GPT-5.2;
    - Google's Gemini-3;

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    - Google's GEMINI-3;
  - **The other model is a general-purpose LLM**: Meta's LLAMA3;
- Experiments were conducted using a timeout of **90s**.

Analysis of LLMs' Reasoning About Code

Large Language Models	CodeGemma	Granite	Qwen3-Coder	Mistral	SemCoder	Llama3	GPT-5.2	Gemini-3
%Failed Predictions	66.8	65.1	49.5	67.4	52.0	61.4	2.5	0.0
%Correct Predictions	33.2	34.9	50.5	32.6	48.0	38.6	97.5	100.0

Robustness to Semantics-Preserving Mutations

LiveCodeBench

LLMs	Original Code	Loop Conversion	Expression Mirroring	Variable Renaming	Swap If-Else	Loop Unrolling
CodeGemma	33.2%	26.3 (-6.9)	31.7 (-1.5)	38.0 (+4.8)	28.4 (-4.8)	10.9 (-22.3)
Granite	34.9%	27.1 (-7.7)	31.3 (-3.5)	38.8 (+4.0)	29.2 (-5.6)	8.4 (-26.5)
Llama3	38.6%	34.4 (-4.2)	34.2 (-4.4)	46.8 (+8.1)	30.1 (-8.6)	9.4 (-29.2)
Mistral	32.6%	24.0 (-8.6)	29.2 (-3.3)	38.2 (+5.6)	27.1 (-5.4)	10.4 (-22.1)
Qwen3-Coder	50.5%	37.8 (-12.7)	44.1 (-6.5)	54.7 (+4.2)	33.2 (-17.3)	15.4 (-35.1)
SemCoder	48.0%	40.1 (-7.9)	48.9 (+0.8)	62.4 (+14.4)	40.3 (-7.7)	15.2 (-32.8)
GPT-5.2	97.1%	**72.4 (-24.6)**	81.0 (-16.1)	98.5 (+1.5)	78.3 (-18.8)	29.0 (-68.1)
Gemini-3	100.0%	**55.3 (-44.7)**	76.0 (-24.0)	68.1 (-31.9)	71.4 (-28.6)	29.6 (-70.4)

Table 1: Output prediction correction rate of each LLM on LiveCodeBench when applying different code mutations: converting for to while loops (F2W), mirroring comparison expressions (MCE), renaming variables (RV), swap if-else statements (SIE), and unroll loops (UL).

Robustness to Semantics-Preserving Mutations

CruxEval

LLMs	Original Code	Loop Conversion	Expression Mirroring	Variable Renaming	Swap If-Else	Loop Unrolling
CodeGemma	30.9%	15.8 (-15.1)	17.6 (-13.3)	34.9 (+4.0)	20.1 (-10.8)	8.9 (-22.0)
Granite	32.6%	14.2 (-18.4)	17.1 (-15.5)	35.4 (+2.8)	19.8 (-12.9)	8.1 (-24.5)
Llama3	26.5%	15.0 (-11.5)	17.4 (-9.1)	37.5 (+11.0)	19.2 (-7.2)	6.6 (-19.9)
Mistral	23.8%	11.0 (-12.8)	13.4 (-10.4)	25.5 (+1.8)	13.9 (-9.9)	6.5 (-17.2)
Qwen3-Coder	48.9%	23.1 (-25.8)	26.2 (-22.6)	49.9 (+1.0)	26.2 (-22.6)	12.5 (-36.4)
SemCoder	50.6%	25.2 (-25.4)	29.9 (-20.8)	55.8 (+5.1)	30.4 (-20.2)	12.8 (-37.9)
GPT-5.2	86.0%	**42.2 (-43.8)**	47.9 (-38.1)	87.0 (+1.0)	52.9 (-33.1)	23.0 (-63.0)
Gemini-3	76.8%	**29.1 (-47.6)**	50.9 (-25.9)	66.2 (-10.5)	41.2 (-35.5)	24.4 (-52.4)

Table 2: Output prediction correction rate of each LLM on CruxEval when applying different code mutations: converting for to while loops (F2W), mirroring comparison expressions (MCE), renaming variables (RV), swap if-else statements (SIE), and unroll loops (UL).

