

Detection of Numerical Bugs using Large Language Models (LLMs)

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Overview

- 1. LLMs Overview
- 2. Testing Infrastructure
- 3. Performance Summary
- 4. Conclusion and Future Research Directions

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What is a Large Language Model (LLM)?

Definition

Al system trained to understand, generate and interact in human language.

Examples

- ChatGPT
- Gemini
- DeepSeek







Inside an LLM

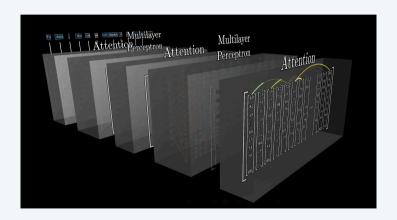


Figure: Source: Transformers, the tech behind LLMs, 3Blue1Brown

LLMs and their significance in code analysis

- **Static vs. Dynamic Analysis**: Static analysis examines code without execution, while dynamic analysis requires runtime testing
- Tool Limitations: Traditional static analysis struggles with input-dependent and complex numerical error patterns
- **Programming Proficiency**: LLMs show promise in coding and static analysis but their numerical error detection capabilities remain unexplored
- Interpretation: Returns outputs interpretable by humans

Research question

Can LLMs detect and classify floating-point errors in code?

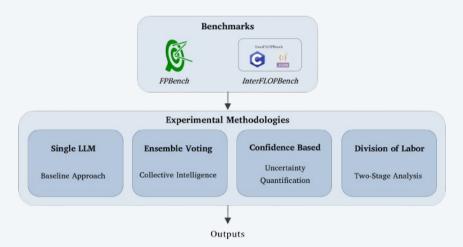
 \Rightarrow Can it detect floating-point errors in small functions?

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Overall Testing Infrastructure



FPBench: A benchmark for validation of numerical accuracy in floating-point computations



- Benchmark: Include benchmarks sourced from recent papers on automatic floating-point verification and accuracy improvement
- Format: Automatic translation from FPCore to C

InterFLOPBench: A benchmark organized into different floating-point error categories

Format Structure



Figure: C source code with accompanying JSON metadata files

Error Categories

Error Category	Benchmark Files	Individual Samples	Total Occurrences
No_error	15	306	480
Comparison	16	247	246
Cancellation	17	181	208
Overflow	13	130	151
Underflow	10	117	83
Div_zero	10	79	70
Nan	9	70	50
Total	90	1130	1288

Experimental Methodology

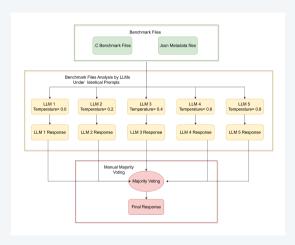
LLMs used

LLM	Developer	Release
Gemini-2.5-flash	Google	Jun 2025
Gemma-3-27B	Google	Mar 2025
Gemini-2.0-flash	Google	Feb 2025
DeepSeek-r1	DeepSeek	Jan 2025
GPT-4o	OpenAI	May 2024

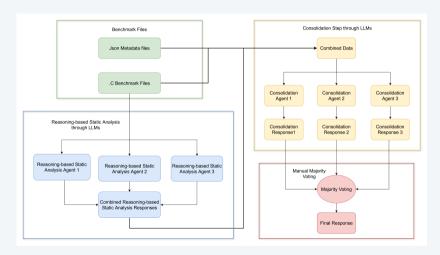
Agent Pipelines

- Single LLM: All five LLMs were considered separately
- Ensemble Voting, Confidence Based, and Division of Labor: Based on Gemini-2.0-flash

Ensemble Voting Pipeline



Division of Labor Pipeline



Evaluation Metrics and Validation

Validation with FPChecker



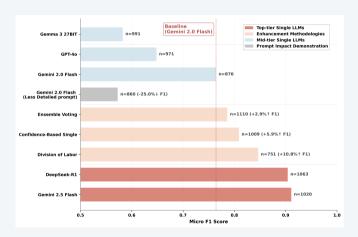
Figure: FPChecker (Floating-Point Checker) is a dynamic analysis tool to detect floating-point errors in HPC applications

Evaluation Metrics

- Micro F1: Aggregates all true/false positives globally before computing F1
- Macro F1: Computes F1 per error type independently, then averages
- Weighted F1: Weights F1 scores by label frequency in dataset
- Sample-wise F1: Averages F1 scores computed per test sample

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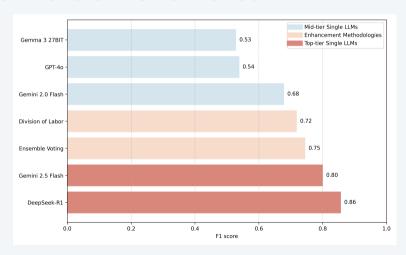
InterFLOPBench - Overall Performance



InterFLOPBench - Per-Category Ranking

Error Category	Avg F1 Score	Difficulty Rank	Best Method F1
Comparison	0.9274	1 (Easiest)	1.0000 (Division of Labor)
Division by Zero	0.9265	2	1.0000 (Division of Labor)
Overflow	0.818	3	0.9524 (Gemini 2.5 Flash)
No Error	0.774	4	0.9402 (Gemini 2.5 Flash)
NaN	0.7122	5	0.9901 (Gemini 2.5 Flash)
Cancellation	0.6521	6	0.8564 (Gemini 2.5 Flash)
Underflow	0.4729	7 (Hardest)	0.9940 (DeepSeek-R1)

FPBench - Overall Performance



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Conclusion - LLM already have some basic numerical knowledge

- Model selection dominates performance (7.6% gap between tiers)
- Sophisticated methodologies enhance mid-tier models
- **Error-specific capabilities**: Explicit operations vs. subtle numerical phenomena
- Prompt engineering is crucial: Simplified prompts cause substantial degradation

Future Research Directions

- How to improve their capability? (more sophisticated reasoning scheme, coupling with tools?)
- How to make them cheaper to use? (get similar quality with small LLM + finetuning)
- How to get a much larger set of FP benchmarks? (synthetic data generation thanks to Floq/HOL)



Thank you for your attention

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References



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Toward a Standard Benchmark Format and Suite for Floating-Point Analysis *Numerical Software Verification*, 63–77.



Laguna, Ignacio (2019)

FPChecker: Detecting Floating-point Exceptions in GPU Applications

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