Robustness to Semantics-Preserving Mutations

Are LLMs robust in understanding code against semantics-preserving mutations?

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Are LLMs robust in understanding code against semantics-preserving mutations?

- LLMs often change predictions in response to our code mutations, indicating **limited robustness in their semantic understanding**.

Verifying LLM-based Code with Formal Methods

P. Orvalho, M. Janota, and V. Manquinho. Counterexample Guided Program Repair Using Zero-Shot Learning and MaxSAT-based Fault localisation. AAAI 2025

Motivation

1: Semantically incorrect program. Faults: {4,8}.

```
1  int main(){ //finds max of 3 nums
2     int f,s,t;
3     scanf("%d%d%d",&f,&s,&t);
4     if (f < s && f >= t)
5        printf("%d",f);
6     else if (s > f && s >= t)
7        printf("%d",s);
8     else if (t < f && t < s)
9        printf("%d",t);
10
11    return 0;
12 }
```

- Symbolic approaches demand an **excessive amount of time to produce an answer**;

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2: Semantically incorrect program. Faults: {4,8}.

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- Symbolic approaches demand an **excessive amount of time to produce an answer**;
- LLMs, while fast, **often produce incorrect or non-minimal fixes**.

Program Sketches

3: Semantically incorrect program. Faults :{4,8}.

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```

4: Program sketch with holes.

```
1  int main(){
2     int f,s,t;
3     scanf("%d%d%d",&f,&s,&t);
4     @ HOLE 1 @
5        printf("%d",f);
6     else if (s > f && s >= t)
7        printf("%d",s);
8     @ HOLE 2 @
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```

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- Combines the strengths of **Formal Methods (FM) and LLM-based approaches**;

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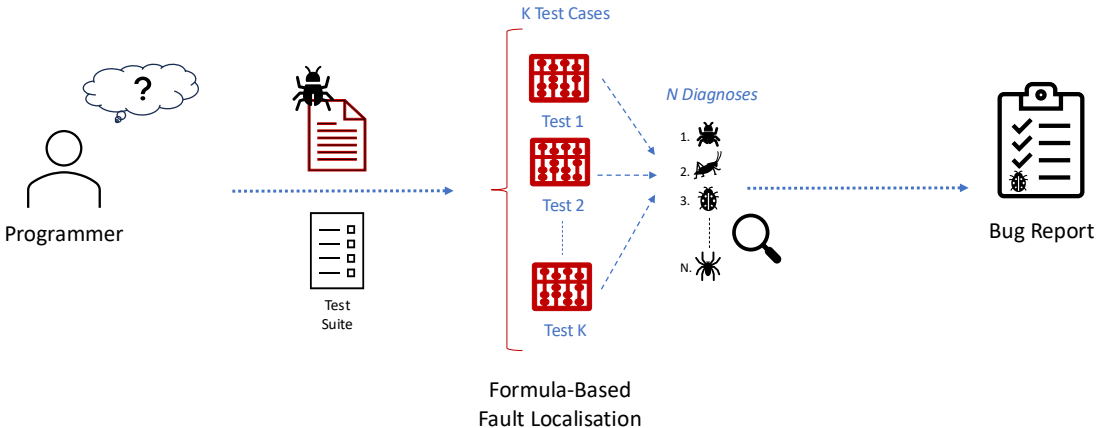
- Combines the strengths of **Formal Methods (FM) and LLM-based approaches**;
- Uses **MaxSAT-based fault localisation to rigorously identify buggy lines**, which can then be highlighted in the LLM prompt;

Formula-Based Fault Localisation (FBFL)

- FBFL methods encode the localisation problem into **several optimisation problems** to identify a minimal set of bugs (diagnoses).



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- We formulate the FL problem as a **single optimisation problem**;

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- We leverage MaxSAT and the theory of *Model-Based Diagnosis (MBD)* [Reiter et al., 1987], **integrating all failing test cases simultaneously**;
- We implement this MBD approach in a publicly available tool called CFaults [Orvalho et al., 2024].

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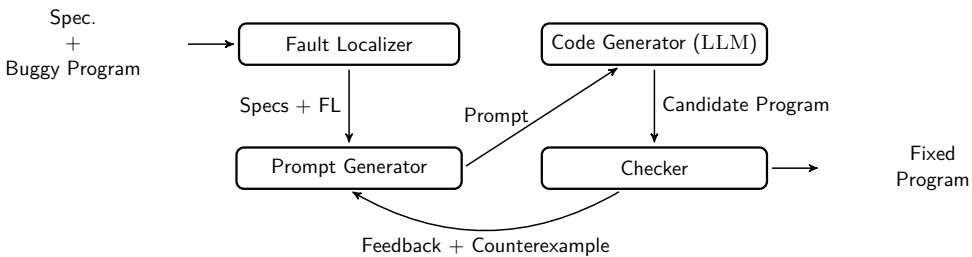
Counterexample Guided Automated Repair



Experimental Setup (2024)

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- **Large Language Models (LLMs):** We evaluated **six different LLMs**.
  - **Three of these models are LLMCs**, i.e., LLMs fine-tuned for coding tasks:
    - IBM's Granite;
    - Google's CodeGemma;
    - Meta's CodeLlama.
  - **The other three models are general-purpose LLMs**:
    - Google's Gemma;
    - Meta's Llama3;
    - Microsoft's Phi3.

LLM-Driven APR with CFaults

LLMs	De-TS	De-TS-CE	FIXME_De-TS	FIXME_De-TS-CE	Sk_De-TS	Sk_De-TS-CE	Portfolio (All Configurations)
CodeGemma	597 (41.7%)	606 (42.3%)	592 (41.4%)	601 (42.0%)	682 (47.7%)	**688 (48.1%)**	823 (57.5%)
CodeLlama	492 (34.4%)	500 (34.9%)	481 (33.6%)	463 (32.4%)	**573 (40.0%)**	561 (39.2%)	712 (49.8%)
Gemma	496 (34.7%)	492 (34.4%)	446 (31.2%)	444 (31.0%)	532 (37.2%)	**534 (37.3%)**	670 (46.8%)
Granite	626 (43.7%)	624 (43.6%)	566 (39.6%)	583 (40.7%)	**691 (48.3%)**	681 (47.6%)	846 (59.1%)
Llama3	564 (39.4%)	590 (41.2%)	535 (37.4%)	557 (38.9%)	578 (40.4%)	**591 (41.3%)**	851 (59.5%)
Phi3	494 (34.5%)	489 (34.2%)	460 (32.1%)	474 (33.1%)	**547 (38.2%)**	535 (37.4%)	621 (43.4%)
Portfolio (All LLMs)	842 (58.8%)	846 (59.1%)	796 (55.6%)	820 (57.3%)	900 (62.9%)	**907 (63.4%)**	1013 (70.8%)

Table 3: The number of programs fixed by each LLM under various configurations. Mapping abbreviations to configuration names: **De** - IPA *Description*, **TS** - *Test Suite*, **CE** - *Counterexample*, **FIXME** - *FIXME Comments*, **SK** - *Sketches*.

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Incorporating **MaxSAT-based Sketches allows LLMs to repair more programs**

On Verifying Python via LLM-Based Transpilation and Bounded Model Checking for C

Pedro Orvalho, Marta Kwiatkowska. On Verifying Python via LLM-Based Transpilation and Bounded Model Checking for C. arXiv:2508.08171 (2025)

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- Yet it **lacks robust tools for formal verification**.
- **Languages such as C benefit from mature model checkers**, for example CBMC [Clarke et al., 2004], which enable exhaustive symbolic reasoning and FL.
- The complexity of Python, coupled with the verbosity of existing transpilers (e.g., Cython), have historically limited the applicability of formal verification to Python.

Motivation

```
1  def distributeCandies(n: int, limit: int) -> int:
2      limit = min(limit, n)
3      ans = 0
4      ans = 0 + 1
5      for i in range(limit + 1):
6          if n - i > limit * 2:
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- For instance, ESBMC-Python **cannot verify this Python program**.

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4. Maps the buggy statements back to the Python code, providing **useful feedback**.

Note: This is an **interim approach** until a robust, native Python symbolic model checker is available. Because PyVeritas **relies on LLMs** for transpilation and for mapping localised statements back to Python, **no completeness guarantees** are provided.

Running Example

- PyVeritas asks an LLM to transpiled this buggy Python program

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9      return ans
10 assert distributeCandies(n = 5, limit = 2) == 3
```

Running Example

- PyVeritas runs CBMC to check that the program is failing the assertion.

```
1  int distributeCandies(int n, int limit) {
2      limit = (limit < n) ? limit : n;
3      int ans = 0;
4      ans = 0 + 1;
5      for (int i = 0; i <= limit; i++) {
6          if (n - i > limit * 2) {
7              continue;
8          }
9          ans += ((limit < n-i) ? limit : (n-i)) -
10         ((n-i-limit > 0) ?(n-i-limit) : 0) + 1;
11     }
12     return ans;
13 }
14 int main() {
15     assert(distributeCandies(5, 2) == 3);
16     return 0;
17 }
```

Running Example

- PyVeritas uses CFaults to localise the buggy assignment in the C code.

```
1  int distributeCandies(int n, int limit) {
2      limit = (limit < n) ? limit : n;
3      int ans = 0;
4      ans = 0 + 1;
5      for (int i = 0; i <= limit; i++) {
6          if (n - i > limit * 2) {
7              continue;
8          }
9          ans += ((limit < n-i) ? limit : (n-i)) -
10         ((n-i-limit > 0) ?(n-i-limit) : 0) + 1;
11     }
12     return ans;
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14 int main() {
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Running Example

- PyVeritas maps the localised buggy statement back to the original Python source code by leveraging the same LLM used during transpilation.

```python
    ans = 0 + 1
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Thus, PyVeritas provides precise localisation for simple bugs in Python.

LLM-based Transpilation of Correct Code

Language Model	LiveCodeBench	Refactory
GPT-5.2	95.2%	97.6%
Qwen3-Coder (30B)	86.6%	95.2%
DeepSeek-Coder-V2 (16B)	65.1%	64.8%
Granite (8B)	55.9%	52.0%
Llama3 (3B)	43.0%	28.0%

Table 4: Verification success rates for each LLM on both benchmarks. Percentages indicate the proportion of C programs that were successfully verified by CBMC and judged semantically equivalent to the original Python code.

MaxSAT-Based Fault Localisation

	Bug: **Wrong Binary Operator (WBO)**			
LLMs	**% Correct Bug Found**	**% Other Bugs**	**% Transpiled Fixed Code**	**% Compilation Err**
GPT-5.2	**77.3%**	14.4%	8.3%	0.0%
Qwen3-Coder (30B)	33.8%	24.4%	41.8%	0.0%
DeepSeek-Coder-V2 (16B)	16.1%	36.8%	42.9%	4.2%
Granite (8B)	41.6%	34.6%	15.2%	8.6%
Llama3 (3B)	22.7%	47.9%	17.7%	11.6%
	Bug: **Assignment Duplication with Constant (ADC)**			
	% Correct Bug Found	**% Other Bugs**	**% Transpiled Fixed Code**	**% Compilation Err**
GPT-5.2	**81.9%**	9.5%	8.6%	0.0%
Qwen3-Coder (30B)	25.7%	6.2%	**68.1%**	0.0%
DeepSeek-Coder-V2 (16B)	6.7%	21.4%	**69.5%**	2.4%
Granite (8B)	39.5%	11.9%	36.7%	11.9%
Llama3 (3B)	18.6%	39.0%	34.3%	8.1%

Table 5: Results of MaxSAT-Based FL with PyVeritas on LiveCodeBench using WBO and ADC bugs.

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- Our novel approach for **verification and fault localisation for Python programs** by leveraging LLM-based transpilation to C.
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- Our novel approach for **verification and fault localisation for Python programs** by leveraging LLM-based transpilation to C.
- We combine **LLM-based code transpilation, bounded model checking** with CBMC, and **MaxSAT-based fault localisation** using CFaults.
- We are able to accurately **verify small yet non-trivial Python programs where native verification tools fall short**.

Thank you!

https://pmorvalho.github.io

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